



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:04 AM UTC

PDB ID : 8XLK / pdb\_00008xk  
EMDB ID : EMD-38451  
Title : Structure of native tri-heteromeric GluN1-GluN2A-GluN2B NMDA receptor  
in rat cortex and hippocampus  
Authors : Zhang, M.; Feng, J.; Li, Y.; Zhu, S.  
Deposited on : 2023-12-26  
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

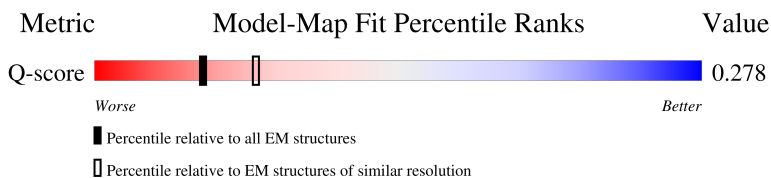
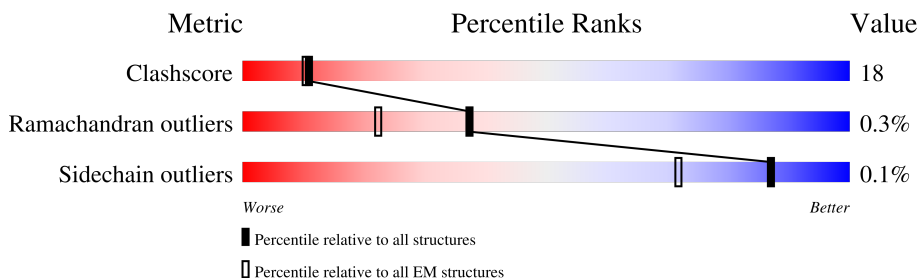
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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.



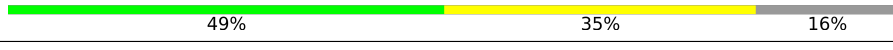
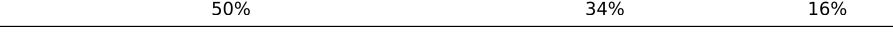
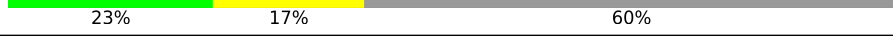
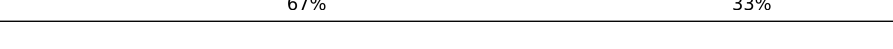
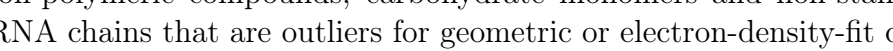
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 5410 ( 3.70 - 4.70 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 938    |                  |
| 1   | C     | 938    |                  |
| 2   | B     | 1464   |                  |
| 3   | D     | 1482   |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | E     | 140    |    |
| 4   | I     | 140    |    |
| 5   | F     | 131    |    |
| 5   | J     | 131    |    |
| 6   | G     | 227    |    |
| 7   | H     | 212    |    |
| 8   | K     | 248    |    |
| 9   | L     | 265    |    |
| 10  | M     | 3      |    |
| 10  | O     | 3      |   |
| 11  | N     | 2      |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 13  | 7RC  | B     | 1504 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 34118 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamate receptor ionotropic, NMDA 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 800      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6322  | 4023 | 1099 | 1165 | 35 |         |       |
| 1   | C     | 800      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6325  | 4025 | 1099 | 1165 | 36 |         |       |

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 792      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6279  | 4051 | 1025 | 1166 | 37 |         |       |

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 2B.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | D     | 792      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6260  | 4026 | 1007 | 1184 | 43 |         |       |

- Molecule 4 is a protein called Heavy Chain of GluN1 Fab, 4F11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | E     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 598 | 150 | 186 | 4 |         |       |
| 4   | I     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 598 | 150 | 186 | 4 |         |       |

- Molecule 5 is a protein called Light Chain of GluN1 Fab, 4F11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | F     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 828   | 518 | 137 | 170 | 3 |         |       |
| 5   | J     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 822   | 512 | 137 | 170 | 3 |         |       |

- Molecule 6 is a protein called Heavy Chain of GluN2A Fab, 28C.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | G     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1693  | 1061 | 294 | 334 | 4 |         |       |

- Molecule 7 is a protein called Light Chain of GluN2A Fab, 28C.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 212      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1576  | 983 | 268 | 320 | 5 |         |       |

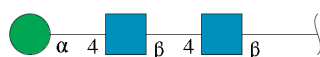
- Molecule 8 is a protein called Heavy Chain of GluN2B Fab2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | K     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 899   | 569 | 152 | 173 | 5 |         |       |

- Molecule 9 is a protein called Light Chain of GluN2B Fab2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | L     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 820   | 520 | 136 | 161 | 3 |         |       |

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



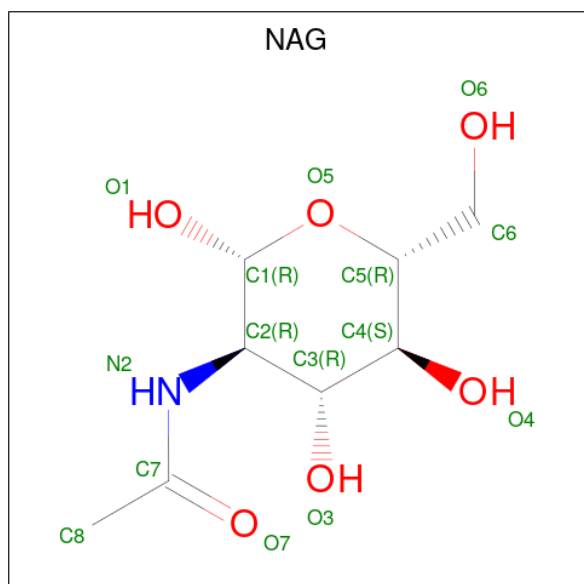
| Mol | Chain | Residues | Atoms |    |   |    |  | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|--|---------|-------|
| 10  | M     | 3        | Total | C  | N | O  |  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |  |         |       |
| 10  | O     | 3        | Total | C  | N | O  |  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |  |         |       |

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 11  | N     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



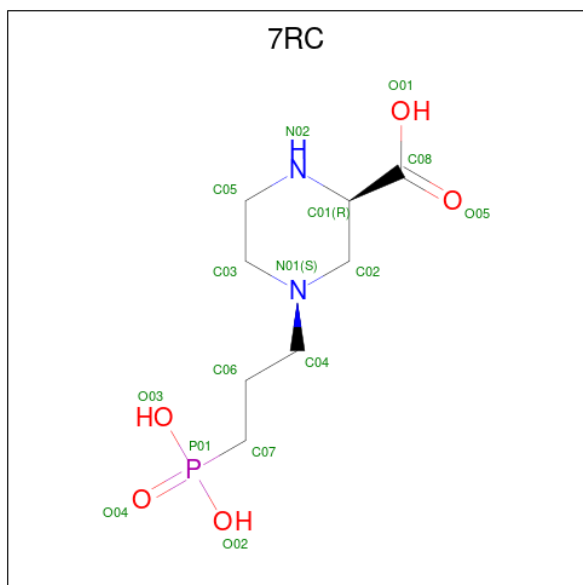
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 12  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 12  | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 12  | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

- Molecule 13 is (2R)-4-(3-phosphonopropyl)piperazine-2-carboxylic acid (CCD ID: 7RC) (formula: C<sub>8</sub>H<sub>17</sub>N<sub>2</sub>O<sub>5</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 13  | B     | 1        | Total | C | N | O | P | 0       |
|     |       |          | 16    | 8 | 2 | 5 | 1 |         |

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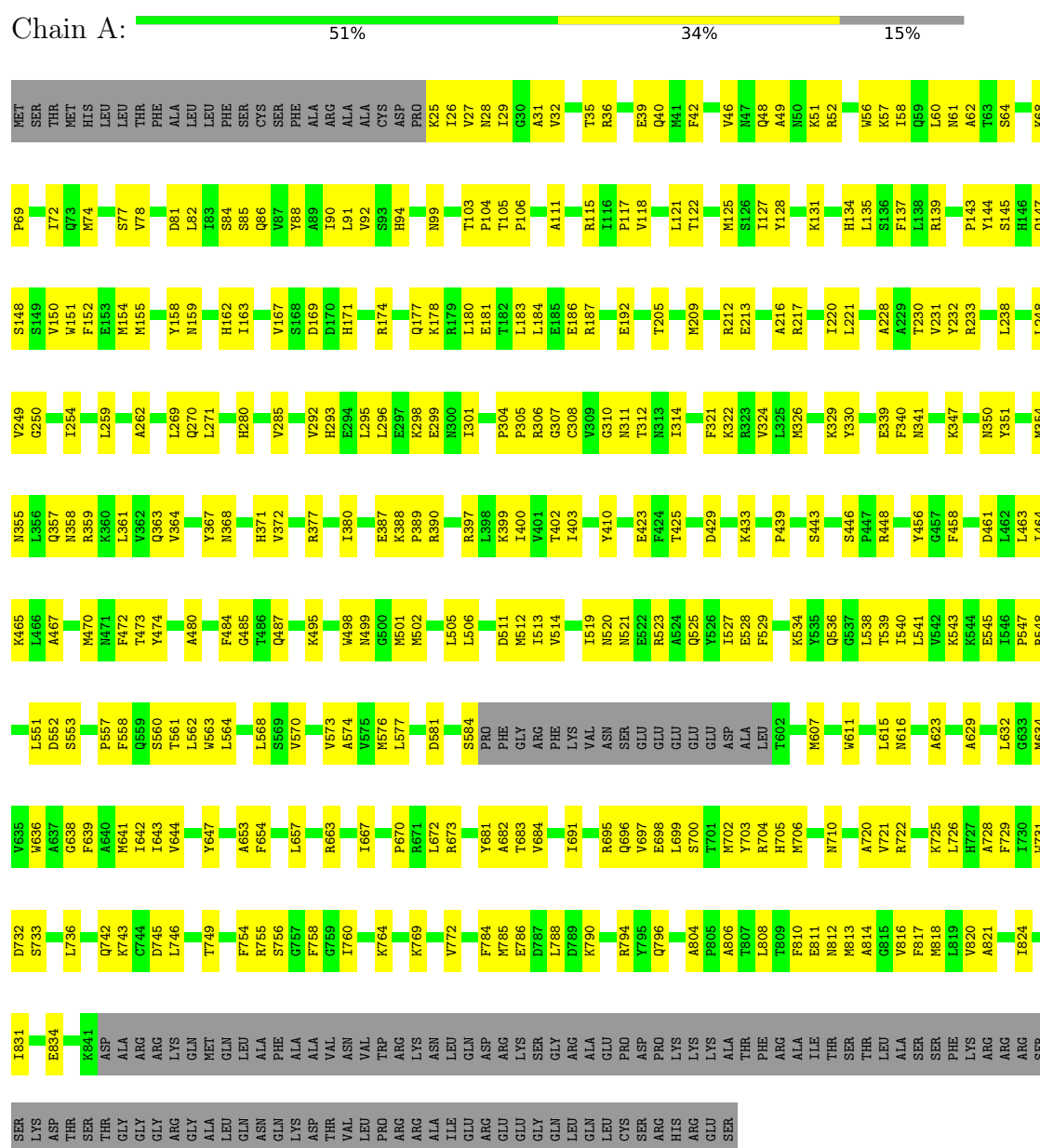
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 13  | D     | 1        | Total | C | N | O | P | 0       |
|     |       |          | 16    | 8 | 2 | 5 | 1 |         |



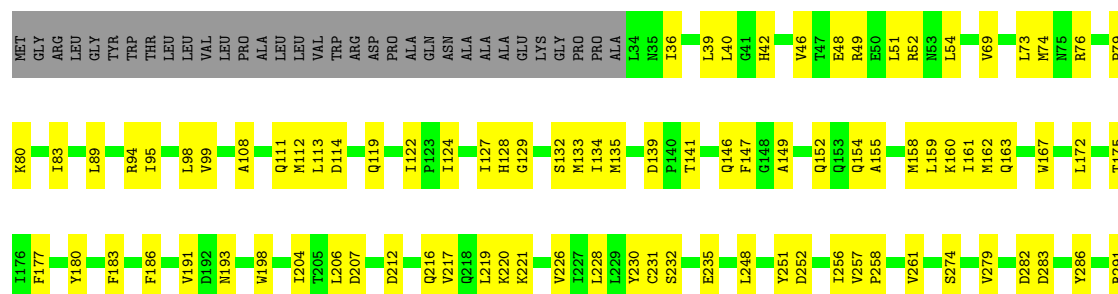
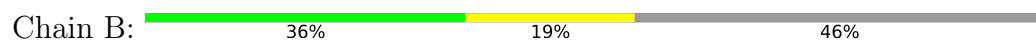
### 3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Glutamate receptor ionotropic, NMDA 1

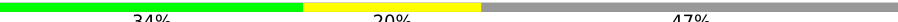


Chain C:  54% 32% 15%



|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |                                                                                                                                                                                                                                                                                                                                                                                                      |
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| GLU<br>HIS<br>VAL<br>MET<br>PRO<br>TYR<br>ALA<br>ASN<br>LYS<br>GLN<br>THR                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | ARG | PRO | PRO | ASP | TYR | LEU | PRO | SER | SER | GLY | ASN | ASN | LEU | THR | GLY | E516 | G602 | E691 | L796 | B691 | A414<br>P415<br>F416<br>V417<br>I418<br>R431<br>N432<br>T433<br>K441<br>I442<br>G449<br>C455<br>C456<br>K457<br>G458<br>F459<br>C460<br>I463<br>L464<br>K465<br>L466<br>L467<br>S468<br>R469<br>T470<br>V471<br>K472<br>D476<br>H485<br>G486<br>K487<br>K488<br>N491<br>V492<br>W493<br>M496<br>I497<br>V500<br>V501<br>Y502<br>Q503<br>R504<br>A505<br>V506<br>M507<br>A508<br>V509<br>I514<br>N515 |
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                    | PRO | PHE | LEU | SER | ALA | TYR | ALA | SER | ALA | ASN | ARG | ARG | LEU | THR | GLY | E517 | K603 | R692 | T797 | N693 |                                                                                                                                                                                                                                                                                                                                                                                                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | HIS | ARG | GLY | HIS | LYS | HIS | THR | ARG | PHE | GLY | SER | GLN | SER | GLY | GLY | R518 | W606 | I694 | R695 | N696 |                                                                                                                                                                                                                                                                                                                                                                                                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | THR | SER | THR | ASP | PHE | HIS | GLY | ARG | CYS | PRO | GLY | GLN | SER | GLY | GLY | V521 | W609 | G695 | N697 | Y698 |                                                                                                                                                                                                                                                                                                                                                                                                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | GLY | ASP | THR | GLN | THR | GLY | GLN | GLN | GLY | GLY | LYS | LYS | ASN | GLN | GLY | V522 | G610 | N697 | L611 | V612 |                                                                                                                                                                                                                                                                                                                                                                                                      |
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                    | LYS | ASP | GLN | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | F528 | F614 | M705 | R707 | F708 |                                                                                                                                                                                                                                                                                                                                                                                                      |
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- Molecule 3: Glutamate receptor ionotropic, NMDA 2B

Chain D:  34% 20% 47%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | LYS | PRO | SER | GLY | GLU | CYS | CYS | SER | PRO | LYS | PHE | TRP | LEU | VAL | LEU | ALA | VAL | ALA | VAL | SER | GLY | SER | LYS | ALA | ARG | VAL | PRO | PRO | PRO | ILE | GLU | G36 | I37 | I40 | L41 | E47 | V48 | A49 | I50 | K51 | D52 | A53 | H60 | H61 | R67 | V71 | A72 | M73 | T76 | D77 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



ARG  
ALA  
PHE  
ASN  
GLY  
SER  
SER  
ASN  
GLY  
HIS  
VAL  
TYR  
GLU  
LYS  
LEU  
SER  
SER  
ILE  
GLU  
SER  
ASP  
VAL

• Molecule 4: Heavy Chain of GluN1 Fab, 4F11

Chain E:



PRO MET VAL SER ILE VAL LEU TYR LEU LEU ALA ALA ALA HIS SER SER ILE GLU SER ASP VAL  
D21 V22 G28 K33 L38 S39 L40 T41 C42 T43 Y47 S48 I49 T50 S51 D52 Y53 A54 W55 I58 R59 Q60 F61 P62 G63 N64 K65 L66 E67 W68 M69 G70 Y71

I72 S73 Y74 S75 G76 G79 N80 Y81 L84 I88 S89 I90 T91 R92 D93 T94 N97 Q98 F99 F100 L101 Q102 L103 N104 S105 D110 Y114 Y121 Y124 G132 V135 S138

• Molecule 4: Heavy Chain of GluN1 Fab, 4F11

Chain I:



PRO MET VAL SER ILE VAL LEU TYR LEU LEU ALA ALA ALA HIS SER SER ILE GLU SER ASP VAL  
D21 V22 Q23 L24 E26 V32 S37 L38 C42 T43 V44 T45 D52 Y53 A54 I58 R59 L66 E67 W68 W69 G70 Y71 I72 S75 T78 G79 Y80

L84 K86 S86 R87 I88 T91 R92 D93 N97 Q98 F99 F100 L101 Q102 L103 N104 S105 V106 T107 T108 T111 A112 T113 Y114 R118 L119 Y120 Y121 Y124 G125 M126 B127 Y128 Q131 T136 V137 S138

• Molecule 5: Light Chain of GluN1 Fab, 4F11

Chain F:



MET VAL SER ILE VAL LEU TYR VAL LEU LEU ALA ALA ALA HIS SER SER ILE GLU SER ASP VAL  
I21 Q25 S26 P27 L30 A31 V32 S33 Q36 R37 A38 T39 L40 V48 Y55 M56 N57 P58 T59 Q60 Q61 K62 Q65 K68 L69 L70 I71 Y72 A73 A74 S75 N76

R64 G67 T95 L96 H97 H99 P100 V101 E102 E103 Y109 Y110 C111 N115 E116 G123 G124 L127 K130

• Molecule 5: Light Chain of GluN1 Fab, 4F11

Chain J:



MET VAL SER ILE VAL LEU TYR VAL LEU LEU ALA ALA ALA HIS SER SER ILE GLU SER ASP VAL  
I21 V22 L23 T24 Q25 A31 V32 S33 L34 C35 Q36 R37 A38 C42 K43 A44 S45 D49 N57 W58 Y59 Q60 Q61 K62 Q65 K68 L69 L70 I71 Y72 E78

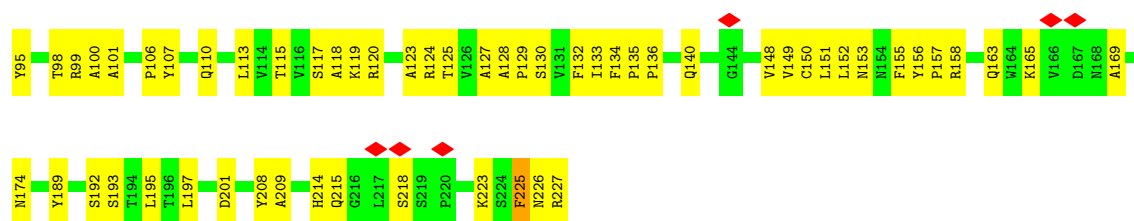
G91 T92 I98 H99 P100 V101 A106 A107 T108 Y109 Y110 C111 Q112 Q113 G114 N115 P119 T120 F121 T125 K126 L127 K130

• Molecule 6: Heavy Chain of GluN2A Fab, 28C

Chain G:

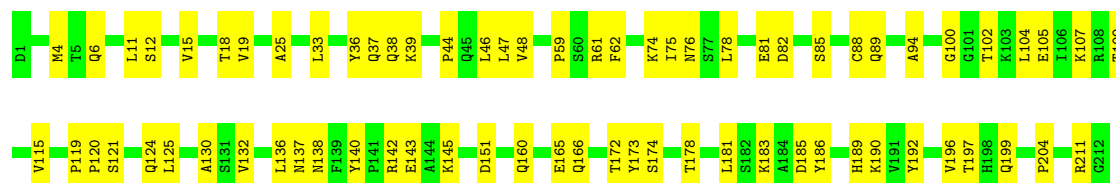


G1 V2 T3 L4 K5 I11 L12 Q13 T17 L18 S23 F24 S25 A29 G33 V34 G37 W38 T39 R40 Q41 P42 K45 G46 L47 W48 W49 H52 T53 A54 A55 Y61 K66 T70 D74 T75 Q79 K83 I84 A85 T89 T92 A93 T94



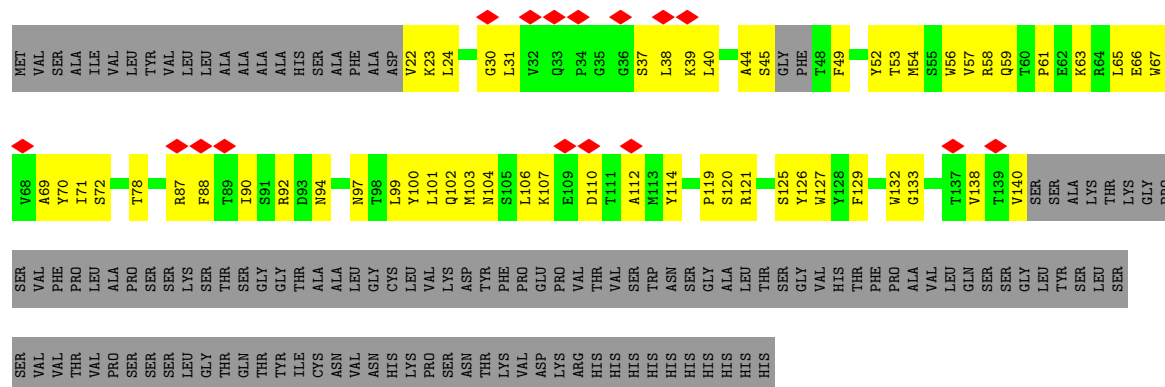
• Molecule 7: Light Chain of GluN2A Fab, 28C

Chain H: 67% 33%



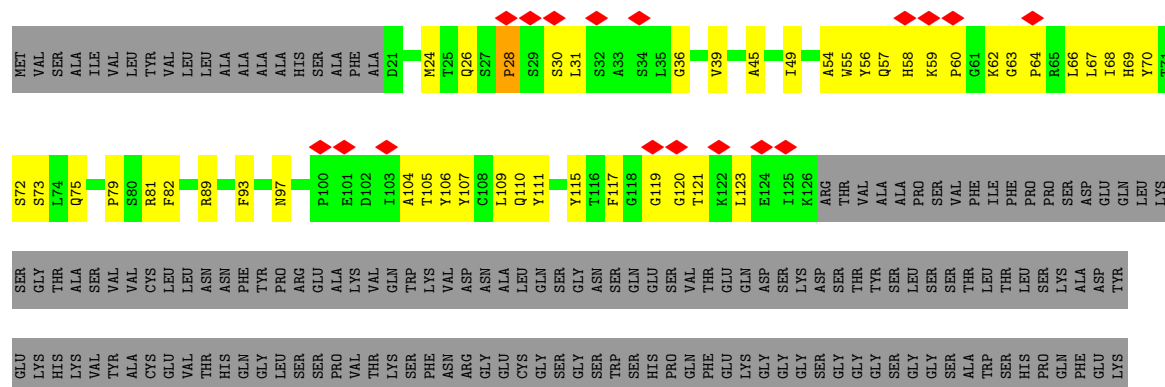
• Molecule 8: Heavy Chain of GluN2B Fab2

Chain K: 6% 24% 23% 53%



• Molecule 9: Light Chain of GluN2B Fab2

Chain L: 6% 23% 17% 60%



- Molecule 10: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  67% 33%

MAG1  
MAG2  
MAG3

- Molecule 10: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  67% 33%

MAG1  
MAG2  
MAG3

- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

MAG1  
MAG2

## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 45676                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI POLARA 300                  | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                              | Depositor |
| Minimum defocus (nm)                 | 1000                            | Depositor |
| Maximum defocus (nm)                 | 2500                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | DIRECT ELECTRON DE-10 (5k x 4k) | Depositor |
| Maximum map value                    | 29.940                          | Depositor |
| Minimum map value                    | -20.122                         | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 1.000                           | Depositor |
| Recommended contour level            | 0.85                            | Depositor |
| Map size ( $\text{\AA}$ )            | 342.72, 342.72, 342.72          | wwPDB     |
| Map dimensions                       | 320, 320, 320                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.071, 1.071, 1.071             | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 7RC, MAN

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     | 0.13         | 0/6464          | 0.38        | 0/8757          |
| 1   | C     | 0.13         | 0/6467          | 0.37        | 0/8760          |
| 2   | B     | 0.13         | 0/6432          | 0.37        | 0/8736          |
| 3   | D     | 0.14         | 0/6401          | 0.40        | 1/8674 (0.0%)   |
| 4   | E     | 0.85         | 7/964 (0.7%)    | 1.00        | 8/1313 (0.6%)   |
| 4   | I     | 0.15         | 0/964           | 0.43        | 0/1313          |
| 5   | F     | 0.14         | 0/847           | 0.37        | 0/1152          |
| 5   | J     | 0.54         | 3/840 (0.4%)    | 0.87        | 6/1143 (0.5%)   |
| 6   | G     | 0.17         | 0/1727          | 0.49        | 0/2349          |
| 7   | H     | 0.13         | 0/1607          | 0.37        | 0/2182          |
| 8   | K     | 0.13         | 0/921           | 0.45        | 0/1247          |
| 9   | L     | 0.15         | 0/840           | 0.47        | 0/1136          |
| All | All   | 0.21         | 10/34474 (0.0%) | 0.44        | 15/46762 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | E     | 0                   | 1                   |
| 9   | L     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4   | E     | 52  | ASP  | CA-CB | -12.42 | 1.34        | 1.53     |
| 4   | E     | 52  | ASP  | CA-C  | -11.53 | 1.37        | 1.53     |
| 4   | E     | 51  | SER  | CA-C  | 10.98  | 1.67        | 1.52     |
| 4   | E     | 52  | ASP  | C-N   | 9.13   | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | J     | 109 | TYR  | CA-C  | 8.18  | 1.63        | 1.52     |
| 5   | J     | 108 | THR  | N-CA  | 6.86  | 1.55        | 1.46     |
| 4   | E     | 52  | ASP  | CB-CG | -6.31 | 1.36        | 1.52     |
| 5   | J     | 109 | TYR  | N-CA  | 5.89  | 1.53        | 1.46     |
| 4   | E     | 51  | SER  | N-CA  | 5.69  | 1.53        | 1.46     |
| 4   | E     | 52  | ASP  | N-CA  | 5.25  | 1.53        | 1.45     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4   | E     | 52  | ASP  | N-CA-CB  | -16.13 | 86.08       | 110.60   |
| 4   | E     | 74  | TYR  | N-CA-C   | -14.42 | 95.82       | 113.41   |
| 4   | E     | 52  | ASP  | CA-C-O   | -13.26 | 103.83      | 121.73   |
| 5   | J     | 110 | TYR  | N-CA-C   | 9.96   | 125.62      | 109.59   |
| 5   | J     | 107 | ALA  | O-C-N    | -9.90  | 112.74      | 123.04   |
| 5   | J     | 110 | TYR  | CA-C-O   | 8.54   | 129.76      | 120.71   |
| 4   | E     | 52  | ASP  | CB-CA-C  | -8.40  | 95.43       | 111.48   |
| 5   | J     | 109 | TYR  | N-CA-C   | 7.64   | 127.07      | 110.80   |
| 4   | E     | 52  | ASP  | CA-C-N   | -7.43  | 107.36      | 121.54   |
| 4   | E     | 52  | ASP  | C-N-CA   | -7.43  | 107.36      | 121.54   |
| 5   | J     | 108 | THR  | CB-CA-C  | -7.22  | 96.04       | 110.42   |
| 3   | D     | 102 | ASP  | N-CA-C   | 6.63   | 117.33      | 108.38   |
| 4   | E     | 52  | ASP  | N-CA-C   | 5.37   | 117.68      | 109.95   |
| 5   | J     | 110 | TYR  | CA-CB-CG | 5.15   | 123.17      | 113.90   |
| 4   | E     | 51  | SER  | O-C-N    | -5.09  | 115.83      | 122.59   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | E     | 52  | ASP  | Mainchain |
| 9   | L     | 28  | PRO  | Peptide   |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6322  | 0        | 6287     | 247     | 0            |
| 1   | C     | 6325  | 0        | 6295     | 235     | 0            |
| 2   | B     | 6279  | 0        | 6193     | 220     | 0            |
| 3   | D     | 6260  | 0        | 6165     | 231     | 0            |
| 4   | E     | 938   | 0        | 883      | 55      | 0            |
| 4   | I     | 938   | 0        | 883      | 37      | 0            |
| 5   | F     | 828   | 0        | 788      | 37      | 0            |
| 5   | J     | 822   | 0        | 781      | 51      | 0            |
| 6   | G     | 1693  | 0        | 1685     | 80      | 0            |
| 7   | H     | 1576  | 0        | 1537     | 53      | 0            |
| 8   | K     | 899   | 0        | 862      | 48      | 0            |
| 9   | L     | 820   | 0        | 799      | 39      | 0            |
| 10  | M     | 39    | 0        | 34       | 0       | 0            |
| 10  | O     | 39    | 0        | 34       | 0       | 0            |
| 11  | N     | 28    | 0        | 25       | 0       | 0            |
| 12  | A     | 98    | 0        | 90       | 0       | 0            |
| 12  | B     | 42    | 0        | 39       | 1       | 0            |
| 12  | C     | 98    | 0        | 91       | 1       | 0            |
| 12  | D     | 42    | 0        | 39       | 1       | 0            |
| 13  | B     | 16    | 0        | 0        | 7       | 0            |
| 13  | D     | 16    | 0        | 0        | 6       | 0            |
| All | All   | 34118 | 0        | 33510    | 1244    | 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 18.

All (1244) 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) |
|-----------------|-------------------|--------------------------|-------------------|
| 3:D:762:TYR:OH  | 13:D:1504:7RC:C05 | 1.93                     | 1.16              |
| 6:G:130:SER:HB2 | 6:G:153:ASN:O     | 1.55                     | 1.05              |
| 1:C:410:TYR:HB2 | 1:C:456:TYR:O     | 1.59                     | 1.02              |
| 1:C:350:ASN:HA  | 1:C:367:TYR:O     | 1.59                     | 1.00              |
| 2:B:485:HIS:CG  | 13:B:1504:7RC:O05 | 2.18                     | 0.97              |
| 2:B:485:HIS:CD2 | 13:B:1504:7RC:C08 | 2.49                     | 0.95              |
| 8:K:22:VAL:HA   | 8:K:45:SER:O      | 1.65                     | 0.94              |
| 6:G:2:VAL:HA    | 6:G:25:SER:O      | 1.67                     | 0.93              |
| 1:A:410:TYR:HB2 | 1:A:456:TYR:O     | 1.69                     | 0.92              |
| 3:D:145:GLN:HG2 | 3:D:147:GLY:H     | 1.34                     | 0.92              |
| 2:B:731:ASP:OD2 | 13:B:1504:7RC:C03 | 2.19                     | 0.90              |
| 7:H:18:THR:HA   | 7:H:75:ILE:O      | 1.70                     | 0.89              |
| 4:E:52:ASP:HB2  | 4:E:53:TYR:CD1    | 2.07                     | 0.89              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:J:60:GLN:HG3   | 5:J:109:TYR:CE2   | 2.08                     | 0.88              |
| 4:E:52:ASP:HB2   | 4:E:53:TYR:CE1    | 2.10                     | 0.87              |
| 4:E:52:ASP:CB    | 4:E:53:TYR:CD1    | 2.58                     | 0.86              |
| 1:C:533:PHE:HB3  | 1:C:776:ILE:HD11  | 1.57                     | 0.85              |
| 4:E:52:ASP:C     | 4:E:53:TYR:CG     | 2.53                     | 0.85              |
| 5:J:110:TYR:HB3  | 5:J:121:PHE:CB    | 2.07                     | 0.84              |
| 1:A:641:MET:HA   | 1:A:644:VAL:HG22  | 1.59                     | 0.84              |
| 6:G:127:ALA:HB1  | 6:G:158:ARG:HD2   | 1.61                     | 0.83              |
| 3:D:519:ARG:HH22 | 13:D:1504:7RC:C08 | 1.92                     | 0.82              |
| 2:B:108:ALA:HA   | 2:B:111:GLN:HE21  | 1.44                     | 0.82              |
| 6:G:150:CYS:HB2  | 6:G:223:LYS:HB3   | 1.62                     | 0.81              |
| 1:C:71:ALA:HA    | 1:C:74:MET:HG2    | 1.64                     | 0.80              |
| 5:F:31:ALA:HA    | 5:F:130:LYS:HE2   | 1.66                     | 0.78              |
| 3:D:684:GLY:HA2  | 3:D:706:MET:HE1   | 1.65                     | 0.77              |
| 5:J:21:ILE:N     | 5:J:45:SER:HG     | 1.82                     | 0.77              |
| 1:A:703:TYR:HA   | 1:A:706:MET:HG2   | 1.65                     | 0.77              |
| 1:C:354:MET:HE1  | 1:C:363:GLN:HG3   | 1.65                     | 0.77              |
| 1:A:541:LEU:HD23 | 1:A:736:LEU:HD11  | 1.67                     | 0.76              |
| 6:G:149:VAL:O    | 6:G:225:PHE:N     | 2.18                     | 0.76              |
| 1:C:570:VAL:HG22 | 1:C:610:SER:HB2   | 1.66                     | 0.76              |
| 4:I:58:ILE:HG22  | 4:I:68:TRP:HA     | 1.66                     | 0.76              |
| 6:G:135:PRO:HD2  | 6:G:226:ASN:HA    | 1.67                     | 0.76              |
| 3:D:116:SER:HB2  | 3:D:142:MET:HB2   | 1.66                     | 0.76              |
| 3:D:519:ARG:NH2  | 13:D:1504:7RC:O05 | 2.17                     | 0.74              |
| 1:A:439:PRO:HG3  | 1:A:480:ALA:HA    | 1.70                     | 0.74              |
| 2:B:666:SER:HB3  | 2:B:756:PHE:HZ    | 1.52                     | 0.74              |
| 8:K:119:PRO:HA   | 8:K:129:PHE:HB3   | 1.70                     | 0.74              |
| 6:G:197:LEU:HD13 | 6:G:201:ASP:HB3   | 1.70                     | 0.73              |
| 4:E:52:ASP:O     | 4:E:53:TYR:CG     | 2.41                     | 0.73              |
| 2:B:36:ILE:HD12  | 2:B:69:VAL:HG22   | 1.70                     | 0.73              |
| 2:B:521:VAL:HG13 | 2:B:522:VAL:HG23  | 1.70                     | 0.73              |
| 1:A:616:ASN:O    | 3:D:616:ASN:ND2   | 2.22                     | 0.72              |
| 2:B:662:VAL:HG22 | 2:B:664:GLY:H     | 1.55                     | 0.72              |
| 1:C:699:LEU:O    | 1:C:702:MET:HB2   | 1.88                     | 0.72              |
| 1:C:513:ILE:HD13 | 1:C:517:LEU:HD22  | 1.70                     | 0.72              |
| 3:D:418:ILE:HB   | 3:D:458:LYS:O     | 1.89                     | 0.72              |
| 3:D:612:LEU:HD23 | 3:D:635:TRP:HD1   | 1.55                     | 0.72              |
| 4:E:38:LEU:HD13  | 4:E:40:LEU:HD23   | 1.70                     | 0.72              |
| 4:E:52:ASP:O     | 4:E:53:TYR:CB     | 2.39                     | 0.71              |
| 4:I:111:THR:HG23 | 4:I:136:THR:HA    | 1.72                     | 0.71              |
| 1:C:439:PRO:HB2  | 1:C:448:ARG:HD2   | 1.72                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:489:ARG:HB2  | 1:C:496:LYS:HE3   | 1.72                     | 0.71              |
| 8:K:129:PHE:O    | 9:L:56:TYR:OH     | 2.07                     | 0.71              |
| 1:A:162:HIS:HB3  | 1:A:192:GLU:HB2   | 1.73                     | 0.71              |
| 3:D:285:TRP:HB2  | 3:D:375:ARG:HH12  | 1.56                     | 0.71              |
| 1:A:86:GLN:HB3   | 1:A:304:PRO:HG2   | 1.72                     | 0.71              |
| 1:C:657:LEU:HD11 | 3:D:655:ILE:HG23  | 1.71                     | 0.71              |
| 2:B:155:ALA:HA   | 2:B:158:MET:HE2   | 1.71                     | 0.71              |
| 2:B:805:ASN:OD1  | 2:B:806:GLU:N     | 2.25                     | 0.70              |
| 3:D:107:ALA:O    | 3:D:110:GLN:HB2   | 1.91                     | 0.70              |
| 4:E:52:ASP:HB3   | 4:E:53:TYR:CD1    | 2.25                     | 0.70              |
| 5:F:48:VAL:HG11  | 5:F:56:MET:HE3    | 1.72                     | 0.70              |
| 4:E:60:GLN:NE2   | 4:E:61:PHE:O      | 2.24                     | 0.70              |
| 3:D:352:SER:N    | 3:D:356:TYR:O     | 2.24                     | 0.70              |
| 2:B:485:HIS:CG   | 13:B:1504:7RC:C08 | 2.74                     | 0.69              |
| 4:I:70:GLY:HA2   | 4:I:80:TYR:HB3    | 1.74                     | 0.69              |
| 5:J:25:GLN:NE2   | 5:J:111:CYS:SG    | 2.64                     | 0.69              |
| 1:A:262:ALA:O    | 1:A:359:ARG:NH1   | 2.22                     | 0.69              |
| 9:L:68:ILE:HG23  | 9:L:72:SER:HA     | 1.75                     | 0.69              |
| 7:H:47:LEU:HD23  | 7:H:48:VAL:HG23   | 1.73                     | 0.69              |
| 5:J:38:ALA:HB3   | 5:J:98:ILE:HB     | 1.75                     | 0.69              |
| 9:L:70:TYR:OH    | 9:L:111:TYR:OH    | 2.09                     | 0.69              |
| 1:A:326:MET:HA   | 1:A:340:PHE:HE2   | 1.58                     | 0.68              |
| 5:J:110:TYR:HB3  | 5:J:121:PHE:N     | 2.09                     | 0.68              |
| 6:G:128:ALA:O    | 6:G:155:PHE:HB2   | 1.94                     | 0.68              |
| 3:D:799:GLY:O    | 3:D:802:HIS:ND1   | 2.25                     | 0.68              |
| 1:C:699:LEU:HB3  | 1:C:702:MET:HG3   | 1.74                     | 0.68              |
| 3:D:316:GLU:O    | 3:D:328:ARG:NH2   | 2.26                     | 0.68              |
| 1:A:158:TYR:O    | 1:A:390:ARG:NH1   | 2.27                     | 0.68              |
| 4:I:32:VAL:HG11  | 4:I:137:VAL:HG22  | 1.74                     | 0.68              |
| 2:B:658:PHE:O    | 2:B:660:ASP:N     | 2.21                     | 0.68              |
| 5:F:115:ASN:OD1  | 5:F:116:GLU:N     | 2.26                     | 0.68              |
| 3:D:275:THR:HA   | 3:D:367:LEU:HB3   | 1.75                     | 0.68              |
| 1:C:541:LEU:HD21 | 1:C:746:LEU:HD13  | 1.76                     | 0.68              |
| 1:C:247:TRP:H    | 1:C:382:PRO:HG2   | 1.59                     | 0.68              |
| 9:L:56:TYR:O     | 9:L:106:TYR:HA    | 1.93                     | 0.68              |
| 1:A:78:VAL:HA    | 1:A:82:LEU:HD23   | 1.76                     | 0.67              |
| 6:G:149:VAL:HG12 | 6:G:150:CYS:H     | 1.59                     | 0.67              |
| 8:K:38:LEU:O     | 8:K:102:GLN:HA    | 1.94                     | 0.67              |
| 1:A:271:LEU:HD12 | 1:A:351:TYR:HE1   | 1.59                     | 0.67              |
| 1:C:124:ARG:NH1  | 1:C:142:PRO:O     | 2.27                     | 0.67              |
| 1:C:672:LEU:HD23 | 1:C:702:MET:HE1   | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:I:66:LEU:HD23  | 5:J:110:TYR:HE1  | 1.57                     | 0.67              |
| 6:G:226:ASN:HD22 | 7:H:121:SER:HB3  | 1.58                     | 0.67              |
| 1:C:259:LEU:HA   | 1:C:262:ALA:HB3  | 1.76                     | 0.67              |
| 3:D:361:LYS:HB2  | 3:D:380:LYS:HE3  | 1.76                     | 0.67              |
| 2:B:692:ARG:HE   | 2:B:695:ARG:HH21 | 1.42                     | 0.66              |
| 3:D:331:GLN:HA   | 3:D:334:MET:HE3  | 1.75                     | 0.66              |
| 4:E:91:THR:HG1   | 4:E:100:PHE:HB2  | 1.59                     | 0.66              |
| 8:K:40:LEU:HD12  | 8:K:99:LEU:HD11  | 1.76                     | 0.66              |
| 9:L:24:MET:HE2   | 9:L:110:GLN:HB2  | 1.77                     | 0.66              |
| 4:E:93:ASP:O     | 4:E:97:ASN:HA    | 1.95                     | 0.66              |
| 8:K:24:LEU:HB2   | 8:K:133:GLY:HA2  | 1.77                     | 0.66              |
| 1:A:28:ASN:ND2   | 1:A:85:SER:O     | 2.29                     | 0.66              |
| 1:C:102:PHE:O    | 1:C:106:PRO:HD2  | 1.96                     | 0.66              |
| 1:A:139:ARG:HD2  | 1:A:143:PRO:HD3  | 1.77                     | 0.65              |
| 5:J:109:TYR:HB2  | 5:J:125:THR:HB   | 1.78                     | 0.65              |
| 2:B:212:ASP:O    | 2:B:216:GLN:NE2  | 2.30                     | 0.65              |
| 3:D:417:VAL:HG13 | 3:D:462:ILE:HD11 | 1.77                     | 0.65              |
| 1:A:295:LEU:HD22 | 1:A:321:PHE:HD1  | 1.61                     | 0.65              |
| 2:B:637:PHE:HZ   | 1:C:819:LEU:HB3  | 1.62                     | 0.65              |
| 5:J:60:GLN:HG3   | 5:J:109:TYR:HE2  | 1.60                     | 0.65              |
| 2:B:135:MET:O    | 2:B:355:TYR:OH   | 2.13                     | 0.65              |
| 1:A:541:LEU:HG   | 1:A:729:PHE:HB3  | 1.77                     | 0.65              |
| 2:B:353:GLU:HG3  | 2:B:355:TYR:HD2  | 1.60                     | 0.65              |
| 1:C:115:ARG:HG3  | 1:C:318:GLY:HA3  | 1.78                     | 0.65              |
| 9:L:58:HIS:HB3   | 9:L:64:PRO:HA    | 1.79                     | 0.65              |
| 1:A:683:THR:HA   | 1:A:729:PHE:HE1  | 1.61                     | 0.65              |
| 4:I:102:GLN:HE22 | 4:I:104:ASN:HD21 | 1.44                     | 0.65              |
| 1:C:547:PRO:HB2  | 1:C:806:ALA:HB2  | 1.79                     | 0.65              |
| 1:A:639:PHE:O    | 1:A:643:ILE:HD12 | 1.97                     | 0.64              |
| 9:L:54:ALA:HB3   | 9:L:109:LEU:HB2  | 1.77                     | 0.64              |
| 2:B:496:MET:HE2  | 2:B:508:ALA:HB1  | 1.78                     | 0.64              |
| 1:C:433:LYS:HD2  | 1:C:454:CYS:HB3  | 1.77                     | 0.64              |
| 1:A:310:GLY:H    | 2:B:76:ARG:HH12  | 1.45                     | 0.64              |
| 1:A:308:CYS:HB2  | 2:B:80:LYS:HE3   | 1.80                     | 0.64              |
| 1:A:731:TRP:HB3  | 1:A:736:LEU:HD21 | 1.79                     | 0.64              |
| 2:B:94:ARG:HH22  | 2:B:318:ALA:HA   | 1.62                     | 0.64              |
| 2:B:331:LEU:O    | 2:B:335:HIS:N    | 2.29                     | 0.64              |
| 1:A:536:GLN:NE2  | 1:A:756:SER:OG   | 2.31                     | 0.64              |
| 6:G:165:LYS:NZ   | 6:G:209:ALA:O    | 2.31                     | 0.64              |
| 6:G:125:THR:HG23 | 6:G:189:TYR:HD1  | 1.62                     | 0.64              |
| 4:E:52:ASP:O     | 4:E:53:TYR:HB2   | 1.96                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:K:63:LYS:HZ3   | 9:L:60:PRO:HG3   | 1.63                     | 0.64              |
| 1:A:216:ALA:O    | 1:A:217:ARG:NH1  | 2.30                     | 0.63              |
| 4:E:43:THR:HB    | 4:E:98:GLN:HB3   | 1.79                     | 0.63              |
| 5:F:58:TRP:HB2   | 5:F:71:ILE:HG22  | 1.80                     | 0.63              |
| 1:A:25:LYS:N     | 1:A:57:LYS:O     | 2.31                     | 0.63              |
| 2:B:431:ARG:O    | 2:B:465:LYS:NZ   | 2.30                     | 0.63              |
| 1:C:270:GLN:NE2  | 1:C:354:MET:SD   | 2.72                     | 0.63              |
| 1:C:347:LYS:HG3  | 1:C:348:PHE:CD2  | 2.34                     | 0.63              |
| 1:C:381:TRP:HB2  | 1:C:385:GLU:HB2  | 1.80                     | 0.63              |
| 3:D:536:VAL:HB   | 3:D:751:ILE:HG21 | 1.79                     | 0.63              |
| 4:E:52:ASP:C     | 4:E:53:TYR:CD1   | 2.76                     | 0.63              |
| 7:H:78:LEU:HD12  | 7:H:82:ASP:HB3   | 1.79                     | 0.63              |
| 4:I:23:GLN:NE2   | 4:I:45:THR:OG1   | 2.31                     | 0.63              |
| 8:K:31:LEU:HD23  | 8:K:140:VAL:HB   | 1.80                     | 0.63              |
| 8:K:44:ALA:HB3   | 8:K:97:ASN:HB3   | 1.80                     | 0.63              |
| 3:D:60:HIS:O     | 3:D:61:HIS:ND1   | 2.31                     | 0.63              |
| 4:I:118:ARG:HD3  | 4:I:128:TYR:HB2  | 1.79                     | 0.63              |
| 1:A:147:GLN:HG3  | 1:A:269:LEU:HD11 | 1.80                     | 0.63              |
| 2:B:773:ARG:NH1  | 1:C:524:ALA:O    | 2.31                     | 0.63              |
| 1:A:667:ILE:HD11 | 1:A:699:LEU:HD21 | 1.79                     | 0.63              |
| 2:B:488:LYS:HD2  | 2:B:491:ASN:HA   | 1.81                     | 0.63              |
| 2:B:536:MET:HG2  | 2:B:735:LEU:HD12 | 1.80                     | 0.63              |
| 3:D:172:VAL:HA   | 3:D:203:LEU:HB2  | 1.81                     | 0.63              |
| 4:E:52:ASP:CB    | 4:E:53:TYR:CE1   | 2.82                     | 0.63              |
| 5:J:108:THR:O    | 5:J:109:TYR:CG   | 2.52                     | 0.63              |
| 8:K:39:LYS:HE2   | 8:K:100:TYR:HB3  | 1.81                     | 0.63              |
| 1:A:813:MET:O    | 1:A:816:VAL:HB   | 2.00                     | 0.62              |
| 2:B:147:PHE:HA   | 2:B:356:GLN:HE22 | 1.64                     | 0.62              |
| 1:C:365:GLY:HA2  | 1:C:374:PRO:HA   | 1.81                     | 0.62              |
| 1:C:559:GLN:HB3  | 1:C:562:LEU:HG   | 1.80                     | 0.62              |
| 1:C:719:GLN:OE1  | 1:C:722:ARG:NH1  | 2.28                     | 0.62              |
| 3:D:429:CYS:O    | 3:D:431:ARG:NH2  | 2.32                     | 0.62              |
| 4:I:38:LEU:HD12  | 4:I:106:VAL:HG11 | 1.80                     | 0.62              |
| 5:J:112:GLN:HA   | 5:J:119:PRO:HB2  | 1.80                     | 0.62              |
| 8:K:121:ARG:HB2  | 8:K:127:TRP:CE3  | 2.33                     | 0.62              |
| 2:B:672:ARG:HH22 | 2:B:674:HIS:HB2  | 1.65                     | 0.62              |
| 5:J:21:ILE:N     | 5:J:45:SER:OG    | 2.31                     | 0.62              |
| 6:G:133:ILE:HG22 | 6:G:134:PHE:H    | 1.64                     | 0.62              |
| 9:L:105:THR:OG1  | 9:L:121:THR:O    | 2.14                     | 0.62              |
| 2:B:719:SER:HB3  | 2:B:724:LYS:HB2  | 1.81                     | 0.62              |
| 3:D:273:PHE:O    | 3:D:371:ARG:NH1  | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:699:LEU:O    | 1:A:703:TYR:N    | 2.27                     | 0.62              |
| 1:C:357:GLN:NE2  | 1:C:378:LYS:O    | 2.33                     | 0.62              |
| 3:D:190:ILE:O    | 3:D:193:SER:OG   | 2.18                     | 0.62              |
| 3:D:203:LEU:HD21 | 3:D:223:LEU:HD21 | 1.82                     | 0.62              |
| 3:D:307:MET:HE1  | 3:D:334:MET:HE1  | 1.82                     | 0.62              |
| 7:H:120:PRO:HD3  | 7:H:132:VAL:HB   | 1.82                     | 0.62              |
| 1:C:198:ASP:O    | 1:C:201:THR:OG1  | 2.17                     | 0.61              |
| 1:A:230:THR:HA   | 1:A:233:ARG:HH11 | 1.66                     | 0.61              |
| 1:C:221:LEU:HB3  | 1:C:249:VAL:HG12 | 1.82                     | 0.61              |
| 2:B:368:LYS:HZ2  | 2:B:394:LYS:H    | 1.46                     | 0.61              |
| 2:B:652:PHE:CE1  | 1:C:805:PRO:HB2  | 2.35                     | 0.61              |
| 3:D:510:VAL:HG12 | 3:D:764:ILE:HD11 | 1.83                     | 0.61              |
| 8:K:57:VAL:O     | 8:K:114:TYR:HA   | 1.99                     | 0.61              |
| 9:L:57:GLN:HG2   | 9:L:67:LEU:HD21  | 1.82                     | 0.61              |
| 1:A:831:ILE:O    | 1:A:834:GLU:HB3  | 2.00                     | 0.61              |
| 2:B:509:VAL:HG23 | 2:B:763:ILE:HG12 | 1.81                     | 0.61              |
| 1:C:448:ARG:NH1  | 1:C:480:ALA:O    | 2.34                     | 0.61              |
| 3:D:148:PRO:HG3  | 3:D:362:LEU:HD11 | 1.82                     | 0.61              |
| 2:B:731:ASP:HB3  | 2:B:734:VAL:HG12 | 1.82                     | 0.61              |
| 1:C:634:MET:HB2  | 3:D:610:TRP:CE2  | 2.35                     | 0.61              |
| 2:B:467:LEU:HD21 | 2:B:775:ILE:HD12 | 1.83                     | 0.61              |
| 3:D:465:LEU:HD12 | 3:D:510:VAL:HG11 | 1.81                     | 0.61              |
| 1:C:28:ASN:ND2   | 1:C:85:SER:O     | 2.32                     | 0.60              |
| 1:C:341:ASN:OD1  | 1:C:345:ASP:N    | 2.33                     | 0.60              |
| 3:D:230:LEU:HB3  | 3:D:258:VAL:HG12 | 1.83                     | 0.60              |
| 3:D:433:THR:HA   | 3:D:457:CYS:O    | 1.99                     | 0.60              |
| 6:G:174:ASN:HB3  | 6:G:195:LEU:HG   | 1.83                     | 0.60              |
| 1:A:448:ARG:NH1  | 1:A:480:ALA:O    | 2.34                     | 0.60              |
| 1:A:764:LYS:O    | 1:A:769:LYS:NZ   | 2.28                     | 0.60              |
| 2:B:175:THR:HG21 | 2:B:235:GLU:HG3  | 1.83                     | 0.60              |
| 1:C:439:PRO:HD2  | 1:C:478:LEU:HB2  | 1.83                     | 0.60              |
| 3:D:131:SER:O    | 3:D:132:MET:HG3  | 2.00                     | 0.60              |
| 3:D:334:MET:O    | 3:D:337:ARG:HB3  | 2.00                     | 0.60              |
| 4:E:51:SER:O     | 4:E:74:TYR:HB3   | 2.01                     | 0.60              |
| 7:H:137:ASN:ND2  | 7:H:138:ASN:OD1  | 2.33                     | 0.60              |
| 1:A:463:LEU:HD22 | 1:A:514:VAL:HG11 | 1.83                     | 0.60              |
| 1:A:721:VAL:HG22 | 1:A:726:LEU:HB3  | 1.82                     | 0.60              |
| 2:B:298:ILE:HG23 | 2:B:341:VAL:HG11 | 1.82                     | 0.60              |
| 1:C:259:LEU:HD13 | 4:I:121:TYR:CE2  | 2.36                     | 0.60              |
| 5:F:33:SER:H     | 5:F:36:GLN:HE22  | 1.50                     | 0.60              |
| 2:B:158:MET:HA   | 2:B:161:ILE:HG22 | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:486:GLY:O    | 2:B:518:ARG:NH2  | 2.34                     | 0.60              |
| 6:G:136:PRO:HA   | 6:G:227:ARG:HH21 | 1.66                     | 0.60              |
| 4:I:72:ILE:HD13  | 4:I:78:THR:HB    | 1.84                     | 0.60              |
| 2:B:228:LEU:HD23 | 2:B:256:ILE:HB   | 1.84                     | 0.60              |
| 3:D:336:ASN:O    | 3:D:340:ILE:N    | 2.34                     | 0.60              |
| 4:E:28:GLY:HA3   | 4:E:40:LEU:HD13  | 1.84                     | 0.60              |
| 6:G:42:PRO:HB2   | 6:G:45:LYS:HB3   | 1.83                     | 0.60              |
| 5:J:61:GLN:HB3   | 5:J:108:THR:OG1  | 2.02                     | 0.60              |
| 2:B:773:ARG:NH2  | 1:C:525:GLN:O    | 2.36                     | 0.59              |
| 6:G:70:THR:HB    | 6:G:83:LYS:HB2   | 1.83                     | 0.59              |
| 8:K:71:ILE:HD11  | 8:K:90:ILE:HD11  | 1.83                     | 0.59              |
| 8:K:58:ARG:NH2   | 8:K:66:GLU:OE1   | 2.35                     | 0.59              |
| 1:C:204:VAL:HG21 | 1:C:231:VAL:HG12 | 1.83                     | 0.59              |
| 1:C:378:LYS:HZ2  | 1:C:380:ILE:HG12 | 1.67                     | 0.59              |
| 2:B:301:THR:HB   | 2:B:341:VAL:HG13 | 1.83                     | 0.59              |
| 2:B:539:ARG:NH2  | 2:B:540:SER:OG   | 2.35                     | 0.59              |
| 2:B:515:ASN:OD1  | 2:B:516:GLU:N    | 2.36                     | 0.59              |
| 2:B:394:LYS:NZ   | 2:B:398:ASP:O    | 2.33                     | 0.59              |
| 1:C:262:ALA:O    | 1:C:359:ARG:NH1  | 2.27                     | 0.59              |
| 3:D:99:PHE:CD2   | 3:D:112:LEU:HD11 | 2.37                     | 0.59              |
| 7:H:38:GLN:HG2   | 7:H:44:PRO:HG3   | 1.84                     | 0.59              |
| 1:A:152:PHE:CZ   | 1:A:187:ARG:HD3  | 2.38                     | 0.58              |
| 1:A:742:GLN:OE1  | 1:A:796:GLN:NE2  | 2.36                     | 0.58              |
| 1:C:351:TYR:HB2  | 1:C:367:TYR:HD2  | 1.68                     | 0.58              |
| 8:K:72:SER:O     | 8:K:92:ARG:NH1   | 2.36                     | 0.58              |
| 1:A:152:PHE:O    | 1:A:155:MET:HG3  | 2.04                     | 0.58              |
| 2:B:279:VAL:HG12 | 2:B:363:VAL:HG22 | 1.85                     | 0.58              |
| 1:A:695:ARG:NH1  | 1:A:696:GLN:OE1  | 2.35                     | 0.58              |
| 2:B:544:VAL:O    | 2:B:816:ASN:ND2  | 2.36                     | 0.58              |
| 3:D:526:SER:HB3  | 3:D:764:ILE:HG22 | 1.86                     | 0.58              |
| 9:L:59:LYS:HD2   | 9:L:62:LYS:HD3   | 1.84                     | 0.58              |
| 4:E:51:SER:O     | 4:E:74:TYR:CD2   | 2.56                     | 0.58              |
| 1:A:545:GLU:OE2  | 1:A:663:ARG:NH2  | 2.37                     | 0.58              |
| 2:B:611:LEU:HD11 | 1:C:618:GLY:H    | 1.68                     | 0.58              |
| 3:D:629:LYS:HA   | 3:D:632:VAL:HG12 | 1.86                     | 0.58              |
| 9:L:69:HIS:HB3   | 9:L:73:SER:HB3   | 1.85                     | 0.58              |
| 2:B:191:VAL:HA   | 2:B:198:TRP:HD1  | 1.68                     | 0.58              |
| 3:D:41:LEU:HD12  | 3:D:72:ALA:HB2   | 1.86                     | 0.58              |
| 7:H:4:MET:HG3    | 7:H:25:ALA:HB2   | 1.85                     | 0.58              |
| 1:A:786:GLU:HG3  | 3:D:757:PHE:CE2  | 2.39                     | 0.58              |
| 2:B:309:LYS:HD2  | 2:B:337:PHE:HZ   | 1.68                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:K:53:THR:OG1   | 8:K:71:ILE:O      | 2.21                     | 0.58              |
| 1:A:364:VAL:HG12 | 1:A:377:ARG:HB2   | 1.86                     | 0.58              |
| 1:C:94:HIS:N     | 1:C:122:THR:OG1   | 2.37                     | 0.58              |
| 1:C:202:LYS:NZ   | 12:C:1002:NAG:O4  | 2.37                     | 0.58              |
| 3:D:508:MET:HG2  | 3:D:766:ILE:HD12  | 1.85                     | 0.58              |
| 6:G:163:GLN:N    | 6:G:163:GLN:OE1   | 2.37                     | 0.58              |
| 1:A:305:PRO:HB2  | 1:A:311:ASN:HD22  | 1.69                     | 0.57              |
| 1:A:339:GLU:O    | 1:A:347:LYS:N     | 2.35                     | 0.57              |
| 2:B:294:ASP:O    | 2:B:298:ILE:HG13  | 2.04                     | 0.57              |
| 4:I:37:SER:HB3   | 4:I:102:GLN:HE21  | 1.69                     | 0.57              |
| 1:A:158:TYR:HB3  | 1:A:390:ARG:HH12  | 1.69                     | 0.57              |
| 1:C:114:TYR:HB2  | 1:C:116:ILE:HD11  | 1.85                     | 0.57              |
| 7:H:160:GLN:NE2  | 7:H:178:THR:OG1   | 2.37                     | 0.57              |
| 7:H:11:LEU:HB2   | 7:H:102:THR:HG21  | 1.85                     | 0.57              |
| 5:J:60:GLN:O     | 5:J:68:LYS:N      | 2.36                     | 0.57              |
| 1:A:558:PHE:HE1  | 2:B:812:LEU:HB2   | 1.68                     | 0.57              |
| 3:D:60:HIS:CD2   | 3:D:61:HIS:H      | 2.22                     | 0.57              |
| 4:I:44:VAL:O     | 4:I:97:ASN:ND2    | 2.37                     | 0.57              |
| 1:A:151:TRP:CD2  | 1:A:220:ILE:HD11  | 2.40                     | 0.57              |
| 1:A:270:GLN:NE2  | 1:A:363:GLN:OE1   | 2.38                     | 0.57              |
| 2:B:654:ILE:HG13 | 2:B:806:GLU:HG3   | 1.86                     | 0.57              |
| 1:C:554:PHE:HD2  | 1:C:816:VAL:HG22  | 1.70                     | 0.57              |
| 3:D:157:MET:HA   | 3:D:160:ILE:HD12  | 1.85                     | 0.57              |
| 4:E:38:LEU:O     | 4:E:102:GLN:HA    | 2.04                     | 0.57              |
| 2:B:433:THR:OG1  | 2:B:455:CYS:SG    | 2.60                     | 0.57              |
| 3:D:91:ASP:HB3   | 3:D:92:ARG:HD3    | 1.86                     | 0.57              |
| 6:G:214:HIS:O    | 6:G:218:SER:N     | 2.38                     | 0.57              |
| 1:A:521:ASN:OD1  | 1:A:525:GLN:NE2   | 2.38                     | 0.57              |
| 1:A:699:LEU:HA   | 1:A:702:MET:HE2   | 1.86                     | 0.57              |
| 2:B:672:ARG:NH2  | 2:B:675:ASP:OD1   | 2.38                     | 0.57              |
| 4:E:89:SER:HB2   | 4:E:102:GLN:HB2   | 1.86                     | 0.57              |
| 1:A:94:HIS:H     | 1:A:122:THR:HB    | 1.69                     | 0.57              |
| 1:A:259:LEU:HD23 | 4:E:121:TYR:HB3   | 1.86                     | 0.57              |
| 2:B:49:ARG:HH12  | 2:B:52:ARG:HD2    | 1.68                     | 0.57              |
| 2:B:485:HIS:NE2  | 13:B:1504:7RC:C01 | 2.67                     | 0.57              |
| 2:B:610:GLY:O    | 2:B:614:ASN:N     | 2.38                     | 0.57              |
| 1:C:630:ARG:NH1  | 3:D:603:GLY:O     | 2.37                     | 0.57              |
| 3:D:500:GLU:OE2  | 3:D:505:ARG:NH2   | 2.38                     | 0.57              |
| 1:A:329:LYS:NZ   | 1:A:330:TYR:O     | 2.38                     | 0.56              |
| 1:A:470:MET:HE3  | 1:A:472:PHE:HE1   | 1.70                     | 0.56              |
| 5:F:25:GLN:HB2   | 5:F:123:GLY:HA3   | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:623:ALA:HB2  | 2:B:617:VAL:HG21 | 1.87                     | 0.56              |
| 2:B:573:VAL:HB   | 2:B:601:ILE:HG22 | 1.87                     | 0.56              |
| 1:A:131:LYS:NZ   | 1:A:137:PHE:O    | 2.33                     | 0.56              |
| 1:A:539:THR:OG1  | 1:A:749:THR:O    | 2.21                     | 0.56              |
| 1:C:555:MET:HE1  | 1:C:563:TRP:CD1  | 2.40                     | 0.56              |
| 1:C:685:LYS:HG3  | 1:C:710:ASN:HB3  | 1.88                     | 0.56              |
| 1:C:815:GLY:HA2  | 1:C:818:MET:HG2  | 1.87                     | 0.56              |
| 5:J:110:TYR:HB3  | 5:J:121:PHE:CA   | 2.34                     | 0.56              |
| 1:A:514:VAL:HA   | 1:A:760:ILE:HG22 | 1.87                     | 0.56              |
| 2:B:497:ILE:HD12 | 2:B:522:VAL:HG21 | 1.88                     | 0.56              |
| 1:C:630:ARG:HH21 | 3:D:604:LYS:HZ3  | 1.54                     | 0.56              |
| 3:D:361:LYS:HA   | 3:D:379:TRP:O    | 2.05                     | 0.56              |
| 1:A:439:PRO:HB2  | 1:A:448:ARG:HD3  | 1.88                     | 0.56              |
| 1:A:653:ALA:HB1  | 2:B:654:ILE:HD13 | 1.88                     | 0.56              |
| 4:E:68:TRP:O     | 4:E:81:ASN:ND2   | 2.29                     | 0.56              |
| 1:A:127:ILE:HG13 | 1:A:171:HIS:ND1  | 2.20                     | 0.56              |
| 1:A:538:LEU:HD23 | 1:A:754:PHE:HB3  | 1.87                     | 0.56              |
| 1:A:638:GLY:O    | 1:A:642:ILE:HG12 | 2.05                     | 0.56              |
| 1:C:203:ASN:OD1  | 1:C:205:THR:HG23 | 2.06                     | 0.56              |
| 1:C:390:ARG:NH1  | 1:C:392:TYR:O    | 2.39                     | 0.56              |
| 3:D:120:LEU:HA   | 3:D:142:MET:HG3  | 1.88                     | 0.56              |
| 3:D:760:THR:HG22 | 3:D:761:GLY:H    | 1.71                     | 0.56              |
| 2:B:139:ASP:OD2  | 2:B:141:THR:OG1  | 2.18                     | 0.56              |
| 2:B:167:TRP:HB3  | 2:B:226:VAL:HG21 | 1.88                     | 0.56              |
| 2:B:543:THR:O    | 2:B:655:GLN:NE2  | 2.39                     | 0.56              |
| 1:C:132:SER:HB3  | 3:D:177:PRO:HB2  | 1.87                     | 0.56              |
| 1:A:56:TRP:CD1   | 1:A:57:LYS:HG3   | 2.41                     | 0.56              |
| 1:A:561:THR:HG23 | 1:A:562:LEU:HD12 | 1.88                     | 0.56              |
| 1:A:634:MET:HE1  | 2:B:606:TRP:HA   | 1.88                     | 0.56              |
| 2:B:459:PHE:HZ   | 2:B:788:MET:HE1  | 1.71                     | 0.56              |
| 3:D:684:GLY:O    | 3:D:730:ILE:N    | 2.39                     | 0.56              |
| 7:H:12:SER:OG    | 7:H:105:GLU:O    | 2.23                     | 0.56              |
| 4:I:54:ALA:HB3   | 4:I:119:LEU:HB3  | 1.87                     | 0.55              |
| 1:A:400:ILE:HD12 | 1:A:512:MET:HB2  | 1.88                     | 0.55              |
| 2:B:134:ILE:HD11 | 2:B:355:TYR:CE1  | 2.42                     | 0.55              |
| 2:B:692:ARG:HH21 | 2:B:695:ARG:HE   | 1.54                     | 0.55              |
| 1:C:311:ASN:O    | 3:D:76:THR:OG1   | 2.22                     | 0.55              |
| 4:E:92:ARG:HH12  | 4:E:99:PHE:HB3   | 1.71                     | 0.55              |
| 6:G:132:PHE:HE2  | 6:G:226:ASN:HB3  | 1.71                     | 0.55              |
| 2:B:500:VAL:HG21 | 2:B:508:ALA:HB2  | 1.88                     | 0.55              |
| 1:C:49:ALA:O     | 1:C:53:HIS:ND1   | 2.26                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:529:PHE:HB2  | 3:D:789:MET:HE2  | 1.89                     | 0.55              |
| 7:H:18:THR:OG1   | 7:H:74:LYS:HE2   | 2.07                     | 0.55              |
| 1:C:79:CYS:HA    | 1:C:83:ILE:HB    | 1.89                     | 0.55              |
| 1:C:238:LEU:HB2  | 1:C:240:MET:HE1  | 1.87                     | 0.55              |
| 1:C:817:PHE:O    | 1:C:820:VAL:HG12 | 2.06                     | 0.55              |
| 5:J:34:LEU:HA    | 5:J:101:VAL:HB   | 1.86                     | 0.55              |
| 5:J:60:GLN:CG    | 5:J:109:TYR:HE2  | 2.19                     | 0.55              |
| 9:L:31:LEU:HB2   | 9:L:123:LEU:HA   | 1.87                     | 0.55              |
| 9:L:45:ALA:O     | 9:L:89:ARG:NH2   | 2.38                     | 0.55              |
| 8:K:88:PHE:HB3   | 8:K:101:LEU:HD11 | 1.87                     | 0.55              |
| 5:J:71:ILE:HA    | 5:J:78:GLU:HB2   | 1.89                     | 0.55              |
| 3:D:174:THR:HA   | 3:D:205:LEU:HB2  | 1.89                     | 0.55              |
| 8:K:40:LEU:HD23  | 8:K:103:MET:HE3  | 1.89                     | 0.55              |
| 1:A:484:PHE:HA   | 1:A:501:MET:HE1  | 1.89                     | 0.55              |
| 1:A:634:MET:HE2  | 2:B:606:TRP:HE3  | 1.72                     | 0.55              |
| 1:A:796:GLN:N    | 1:A:796:GLN:OE1  | 2.40                     | 0.55              |
| 2:B:656:GLU:HB2  | 2:B:806:GLU:HA   | 1.89                     | 0.55              |
| 1:C:44:GLU:OE2   | 1:C:48:GLN:NE2   | 2.40                     | 0.55              |
| 3:D:164:TYR:OH   | 3:D:386:MET:SD   | 2.63                     | 0.55              |
| 5:J:60:GLN:CG    | 5:J:109:TYR:CE2  | 2.88                     | 0.55              |
| 2:B:219:LEU:HD11 | 2:B:248:LEU:HG   | 1.89                     | 0.55              |
| 6:G:130:SER:N    | 6:G:155:PHE:HB3  | 2.21                     | 0.55              |
| 6:G:149:VAL:HB   | 6:G:225:PHE:CZ   | 2.42                     | 0.55              |
| 2:B:785:ASP:O    | 1:C:696:GLN:NE2  | 2.32                     | 0.54              |
| 2:B:784:GLY:HA2  | 1:C:754:PHE:HE1  | 1.73                     | 0.54              |
| 1:C:264:ASP:HA   | 1:C:356:LEU:HD23 | 1.88                     | 0.54              |
| 1:C:341:ASN:OD1  | 1:C:344:GLY:N    | 2.40                     | 0.54              |
| 7:H:120:PRO:HG3  | 7:H:130:ALA:HB1  | 1.88                     | 0.54              |
| 9:L:66:LEU:O     | 9:L:75:GLN:NE2   | 2.40                     | 0.54              |
| 1:A:68:LYS:HB3   | 1:A:74:MET:HB2   | 1.90                     | 0.54              |
| 2:B:146:GLN:O    | 2:B:356:GLN:NE2  | 2.41                     | 0.54              |
| 2:B:212:ASP:HB3  | 2:B:216:GLN:HE22 | 1.72                     | 0.54              |
| 3:D:533:GLY:O    | 3:D:733:ALA:N    | 2.41                     | 0.54              |
| 8:K:30:GLY:H     | 8:K:138:VAL:HG22 | 1.73                     | 0.54              |
| 1:A:46:VAL:HA    | 1:A:285:VAL:HG11 | 1.89                     | 0.54              |
| 1:A:458:PHE:CE1  | 1:A:788:LEU:HB3  | 2.43                     | 0.54              |
| 1:C:225:GLU:OE2  | 1:C:258:ALA:N    | 2.40                     | 0.54              |
| 3:D:110:GLN:NE2  | 3:D:134:MET:HE1  | 2.22                     | 0.54              |
| 3:D:166:TRP:HB3  | 3:D:227:ILE:HD13 | 1.88                     | 0.54              |
| 3:D:233:THR:O    | 3:D:237:ALA:N    | 2.40                     | 0.54              |
| 3:D:367:LEU:HG   | 3:D:371:ARG:HA   | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:51:SER:O     | 4:E:74:TYR:CB    | 2.54                     | 0.54              |
| 4:E:55:TRP:O     | 4:E:71:TYR:HA    | 2.07                     | 0.54              |
| 1:A:68:LYS:HD2   | 1:A:69:PRO:HD2   | 1.90                     | 0.54              |
| 1:A:397:ARG:HH11 | 1:A:473:THR:HB   | 1.71                     | 0.54              |
| 6:G:92:THR:HG23  | 6:G:115:THR:HA   | 1.89                     | 0.54              |
| 6:G:192:SER:OG   | 6:G:193:SER:N    | 2.41                     | 0.54              |
| 4:I:23:GLN:NE2   | 4:I:25:GLN:OE1   | 2.40                     | 0.54              |
| 1:C:731:TRP:CD1  | 1:C:732:ASP:H    | 2.25                     | 0.54              |
| 4:E:124:TYR:OH   | 5:F:73:ALA:HB2   | 2.08                     | 0.54              |
| 2:B:129:GLY:O    | 2:B:132:SER:OG   | 2.24                     | 0.54              |
| 3:D:831:LEU:HA   | 3:D:834:ILE:HG12 | 1.89                     | 0.54              |
| 6:G:165:LYS:HE3  | 6:G:208:TYR:HD2  | 1.73                     | 0.54              |
| 7:H:165:GLU:N    | 7:H:165:GLU:OE2  | 2.39                     | 0.54              |
| 3:D:331:GLN:O    | 3:D:335:LEU:N    | 2.33                     | 0.54              |
| 3:D:793:GLU:HB2  | 3:D:797:LEU:HG   | 1.91                     | 0.53              |
| 4:E:38:LEU:HD11  | 4:E:103:LEU:HB3  | 1.89                     | 0.53              |
| 6:G:169:ALA:O    | 6:G:174:ASN:ND2  | 2.35                     | 0.53              |
| 2:B:274:SER:HA   | 2:B:366:LEU:HB3  | 1.90                     | 0.53              |
| 1:C:34:SER:H     | 1:C:67:HIS:HD2   | 1.53                     | 0.53              |
| 1:C:531:LYS:HE2  | 1:C:532:PRO:HD2  | 1.90                     | 0.53              |
| 3:D:685:THR:HB   | 3:D:730:ILE:HB   | 1.89                     | 0.53              |
| 7:H:119:PRO:HA   | 7:H:132:VAL:HG23 | 1.90                     | 0.53              |
| 7:H:181:LEU:HD11 | 7:H:185:ASP:HB3  | 1.90                     | 0.53              |
| 5:J:69:LEU:HD21  | 5:J:72:TYR:HB3   | 1.89                     | 0.53              |
| 1:C:165:LEU:HD13 | 1:C:220:ILE:HB   | 1.90                     | 0.53              |
| 8:K:58:ARG:HD3   | 8:K:106:LEU:HD22 | 1.90                     | 0.53              |
| 1:A:573:VAL:O    | 1:A:577:LEU:HG   | 2.09                     | 0.53              |
| 2:B:564:MET:HA   | 2:B:567:ILE:HG12 | 1.90                     | 0.53              |
| 2:B:698:TYR:HB3  | 2:B:701:MET:HB3  | 1.89                     | 0.53              |
| 1:C:32:VAL:HG12  | 1:C:67:HIS:CE1   | 2.44                     | 0.53              |
| 1:C:533:PHE:HA   | 1:C:780:HIS:NE2  | 2.23                     | 0.53              |
| 3:D:108:ILE:O    | 3:D:111:ILE:HB   | 2.07                     | 0.53              |
| 3:D:503:MET:HE3  | 3:D:503:MET:HA   | 1.89                     | 0.53              |
| 5:F:27:PRO:HG2   | 5:F:30:LEU:HB3   | 1.90                     | 0.53              |
| 6:G:89:THR:HG23  | 6:G:117:SER:HA   | 1.91                     | 0.53              |
| 1:A:543:LYS:HA   | 1:A:746:LEU:HD13 | 1.90                     | 0.53              |
| 1:A:702:MET:O    | 1:A:705:HIS:HB3  | 2.09                     | 0.53              |
| 3:D:244:ALA:HB1  | 3:D:249:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:145:SER:O    | 1:A:148:SER:OG   | 2.22                     | 0.53              |
| 5:J:113:GLN:HG3  | 5:J:119:PRO:HB3  | 1.91                     | 0.53              |
| 1:A:357:GLN:HA   | 1:A:380:ILE:HD12 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:252:ASP:N    | 2:B:252:ASP:OD1  | 2.40                     | 0.53              |
| 3:D:430:MET:SD   | 3:D:430:MET:N    | 2.77                     | 0.53              |
| 7:H:121:SER:H    | 7:H:124:GLN:NE2  | 2.06                     | 0.53              |
| 8:K:70:TYR:CE1   | 9:L:115:TYR:HB2  | 2.44                     | 0.53              |
| 2:B:600:THR:HG23 | 2:B:603:LYS:HE2  | 1.89                     | 0.53              |
| 1:C:700:SER:OG   | 1:C:704:ARG:NH2  | 2.40                     | 0.53              |
| 1:C:830:LEU:O    | 1:C:833:ILE:HB   | 2.09                     | 0.53              |
| 5:J:25:GLN:HG2   | 5:J:42:CYS:HA    | 1.91                     | 0.53              |
| 8:K:87:ARG:O     | 8:K:104:ASN:ND2  | 2.42                     | 0.53              |
| 2:B:460:CYS:HA   | 2:B:463:ILE:HG22 | 1.91                     | 0.53              |
| 4:I:92:ARG:HD3   | 4:I:99:PHE:HB3   | 1.91                     | 0.53              |
| 3:D:73:MET:HE3   | 3:D:80:SER:HB3   | 1.91                     | 0.53              |
| 8:K:58:ARG:HG3   | 8:K:112:ALA:HB1  | 1.91                     | 0.53              |
| 2:B:624:GLY:O    | 2:B:627:SER:N    | 2.40                     | 0.52              |
| 3:D:684:GLY:CA   | 3:D:706:MET:HE1  | 2.38                     | 0.52              |
| 5:F:33:SER:OG    | 5:F:36:GLN:NE2   | 2.42                     | 0.52              |
| 7:H:15:VAL:HA    | 7:H:78:LEU:HD23  | 1.91                     | 0.52              |
| 8:K:37:SER:HB2   | 8:K:102:GLN:HB3  | 1.90                     | 0.52              |
| 1:A:209:MET:O    | 1:A:212:ARG:HG2  | 2.09                     | 0.52              |
| 2:B:134:ILE:HD11 | 2:B:355:TYR:HE1  | 1.74                     | 0.52              |
| 1:C:345:ASP:OD1  | 1:C:346:ARG:N    | 2.43                     | 0.52              |
| 1:C:544:LYS:O    | 1:C:545:GLU:HG3  | 2.08                     | 0.52              |
| 3:D:328:ARG:O    | 3:D:332:SER:N    | 2.38                     | 0.52              |
| 3:D:448:GLU:HG3  | 3:D:449:GLU:H    | 1.74                     | 0.52              |
| 6:G:40:ARG:HD3   | 6:G:95:TYR:CE1   | 2.44                     | 0.52              |
| 1:A:148:SER:HA   | 1:A:151:TRP:CE3  | 2.45                     | 0.52              |
| 3:D:60:HIS:CG    | 3:D:61:HIS:H     | 2.27                     | 0.52              |
| 4:I:126:MET:HB3  | 5:J:59:TYR:HE2   | 1.75                     | 0.52              |
| 9:L:107:TYR:CE1  | 9:L:120:GLY:HA3  | 2.44                     | 0.52              |
| 2:B:79:PRO:O     | 2:B:83:ILE:HG12  | 2.09                     | 0.52              |
| 1:C:662:GLU:O    | 1:C:671:ARG:NH1  | 2.43                     | 0.52              |
| 3:D:226:PRO:HA   | 3:D:254:TYR:HD1  | 1.73                     | 0.52              |
| 4:I:26:GLU:H     | 4:I:131:GLN:HE22 | 1.58                     | 0.52              |
| 3:D:668:ASP:OD1  | 3:D:669:LYS:N    | 2.43                     | 0.52              |
| 1:A:672:LEU:O    | 1:A:681:TYR:OH   | 2.26                     | 0.52              |
| 2:B:160:LYS:O    | 2:B:163:GLN:HG3  | 2.09                     | 0.52              |
| 1:C:552:ASP:OD1  | 1:C:553:SER:N    | 2.43                     | 0.52              |
| 3:D:565:MET:HA   | 3:D:568:ILE:HG12 | 1.91                     | 0.52              |
| 3:D:631:MET:HE3  | 3:D:631:MET:HA   | 1.90                     | 0.52              |
| 2:B:172:LEU:HD11 | 2:B:183:PHE:HE2  | 1.75                     | 0.52              |
| 1:A:42:PHE:HE2   | 1:A:62:ALA:HB1   | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:576:MET:HE2  | 2:B:828:MET:SD   | 2.49                     | 0.52              |
| 1:C:34:SER:HB3   | 1:C:67:HIS:H     | 1.74                     | 0.52              |
| 1:C:415:MET:SD   | 1:C:419:THR:OG1  | 2.68                     | 0.52              |
| 3:D:191:GLU:OE2  | 3:D:192:ASN:ND2  | 2.43                     | 0.52              |
| 7:H:12:SER:HA    | 7:H:104:LEU:HD13 | 1.92                     | 0.52              |
| 7:H:59:PRO:HG2   | 7:H:62:PHE:HE2   | 1.75                     | 0.52              |
| 1:A:350:ASN:HA   | 1:A:367:TYR:O    | 2.09                     | 0.52              |
| 1:C:260:ARG:NH2  | 5:J:115:ASN:O    | 2.43                     | 0.52              |
| 3:D:437:GLN:HE22 | 3:D:439:ARG:HH21 | 1.58                     | 0.52              |
| 3:D:658:GLU:HB3  | 3:D:808:VAL:HG12 | 1.92                     | 0.52              |
| 6:G:23:SER:HA    | 6:G:79:GLN:HA    | 1.91                     | 0.52              |
| 2:B:113:LEU:HD22 | 2:B:124:ILE:HG21 | 1.90                     | 0.52              |
| 3:D:96:GLY:HA3   | 3:D:300:ILE:HG21 | 1.92                     | 0.52              |
| 3:D:557:ASP:O    | 3:D:561:MET:HG2  | 2.09                     | 0.52              |
| 6:G:4:LEU:O      | 6:G:110:GLN:NE2  | 2.43                     | 0.52              |
| 1:A:312:THR:HG23 | 2:B:76:ARG:HH21  | 1.75                     | 0.51              |
| 1:A:697:VAL:HA   | 1:A:700:SER:HB3  | 1.91                     | 0.51              |
| 1:C:486:THR:OG1  | 1:C:488:GLU:OE2  | 2.21                     | 0.51              |
| 3:D:125:GLY:HA2  | 3:D:130:SER:HB2  | 1.91                     | 0.51              |
| 3:D:406:LEU:HD22 | 3:D:507:TYR:CG   | 2.44                     | 0.51              |
| 5:J:57:ASN:ND2   | 5:J:59:TYR:OH    | 2.43                     | 0.51              |
| 9:L:49:ILE:HG12  | 9:L:89:ARG:HA    | 1.92                     | 0.51              |
| 1:A:821:ALA:HA   | 1:A:824:ILE:HG12 | 1.92                     | 0.51              |
| 3:D:433:THR:HG22 | 3:D:458:LYS:HB2  | 1.92                     | 0.51              |
| 5:F:74:ALA:HB1   | 5:F:87:GLY:HA3   | 1.92                     | 0.51              |
| 2:B:161:ILE:HD13 | 2:B:383:LEU:HD21 | 1.92                     | 0.51              |
| 1:C:528:GLU:HG2  | 1:C:769:LYS:HE2  | 1.91                     | 0.51              |
| 3:D:226:PRO:O    | 3:D:255:THR:N    | 2.36                     | 0.51              |
| 4:E:110:ASP:HB2  | 4:E:138:SER:HB3  | 1.91                     | 0.51              |
| 6:G:98:THR:HG1   | 6:G:107:TYR:C    | 2.16                     | 0.51              |
| 6:G:117:SER:OG   | 6:G:118:ALA:N    | 2.44                     | 0.51              |
| 7:H:143:GLU:HG2  | 7:H:199:GLN:HB3  | 1.92                     | 0.51              |
| 1:C:479:VAL:HG13 | 1:C:482:GLY:H    | 1.74                     | 0.51              |
| 1:C:731:TRP:HB3  | 1:C:736:LEU:HD21 | 1.92                     | 0.51              |
| 7:H:138:ASN:HA   | 7:H:172:THR:HB   | 1.93                     | 0.51              |
| 5:J:44:ALA:N     | 5:J:92:THR:O     | 2.38                     | 0.51              |
| 4:E:51:SER:O     | 4:E:74:TYR:CG    | 2.63                     | 0.51              |
| 2:B:516:GLU:HG2  | 1:C:778:LYS:HE2  | 1.92                     | 0.51              |
| 1:C:263:PRO:HG2  | 1:C:266:ILE:HD11 | 1.93                     | 0.51              |
| 1:C:702:MET:O    | 1:C:706:MET:HE3  | 2.11                     | 0.51              |
| 1:C:714:ALA:O    | 1:C:718:ILE:HG12 | 2.10                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:186:ILE:O    | 3:D:190:ILE:HG12  | 2.11                     | 0.51              |
| 3:D:561:MET:HA   | 3:D:564:VAL:HG22  | 1.93                     | 0.51              |
| 1:A:163:ILE:H    | 1:A:192:GLU:H     | 1.58                     | 0.51              |
| 1:A:551:LEU:HD12 | 1:A:654:PHE:HE2   | 1.75                     | 0.51              |
| 1:A:742:GLN:HA   | 1:A:796:GLN:HE21  | 1.76                     | 0.51              |
| 2:B:40:LEU:HB2   | 2:B:73:LEU:HD23   | 1.92                     | 0.51              |
| 2:B:293:ARG:NH2  | 2:B:296:LEU:HD13  | 2.26                     | 0.51              |
| 2:B:332:HIS:O    | 2:B:335:HIS:HB3   | 2.11                     | 0.51              |
| 1:C:225:GLU:OE2  | 1:C:257:ASN:N     | 2.38                     | 0.51              |
| 1:C:405:GLN:HG2  | 1:C:516:PRO:HG3   | 1.92                     | 0.51              |
| 1:C:773:SER:O    | 1:C:776:ILE:HG22  | 2.11                     | 0.51              |
| 3:D:95:GLN:NE2   | 3:D:315:PRO:O     | 2.44                     | 0.51              |
| 3:D:103:THR:H    | 3:D:128:GLY:HA3   | 1.76                     | 0.51              |
| 3:D:414:ALA:HB2  | 3:D:418:ILE:HD11  | 1.93                     | 0.51              |
| 3:D:612:LEU:HD23 | 3:D:635:TRP:CD1   | 2.41                     | 0.51              |
| 7:H:4:MET:HE2    | 7:H:88:CYS:SG     | 2.51                     | 0.51              |
| 8:K:90:ILE:HD13  | 8:K:101:LEU:HD13  | 1.91                     | 0.51              |
| 1:A:814:ALA:HA   | 1:A:817:PHE:HD2   | 1.76                     | 0.51              |
| 1:C:258:ALA:N    | 4:I:121:TYR:OH    | 2.44                     | 0.51              |
| 3:D:134:MET:HB3  | 3:D:145:GLN:OE1   | 2.11                     | 0.51              |
| 2:B:122:ILE:HG23 | 2:B:124:ILE:HD11  | 1.94                     | 0.50              |
| 1:C:216:ALA:O    | 1:C:217:ARG:NH1   | 2.44                     | 0.50              |
| 1:C:546:ILE:HD12 | 1:C:547:PRO:HD2   | 1.92                     | 0.50              |
| 7:H:4:MET:O      | 7:H:6:GLN:NE2     | 2.41                     | 0.50              |
| 4:I:102:GLN:HE22 | 4:I:104:ASN:ND2   | 2.08                     | 0.50              |
| 1:A:135:LEU:O    | 1:A:322:LYS:HE3   | 2.11                     | 0.50              |
| 1:A:58:ILE:HD13  | 1:A:292:VAL:HG12  | 1.93                     | 0.50              |
| 1:A:128:TYR:HA   | 1:A:134:HIS:ND1   | 2.27                     | 0.50              |
| 9:L:24:MET:CE    | 9:L:110:GLN:HB2   | 2.40                     | 0.50              |
| 1:C:258:ALA:O    | 1:C:262:ALA:N     | 2.41                     | 0.50              |
| 1:C:495:LYS:HZ2  | 1:C:497:GLU:HB3   | 1.76                     | 0.50              |
| 3:D:530:ILE:HD11 | 3:D:762:TYR:HD2   | 1.77                     | 0.50              |
| 3:D:762:TYR:CZ   | 13:D:1504:7RC:C05 | 2.91                     | 0.50              |
| 8:K:54:MET:SD    | 8:K:99:LEU:HB3    | 2.51                     | 0.50              |
| 1:A:31:ALA:O     | 1:A:64:SER:HA     | 2.11                     | 0.50              |
| 2:B:251:TYR:HE1  | 2:B:394:LYS:HD3   | 1.76                     | 0.50              |
| 2:B:374:LYS:HZ3  | 2:B:377:LYS:HB2   | 1.76                     | 0.50              |
| 3:D:171:ILE:HG23 | 3:D:229:LEU:HD11  | 1.94                     | 0.50              |
| 3:D:509:ALA:HB3  | 3:D:765:ALA:HB3   | 1.93                     | 0.50              |
| 4:I:32:VAL:HG21  | 4:I:137:VAL:HG13  | 1.93                     | 0.50              |
| 5:J:62:LYS:HB2   | 5:J:65:GLN:HB2    | 1.94                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:36:ARG:NH2   | 1:A:39:GLU:OE2    | 2.36                     | 0.50              |
| 1:A:423:GLU:OE1  | 1:A:433:LYS:NZ    | 2.36                     | 0.50              |
| 2:B:708:PHE:O    | 2:B:710:GLN:NE2   | 2.43                     | 0.50              |
| 3:D:609:LEU:O    | 3:D:613:VAL:HG23  | 2.12                     | 0.50              |
| 1:A:48:GLN:HE22  | 1:A:52:ARG:HD3    | 1.77                     | 0.50              |
| 1:A:682:ALA:HB1  | 1:A:710:ASN:HA    | 1.94                     | 0.50              |
| 2:B:514:ILE:HG21 | 1:C:531:LYS:HZ1   | 1.77                     | 0.50              |
| 3:D:337:ARG:O    | 3:D:340:ILE:HG22  | 2.12                     | 0.50              |
| 4:E:41:THR:HG23  | 4:E:100:PHE:HE1   | 1.76                     | 0.50              |
| 6:G:5:LYS:HG2    | 6:G:23:SER:OG     | 2.12                     | 0.50              |
| 6:G:17:THR:HA    | 6:G:85:ALA:HA     | 1.94                     | 0.50              |
| 1:A:221:LEU:HB3  | 1:A:249:VAL:HG12  | 1.93                     | 0.50              |
| 1:A:183:LEU:HB3  | 1:A:187:ARG:CZ    | 2.42                     | 0.50              |
| 1:A:541:LEU:HB3  | 1:A:736:LEU:HD12  | 1.94                     | 0.50              |
| 1:A:581:ASP:HA   | 1:A:584:SER:HB2   | 1.94                     | 0.49              |
| 1:C:296:LEU:HA   | 1:C:301:ILE:HD12  | 1.94                     | 0.49              |
| 3:D:601:THR:O    | 3:D:605:ALA:N     | 2.44                     | 0.49              |
| 3:D:672:GLN:HG3  | 3:D:673:ARG:HG2   | 1.94                     | 0.49              |
| 5:J:60:GLN:HB2   | 5:J:70:LEU:HG     | 1.95                     | 0.49              |
| 2:B:485:HIS:CE1  | 13:B:1504:7RC:C01 | 2.96                     | 0.49              |
| 1:C:128:TYR:HA   | 1:C:134:HIS:ND1   | 2.27                     | 0.49              |
| 6:G:127:ALA:HB3  | 6:G:156:TYR:O     | 2.12                     | 0.49              |
| 1:C:34:SER:HB3   | 1:C:67:HIS:HB2    | 1.92                     | 0.49              |
| 6:G:134:PHE:HE1  | 6:G:225:PHE:HB2   | 1.75                     | 0.49              |
| 1:A:560:SER:HA   | 1:A:563:TRP:HD1   | 1.77                     | 0.49              |
| 1:C:58:ILE:HB    | 1:C:293:HIS:CE1   | 2.47                     | 0.49              |
| 1:C:489:ARG:HD2  | 1:C:492:ASN:HA    | 1.94                     | 0.49              |
| 5:J:49:ASP:OD2   | 5:J:91:GLY:N      | 2.46                     | 0.49              |
| 5:J:110:TYR:HB3  | 5:J:121:PHE:H     | 1.78                     | 0.49              |
| 8:K:65:LEU:HB2   | 9:L:117:PHE:CZ    | 2.47                     | 0.49              |
| 2:B:637:PHE:CZ   | 1:C:819:LEU:HB3   | 2.44                     | 0.49              |
| 2:B:780:LEU:HD11 | 1:C:519:ILE:HG22  | 1.94                     | 0.49              |
| 1:C:30:GLY:N     | 1:C:89:ALA:O      | 2.45                     | 0.49              |
| 1:A:355:ASN:HD21 | 1:A:380:ILE:H     | 1.61                     | 0.49              |
| 1:A:367:TYR:HB2  | 1:A:372:VAL:HG22  | 1.93                     | 0.49              |
| 3:D:105:GLN:O    | 3:D:108:ILE:HG12  | 2.12                     | 0.49              |
| 4:E:66:LEU:HD23  | 5:F:110:TYR:CE2   | 2.47                     | 0.49              |
| 1:A:470:MET:HE3  | 1:A:472:PHE:CE1   | 2.47                     | 0.49              |
| 1:C:555:MET:HE3  | 1:C:555:MET:HA    | 1.94                     | 0.49              |
| 5:F:60:GLN:HB3   | 5:F:70:LEU:HD11   | 1.93                     | 0.49              |
| 1:A:103:THR:O    | 1:A:106:PRO:HD2   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:341:ASN:HB3  | 1:A:347:LYS:HE3   | 1.95                     | 0.49              |
| 1:C:502:MET:HE2  | 1:C:502:MET:HA    | 1.95                     | 0.49              |
| 6:G:61:TYR:HB2   | 6:G:66:LYS:HE2    | 1.95                     | 0.49              |
| 3:D:95:GLN:HE21  | 3:D:315:PRO:HB2   | 1.77                     | 0.49              |
| 3:D:138:ASP:OD1  | 3:D:139:GLU:N     | 2.46                     | 0.49              |
| 5:J:33:SER:OG    | 5:J:36:GLN:OE1    | 2.26                     | 0.49              |
| 5:J:61:GLN:NE2   | 5:J:62:LYS:O      | 2.46                     | 0.49              |
| 1:A:49:ALA:HA    | 1:A:52:ARG:HG2    | 1.94                     | 0.49              |
| 1:A:564:LEU:HD23 | 1:A:568:LEU:HD23  | 1.95                     | 0.49              |
| 3:D:407:SER:O    | 3:D:507:TYR:N     | 2.43                     | 0.49              |
| 1:A:121:LEU:HD12 | 1:A:280:HIS:HB3   | 1.96                     | 0.48              |
| 1:A:312:THR:HG21 | 2:B:42:HIS:CE1    | 2.48                     | 0.48              |
| 2:B:406:LEU:HD23 | 2:B:506:VAL:HG11  | 1.95                     | 0.48              |
| 5:F:37:ARG:H     | 5:F:37:ARG:HD3    | 1.78                     | 0.48              |
| 4:I:91:THR:OG1   | 4:I:100:PHE:HB2   | 2.13                     | 0.48              |
| 4:I:93:ASP:OD1   | 4:I:98:GLN:HB3    | 2.13                     | 0.48              |
| 9:L:26:GLN:HB2   | 9:L:120:GLY:H     | 1.78                     | 0.48              |
| 2:B:485:HIS:CB   | 13:B:1504:7RC:O05 | 2.61                     | 0.48              |
| 1:C:139:ARG:NH1  | 1:C:143:PRO:HB3   | 2.29                     | 0.48              |
| 1:C:630:ARG:HD3  | 3:D:607:TRP:HB2   | 1.94                     | 0.48              |
| 4:E:74:TYR:C     | 4:E:76:GLY:H      | 2.22                     | 0.48              |
| 6:G:149:VAL:HG22 | 6:G:195:LEU:HD13  | 1.94                     | 0.48              |
| 6:G:156:TYR:N    | 6:G:157:PRO:HD3   | 2.29                     | 0.48              |
| 8:K:31:LEU:HB2   | 8:K:138:VAL:HG13  | 1.94                     | 0.48              |
| 1:A:502:MET:HE1  | 1:A:523:ARG:HG2   | 1.95                     | 0.48              |
| 1:A:616:ASN:OD1  | 2:B:614:ASN:ND2   | 2.38                     | 0.48              |
| 2:B:204:ILE:HB   | 2:B:206:LEU:HD23  | 1.95                     | 0.48              |
| 2:B:361:LEU:HB3  | 2:B:378:TRP:HB3   | 1.96                     | 0.48              |
| 2:B:466:LYS:HD2  | 2:B:791:LEU:HD11  | 1.94                     | 0.48              |
| 1:C:38:HIS:HA    | 1:C:41:MET:HG3    | 1.94                     | 0.48              |
| 3:D:131:SER:C    | 3:D:133:ILE:H     | 2.21                     | 0.48              |
| 3:D:233:THR:HG22 | 3:D:261:LEU:HD21  | 1.94                     | 0.48              |
| 3:D:689:GLY:HA3  | 13:D:1504:7RC:O02 | 2.13                     | 0.48              |
| 4:E:50:THR:HB    | 4:E:74:TYR:CD1    | 2.49                     | 0.48              |
| 1:A:26:ILE:HD11  | 1:A:61:ASN:HB2    | 1.94                     | 0.48              |
| 1:A:169:ASP:O    | 1:A:174:ARG:NH2   | 2.36                     | 0.48              |
| 2:B:333:THR:O    | 2:B:336:GLN:HG3   | 2.13                     | 0.48              |
| 1:C:71:ALA:HA    | 1:C:74:MET:CG     | 2.40                     | 0.48              |
| 6:G:129:PRO:HB3  | 6:G:152:LEU:HD12  | 1.94                     | 0.48              |
| 8:K:67:TRP:CD1   | 9:L:117:PHE:HB2   | 2.48                     | 0.48              |
| 3:D:702:MET:O    | 3:D:706:MET:HG2   | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:133:MET:O    | 2:B:146:GLN:NE2  | 2.47                     | 0.48              |
| 2:B:159:LEU:O    | 2:B:162:MET:HE3  | 2.13                     | 0.48              |
| 1:C:400:ILE:HD13 | 1:C:512:MET:HB2  | 1.95                     | 0.48              |
| 1:C:825:VAL:O    | 1:C:828:ILE:HG12 | 2.14                     | 0.48              |
| 3:D:760:THR:HG22 | 3:D:761:GLY:N    | 2.29                     | 0.48              |
| 5:J:106:ALA:HA   | 5:J:127:LEU:HB3  | 1.96                     | 0.48              |
| 9:L:56:TYR:CD1   | 9:L:64:PRO:HB2   | 2.48                     | 0.48              |
| 1:A:35:THR:HG21  | 4:E:94:THR:O     | 2.14                     | 0.48              |
| 1:A:90:ILE:HB    | 1:A:118:VAL:HG23 | 1.95                     | 0.48              |
| 2:B:99:VAL:HB    | 2:B:127:ILE:HD11 | 1.95                     | 0.48              |
| 2:B:149:ALA:HB3  | 2:B:154:GLN:NE2  | 2.27                     | 0.48              |
| 1:C:544:LYS:HE2  | 1:C:747:VAL:HG13 | 1.95                     | 0.48              |
| 3:D:157:MET:O    | 3:D:161:MET:HG2  | 2.13                     | 0.48              |
| 3:D:226:PRO:HA   | 3:D:254:TYR:CD1  | 2.47                     | 0.48              |
| 3:D:306:ASP:HB2  | 3:D:338:TYR:HB3  | 1.96                     | 0.48              |
| 6:G:40:ARG:CZ    | 6:G:93:ALA:HB3   | 2.43                     | 0.48              |
| 7:H:136:LEU:O    | 7:H:174:SER:HA   | 2.13                     | 0.48              |
| 2:B:508:ALA:HB3  | 2:B:764:ALA:HB3  | 1.96                     | 0.48              |
| 1:C:414:THR:HG23 | 1:C:453:GLN:HA   | 1.96                     | 0.48              |
| 6:G:74:ASP:HB3   | 6:G:79:GLN:HE21  | 1.79                     | 0.48              |
| 6:G:150:CYS:CB   | 6:G:223:LYS:HB3  | 2.40                     | 0.48              |
| 4:I:80:TYR:CZ    | 4:I:88:ILE:HB    | 2.49                     | 0.48              |
| 5:J:59:TYR:HA    | 5:J:69:LEU:HA    | 1.95                     | 0.48              |
| 1:A:355:ASN:ND2  | 1:A:380:ILE:H    | 2.12                     | 0.48              |
| 1:A:629:ALA:HA   | 1:A:632:LEU:HD12 | 1.95                     | 0.48              |
| 2:B:637:PHE:CE2  | 1:C:820:VAL:HB   | 2.49                     | 0.48              |
| 4:E:91:THR:OG1   | 4:E:100:PHE:HB2  | 2.14                     | 0.48              |
| 4:I:26:GLU:N     | 4:I:131:GLN:HE22 | 2.11                     | 0.48              |
| 4:I:71:TYR:O     | 4:I:78:THR:HA    | 2.14                     | 0.48              |
| 8:K:132:TRP:CH2  | 9:L:63:GLY:HA3   | 2.49                     | 0.48              |
| 9:L:26:GLN:H     | 9:L:119:GLY:H    | 1.62                     | 0.48              |
| 1:C:447:PRO:HB2  | 1:C:449:HIS:CE1  | 2.49                     | 0.47              |
| 3:D:37:ILE:HG21  | 3:D:297:ILE:HG12 | 1.96                     | 0.47              |
| 3:D:686:VAL:HG23 | 3:D:729:PHE:HZ   | 1.79                     | 0.47              |
| 8:K:63:LYS:O     | 9:L:107:TYR:OH   | 2.26                     | 0.47              |
| 9:L:82:PHE:HB3   | 9:L:93:PHE:CE1   | 2.49                     | 0.47              |
| 3:D:49:ALA:O     | 3:D:53:ALA:HB3   | 2.14                     | 0.47              |
| 7:H:190:LYS:NZ   | 7:H:211:ARG:HE   | 2.12                     | 0.47              |
| 8:K:61:PRO:HD3   | 8:K:110:ASP:OD1  | 2.15                     | 0.47              |
| 1:A:639:PHE:CZ   | 1:A:643:ILE:HD11 | 2.49                     | 0.47              |
| 1:C:99:ASN:OD1   | 4:I:75:SER:OG    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:185:GLU:HG2  | 1:C:190:LYS:HE3  | 1.95                     | 0.47              |
| 1:C:470:MET:SD   | 1:C:771:ASN:HB3  | 2.54                     | 0.47              |
| 3:D:151:GLU:OE1  | 3:D:151:GLU:N    | 2.47                     | 0.47              |
| 5:F:30:LEU:HD23  | 5:F:30:LEU:H     | 1.79                     | 0.47              |
| 1:A:42:PHE:CE2   | 1:A:62:ALA:HB1   | 2.49                     | 0.47              |
| 1:A:69:PRO:HB3   | 1:A:99:ASN:HD22  | 1.79                     | 0.47              |
| 2:B:441:LYS:HA   | 2:B:449:GLY:HA3  | 1.95                     | 0.47              |
| 1:C:48:GLN:O     | 1:C:52:ARG:HG2   | 2.14                     | 0.47              |
| 3:D:213:ASP:HA   | 3:D:216:ILE:HB   | 1.96                     | 0.47              |
| 3:D:333:ASN:O    | 3:D:337:ARG:N    | 2.46                     | 0.47              |
| 3:D:786:ASP:HB2  | 3:D:788:GLU:OE1  | 2.14                     | 0.47              |
| 8:K:126:TYR:HB3  | 9:L:115:TYR:CZ   | 2.49                     | 0.47              |
| 1:A:104:PRO:HB2  | 1:A:128:TYR:CZ   | 2.50                     | 0.47              |
| 1:A:501:MET:HB3  | 1:A:513:ILE:HD12 | 1.95                     | 0.47              |
| 1:A:755:ARG:NH2  | 3:D:531:GLU:HB3  | 2.29                     | 0.47              |
| 2:B:128:HIS:HA   | 2:B:132:SER:HB3  | 1.96                     | 0.47              |
| 2:B:718:VAL:HA   | 2:B:721:LYS:HD3  | 1.96                     | 0.47              |
| 1:A:32:VAL:HB    | 1:A:92:VAL:HG22  | 1.95                     | 0.47              |
| 1:A:115:ARG:HG2  | 1:A:314:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:720:ALA:HB1  | 1:A:725:LYS:HB2  | 1.96                     | 0.47              |
| 2:B:693:ASN:OD1  | 2:B:697:ASN:ND2  | 2.47                     | 0.47              |
| 1:C:148:SER:HA   | 1:C:151:TRP:CE3  | 2.49                     | 0.47              |
| 3:D:278:ILE:HD11 | 3:D:364:ILE:HG22 | 1.97                     | 0.47              |
| 6:G:40:ARG:HG3   | 6:G:42:PRO:HD3   | 1.97                     | 0.47              |
| 6:G:149:VAL:HG12 | 6:G:150:CYS:N    | 2.27                     | 0.47              |
| 2:B:658:PHE:C    | 2:B:660:ASP:H    | 2.16                     | 0.47              |
| 2:B:811:GLN:OE1  | 2:B:811:GLN:N    | 2.40                     | 0.47              |
| 1:C:668:ASN:HA   | 1:C:673:ARG:HD3  | 1.97                     | 0.47              |
| 3:D:87:ASP:HB3   | 3:D:92:ARG:HH12  | 1.80                     | 0.47              |
| 3:D:613:VAL:HG23 | 3:D:635:TRP:HE1  | 1.79                     | 0.47              |
| 9:L:28:PRO:O     | 9:L:30:SER:N     | 2.47                     | 0.47              |
| 1:A:388:LYS:HB2  | 1:A:390:ARG:NH2  | 2.28                     | 0.47              |
| 1:A:611:TRP:O    | 1:A:615:LEU:HD23 | 2.15                     | 0.47              |
| 1:A:307:GLY:O    | 1:A:311:ASN:ND2  | 2.48                     | 0.47              |
| 2:B:39:LEU:HD22  | 2:B:74:MET:HE1   | 1.95                     | 0.47              |
| 1:C:411:VAL:HG12 | 1:C:455:CYS:SG   | 2.55                     | 0.47              |
| 1:C:520:ASN:ND2  | 1:C:522:GLU:OE2  | 2.48                     | 0.47              |
| 4:E:64:ASN:O     | 5:F:110:TYR:OH   | 2.33                     | 0.47              |
| 4:I:126:MET:HB3  | 5:J:59:TYR:CE2   | 2.50                     | 0.47              |
| 1:A:250:GLY:O    | 1:A:254:ILE:HG23 | 2.15                     | 0.47              |
| 2:B:514:ILE:HD13 | 1:C:531:LYS:HZ2  | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:612:VAL:HA   | 2:B:638:ALA:HB1  | 1.96                     | 0.47              |
| 1:C:42:PHE:HD1   | 1:C:281:ILE:HG23 | 1.80                     | 0.47              |
| 1:C:187:ARG:O    | 1:C:187:ARG:HG3  | 2.15                     | 0.47              |
| 3:D:460:PHE:HE1  | 3:D:792:LEU:HB3  | 1.80                     | 0.47              |
| 3:D:662:GLN:N    | 3:D:662:GLN:OE1  | 2.48                     | 0.47              |
| 4:E:81:ASN:HB2   | 4:E:84:LEU:HB3   | 1.97                     | 0.47              |
| 6:G:136:PRO:HA   | 6:G:227:ARG:NH2  | 2.30                     | 0.47              |
| 9:L:55:TRP:HA    | 9:L:107:TYR:O    | 2.14                     | 0.47              |
| 2:B:334:LEU:HA   | 2:B:337:PHE:HB2  | 1.96                     | 0.46              |
| 1:C:253:GLU:CD   | 1:C:253:GLU:H    | 2.22                     | 0.46              |
| 3:D:788:GLU:O    | 3:D:792:LEU:HG   | 2.14                     | 0.46              |
| 6:G:124:ARG:HH11 | 6:G:125:THR:HB   | 1.79                     | 0.46              |
| 1:A:523:ARG:O    | 1:A:527:ILE:HG22 | 2.15                     | 0.46              |
| 1:A:732:ASP:O    | 1:A:736:LEU:HD23 | 2.15                     | 0.46              |
| 2:B:152:GLN:HG3  | 2:B:186:PHE:CG   | 2.51                     | 0.46              |
| 2:B:476:ASP:N    | 2:B:476:ASP:OD1  | 2.48                     | 0.46              |
| 2:B:542:GLY:H    | 2:B:807:VAL:HG11 | 1.79                     | 0.46              |
| 2:B:576:PHE:HE1  | 2:B:623:LYS:HG3  | 1.80                     | 0.46              |
| 1:C:68:LYS:H     | 1:C:74:MET:HE1   | 1.79                     | 0.46              |
| 1:C:125:MET:SD   | 1:C:125:MET:N    | 2.88                     | 0.46              |
| 1:C:701:THR:HG23 | 1:C:704:ARG:HH21 | 1.79                     | 0.46              |
| 3:D:552:GLU:N    | 3:D:553:PRO:HD2  | 2.31                     | 0.46              |
| 5:F:55:TYR:O     | 5:F:56:MET:HE2   | 2.14                     | 0.46              |
| 4:I:59:ARG:HB2   | 4:I:114:TYR:CE1  | 2.50                     | 0.46              |
| 1:A:485:GLY:HA2  | 1:A:499:ASN:OD1  | 2.16                     | 0.46              |
| 2:B:172:LEU:HD11 | 2:B:183:PHE:CE2  | 2.50                     | 0.46              |
| 5:F:37:ARG:HA    | 5:F:98:ILE:O     | 2.15                     | 0.46              |
| 2:B:416:PHE:HB3  | 2:B:460:CYS:SG   | 2.56                     | 0.46              |
| 1:C:71:ALA:HB3   | 3:D:114:PHE:CE1  | 2.51                     | 0.46              |
| 1:C:483:LYS:HZ1  | 1:C:499:ASN:HB2  | 1.81                     | 0.46              |
| 1:C:577:LEU:HD11 | 1:C:629:ALA:HB2  | 1.96                     | 0.46              |
| 3:D:442:SER:HB2  | 3:D:446:THR:HA   | 1.97                     | 0.46              |
| 3:D:490:ILE:N    | 3:D:493:THR:O    | 2.41                     | 0.46              |
| 6:G:46:GLY:C     | 6:G:47:LEU:HD12  | 2.41                     | 0.46              |
| 1:A:298:LYS:HG3  | 1:A:299:GLU:HG2  | 1.97                     | 0.46              |
| 2:B:493:TRP:NE1  | 2:B:521:VAL:HG11 | 2.31                     | 0.46              |
| 2:B:636:PHE:CE1  | 2:B:640:ILE:HD11 | 2.51                     | 0.46              |
| 3:D:102:ASP:OD1  | 3:D:102:ASP:N    | 2.47                     | 0.46              |
| 3:D:526:SER:OG   | 3:D:527:VAL:N    | 2.46                     | 0.46              |
| 3:D:772:TRP:O    | 3:D:776:VAL:HG22 | 2.16                     | 0.46              |
| 6:G:129:PRO:CB   | 6:G:152:LEU:HD12 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:31:ALA:HA    | 5:J:130:LYS:HD3  | 1.97                     | 0.46              |
| 1:A:743:LYS:HB3  | 1:A:745:ASP:OD1  | 2.16                     | 0.46              |
| 1:A:817:PHE:HA   | 1:A:820:VAL:HG12 | 1.98                     | 0.46              |
| 1:C:253:GLU:OE1  | 1:C:253:GLU:N    | 2.49                     | 0.46              |
| 3:D:302:THR:HG21 | 3:D:344:PHE:HB2  | 1.98                     | 0.46              |
| 7:H:19:VAL:HG12  | 7:H:75:ILE:HB    | 1.96                     | 0.46              |
| 1:A:683:THR:HG22 | 1:A:706:MET:HE2  | 1.98                     | 0.46              |
| 1:A:731:TRP:CG   | 1:A:732:ASP:H    | 2.33                     | 0.46              |
| 1:A:808:LEU:HB2  | 3:D:649:ASN:HD21 | 1.79                     | 0.46              |
| 2:B:722:THR:HG23 | 2:B:724:LYS:HG2  | 1.97                     | 0.46              |
| 1:C:156:ARG:NH2  | 1:C:159:ASN:OD1  | 2.35                     | 0.46              |
| 3:D:150:ILE:HA   | 3:D:153:GLN:NE2  | 2.30                     | 0.46              |
| 8:K:120:SER:HB3  | 8:K:129:PHE:HA   | 1.98                     | 0.46              |
| 1:A:91:LEU:HD12  | 1:A:121:LEU:HD21 | 1.97                     | 0.46              |
| 2:B:301:THR:HG21 | 2:B:342:THR:H    | 1.81                     | 0.46              |
| 1:C:295:LEU:HD13 | 1:C:324:VAL:HG21 | 1.98                     | 0.46              |
| 1:C:577:LEU:HD22 | 1:C:632:LEU:HD23 | 1.96                     | 0.46              |
| 3:D:207:MET:HE2  | 3:D:239:TYR:HD2  | 1.81                     | 0.46              |
| 3:D:415:PRO:HD3  | 3:D:738:TYR:CD2  | 2.50                     | 0.46              |
| 4:E:84:LEU:HD23  | 4:E:88:ILE:HD13  | 1.98                     | 0.46              |
| 4:E:93:ASP:O     | 4:E:97:ASN:CA    | 2.63                     | 0.46              |
| 9:L:69:HIS:CG    | 9:L:70:TYR:H     | 2.33                     | 0.46              |
| 1:A:36:ARG:O     | 1:A:40:GLN:HG2   | 2.15                     | 0.46              |
| 1:A:58:ILE:HB    | 1:A:293:HIS:CE1  | 2.51                     | 0.46              |
| 1:A:551:LEU:HB3  | 1:A:812:ASN:HD22 | 1.81                     | 0.46              |
| 1:C:235:ALA:HA   | 1:C:240:MET:HE2  | 1.98                     | 0.46              |
| 1:C:444:PRO:HA   | 1:C:448:ARG:HH21 | 1.80                     | 0.46              |
| 1:C:541:LEU:HD11 | 1:C:746:LEU:HB3  | 1.98                     | 0.46              |
| 5:F:38:ALA:HB3   | 5:F:98:ILE:HB    | 1.98                     | 0.46              |
| 5:F:103:GLU:OE2  | 5:F:103:GLU:N    | 2.48                     | 0.46              |
| 1:A:144:TYR:HD1  | 1:A:147:GLN:HE22 | 1.63                     | 0.46              |
| 3:D:794:ALA:O    | 3:D:798:THR:OG1  | 2.35                     | 0.46              |
| 1:A:209:MET:HE3  | 1:A:238:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:641:MET:HE1  | 2:B:613:PHE:C    | 2.40                     | 0.45              |
| 1:A:818:MET:O    | 1:A:821:ALA:HB3  | 2.15                     | 0.45              |
| 2:B:207:ASP:OD1  | 2:B:207:ASP:N    | 2.49                     | 0.45              |
| 1:C:171:HIS:N    | 3:D:139:GLU:OE2  | 2.49                     | 0.45              |
| 3:D:168:ILE:HG13 | 3:D:227:ILE:HD12 | 1.98                     | 0.45              |
| 4:E:74:TYR:C     | 4:E:76:GLY:N     | 2.73                     | 0.45              |
| 4:I:80:TYR:OH    | 4:I:85:LYS:O     | 2.34                     | 0.45              |
| 1:A:232:TYR:CD2  | 1:A:262:ALA:HA   | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:683:THR:HA   | 1:A:729:PHE:CE1  | 2.46                     | 0.45              |
| 1:C:334:VAL:HG23 | 1:C:335:THR:HG23 | 1.97                     | 0.45              |
| 1:C:519:ILE:HG12 | 1:C:529:PHE:CG   | 2.52                     | 0.45              |
| 3:D:132:MET:H    | 3:D:145:GLN:NE2  | 2.14                     | 0.45              |
| 5:F:30:LEU:HG    | 5:F:32:VAL:HG23  | 1.99                     | 0.45              |
| 5:J:60:GLN:CB    | 5:J:109:TYR:HE2  | 2.30                     | 0.45              |
| 1:A:151:TRP:HA   | 1:A:154:MET:SD   | 2.57                     | 0.45              |
| 1:A:498:TRP:HB2  | 1:A:506:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:520:ASN:HD21 | 1:A:691:ILE:HD11 | 1.81                     | 0.45              |
| 3:D:481:VAL:HG11 | 3:D:496:GLY:HA2  | 1.97                     | 0.45              |
| 7:H:166:GLN:HA   | 7:H:173:TYR:HE1  | 1.80                     | 0.45              |
| 2:B:257:VAL:HB   | 2:B:261:VAL:HG21 | 1.98                     | 0.45              |
| 1:C:387:GLU:OE1  | 1:C:387:GLU:N    | 2.50                     | 0.45              |
| 1:C:401:VAL:HG13 | 1:C:501:MET:HE1  | 1.98                     | 0.45              |
| 4:E:22:VAL:HG22  | 4:E:47:TYR:HB2   | 1.97                     | 0.45              |
| 8:K:56:TRP:CE3   | 8:K:99:LEU:HD22  | 2.52                     | 0.45              |
| 1:A:48:GLN:HG2   | 1:A:51:LYS:HE3   | 1.98                     | 0.45              |
| 2:B:160:LYS:HD3  | 2:B:378:TRP:CZ3  | 2.52                     | 0.45              |
| 2:B:217:VAL:O    | 2:B:221:LYS:HG2  | 2.16                     | 0.45              |
| 5:J:59:TYR:CE2   | 5:J:69:LEU:HD13  | 2.52                     | 0.45              |
| 8:K:53:THR:HG23  | 8:K:119:PRO:HG2  | 1.97                     | 0.45              |
| 8:K:59:GLN:HG2   | 8:K:65:LEU:HD23  | 1.99                     | 0.45              |
| 2:B:680:PHE:O    | 2:B:704:TYR:OH   | 2.32                     | 0.45              |
| 1:C:75:ALA:HA    | 1:C:78:VAL:HG12  | 1.99                     | 0.45              |
| 1:C:119:LEU:HD13 | 1:C:138:LEU:HB2  | 1.98                     | 0.45              |
| 1:C:523:ARG:HH12 | 1:C:688:SER:HB3  | 1.82                     | 0.45              |
| 1:C:555:MET:HE1  | 1:C:563:TRP:HD1  | 1.80                     | 0.45              |
| 1:A:58:ILE:HD12  | 1:A:293:HIS:HA   | 1.98                     | 0.45              |
| 1:A:127:ILE:HA   | 1:A:171:HIS:CE1  | 2.52                     | 0.45              |
| 1:A:295:LEU:HD22 | 1:A:321:PHE:CD1  | 2.47                     | 0.45              |
| 2:B:701:MET:O    | 2:B:705:MET:HG2  | 2.17                     | 0.45              |
| 1:C:35:THR:OG1   | 1:C:38:HIS:HB2   | 2.16                     | 0.45              |
| 3:D:41:LEU:HD11  | 3:D:50:ILE:HG21  | 1.99                     | 0.45              |
| 3:D:344:PHE:CD2  | 3:D:345:GLU:HG3  | 2.52                     | 0.45              |
| 3:D:654:MET:O    | 3:D:654:MET:HG2  | 2.17                     | 0.45              |
| 1:A:813:MET:HE2  | 1:A:813:MET:HA   | 1.98                     | 0.45              |
| 2:B:114:ASP:OD2  | 2:B:135:MET:HE3  | 2.17                     | 0.45              |
| 2:B:232:SER:OG   | 2:B:235:GLU:OE1  | 2.34                     | 0.45              |
| 2:B:339:VAL:HG13 | 2:B:350:PHE:O    | 2.16                     | 0.45              |
| 3:D:213:ASP:O    | 3:D:217:GLN:NE2  | 2.50                     | 0.45              |
| 6:G:39:ILE:HG13  | 6:G:47:LEU:HD23  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:G:214:HIS:O    | 6:G:218:SER:CA   | 2.65                     | 0.45              |
| 1:C:609:PHE:HE1  | 3:D:619:PRO:HD2  | 1.82                     | 0.45              |
| 3:D:332:SER:OG   | 3:D:333:ASN:N    | 2.50                     | 0.45              |
| 3:D:537:MET:HB2  | 3:D:736:LEU:HD11 | 1.99                     | 0.45              |
| 3:D:540:ARG:NE   | 3:D:746:CYS:O    | 2.49                     | 0.45              |
| 5:F:55:TYR:HD2   | 5:F:115:ASN:HA   | 1.82                     | 0.45              |
| 8:K:38:LEU:HB2   | 8:K:103:MET:SD   | 2.57                     | 0.45              |
| 1:A:58:ILE:HD11  | 1:A:296:LEU:HB2  | 1.97                     | 0.45              |
| 1:A:399:LYS:N    | 1:A:511:ASP:OD2  | 2.36                     | 0.45              |
| 1:A:667:ILE:HD12 | 1:A:672:LEU:HG   | 1.98                     | 0.45              |
| 2:B:46:VAL:HG12  | 2:B:51:LEU:HG    | 1.99                     | 0.45              |
| 2:B:564:MET:O    | 2:B:568:VAL:HG22 | 2.16                     | 0.45              |
| 2:B:792:GLU:O    | 2:B:796:LEU:HB2  | 2.17                     | 0.45              |
| 2:B:817:MET:O    | 2:B:820:VAL:HG22 | 2.16                     | 0.45              |
| 4:E:43:THR:HB    | 4:E:98:GLN:CB    | 2.46                     | 0.45              |
| 6:G:94:THR:HA    | 6:G:113:LEU:HA   | 1.99                     | 0.45              |
| 6:G:132:PHE:HB3  | 6:G:151:LEU:HB3  | 1.99                     | 0.45              |
| 6:G:215:GLN:OE1  | 6:G:215:GLN:N    | 2.47                     | 0.45              |
| 7:H:37:GLN:O     | 7:H:39:LYS:NZ    | 2.50                     | 0.45              |
| 5:J:35:GLY:HA2   | 5:J:100:PRO:HB3  | 1.99                     | 0.45              |
| 1:A:205:THR:O    | 1:A:209:MET:HG2  | 2.17                     | 0.44              |
| 1:A:487:GLN:HG3  | 1:A:498:TRP:CZ2  | 2.53                     | 0.44              |
| 1:C:670:PRO:HG3  | 3:D:800:ILE:HG21 | 1.99                     | 0.44              |
| 3:D:67:ARG:HA    | 8:K:127:TRP:HZ2  | 1.81                     | 0.44              |
| 5:F:39:THR:HG23  | 5:F:95:THR:HG23  | 1.99                     | 0.44              |
| 6:G:11:ILE:HD11  | 6:G:119:LYS:HB3  | 1.99                     | 0.44              |
| 7:H:38:GLN:HB3   | 7:H:85:SER:HB3   | 1.98                     | 0.44              |
| 4:I:84:LEU:HB3   | 4:I:87:ARG:HB2   | 1.98                     | 0.44              |
| 1:A:458:PHE:HZ   | 1:A:785:MET:HE1  | 1.83                     | 0.44              |
| 3:D:682:ARG:O    | 3:D:727:ASP:HB2  | 2.17                     | 0.44              |
| 4:E:92:ARG:NH1   | 4:E:99:PHE:HB3   | 2.33                     | 0.44              |
| 5:F:84:ARG:NH2   | 5:F:100:PRO:HG2  | 2.33                     | 0.44              |
| 5:J:130:LYS:HD2  | 5:J:130:LYS:N    | 2.31                     | 0.44              |
| 2:B:127:ILE:HA   | 2:B:147:PHE:HD2  | 1.81                     | 0.44              |
| 2:B:504:ARG:HH21 | 6:G:52:HIS:CD2   | 2.35                     | 0.44              |
| 1:C:347:LYS:HG3  | 1:C:348:PHE:HD2  | 1.82                     | 0.44              |
| 1:C:612:GLY:O    | 1:C:616:ASN:N    | 2.51                     | 0.44              |
| 3:D:109:ALA:O    | 3:D:113:ASP:N    | 2.44                     | 0.44              |
| 3:D:237:ALA:HA   | 3:D:240:ILE:HG22 | 1.99                     | 0.44              |
| 5:F:25:GLN:OE1   | 5:F:124:GLY:N    | 2.50                     | 0.44              |
| 1:A:180:LEU:HA   | 1:A:183:LEU:HD12 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:547:PRO:HG3  | 1:A:804:ALA:HB3  | 1.97                     | 0.44              |
| 2:B:135:MET:N    | 2:B:146:GLN:OE1  | 2.48                     | 0.44              |
| 5:F:84:ARG:CZ    | 5:F:102:GLU:HG3  | 2.48                     | 0.44              |
| 8:K:49:PHE:HA    | 8:K:52:TYR:HB2   | 1.99                     | 0.44              |
| 1:A:368:ASN:OD1  | 1:A:371:HIS:N    | 2.44                     | 0.44              |
| 1:A:790:LYS:NZ   | 1:A:794:ARG:HE   | 2.16                     | 0.44              |
| 2:B:54:LEU:HD22  | 2:B:293:ARG:HD2  | 2.00                     | 0.44              |
| 3:D:565:MET:HE2  | 3:D:635:TRP:CZ3  | 2.53                     | 0.44              |
| 3:D:789:MET:O    | 3:D:792:LEU:N    | 2.50                     | 0.44              |
| 6:G:128:ALA:C    | 6:G:155:PHE:HB2  | 2.42                     | 0.44              |
| 5:J:108:THR:HB   | 5:J:109:TYR:H    | 1.27                     | 0.44              |
| 2:B:108:ALA:O    | 2:B:112:MET:HG3  | 2.17                     | 0.44              |
| 2:B:464:LEU:HD22 | 2:B:509:VAL:HG11 | 2.00                     | 0.44              |
| 2:B:606:TRP:CD1  | 2:B:619:VAL:HG11 | 2.52                     | 0.44              |
| 1:C:481:ASP:N    | 1:C:481:ASP:OD1  | 2.51                     | 0.44              |
| 1:C:667:ILE:O    | 1:C:672:LEU:HD22 | 2.18                     | 0.44              |
| 4:E:98:GLN:N     | 4:E:98:GLN:OE1   | 2.50                     | 0.44              |
| 6:G:42:PRO:HD2   | 6:G:46:GLY:O     | 2.16                     | 0.44              |
| 7:H:62:PHE:HE1   | 7:H:82:ASP:CG    | 2.24                     | 0.44              |
| 2:B:54:LEU:O     | 2:B:293:ARG:NH1  | 2.51                     | 0.44              |
| 2:B:380:ASN:HB2  | 12:B:1503:NAG:O5 | 2.16                     | 0.44              |
| 5:J:112:GLN:NE2  | 5:J:119:PRO:HG2  | 2.33                     | 0.44              |
| 8:K:125:SER:HB2  | 8:K:127:TRP:CZ2  | 2.53                     | 0.44              |
| 9:L:79:PRO:HG2   | 9:L:81:ARG:NH1   | 2.32                     | 0.44              |
| 9:L:105:THR:HG23 | 9:L:107:TYR:HE2  | 1.83                     | 0.44              |
| 1:A:634:MET:HE2  | 2:B:606:TRP:CE3  | 2.51                     | 0.44              |
| 3:D:289:LEU:HA   | 3:D:292:ARG:HE   | 1.83                     | 0.44              |
| 4:E:114:TYR:CD1  | 4:E:135:VAL:HB   | 2.53                     | 0.44              |
| 6:G:29:ALA:HB3   | 6:G:75:THR:HG22  | 2.00                     | 0.44              |
| 7:H:33:LEU:HG    | 7:H:89:GLN:O     | 2.17                     | 0.44              |
| 5:J:110:TYR:CB   | 5:J:121:PHE:N    | 2.79                     | 0.44              |
| 1:A:764:LYS:HZ1  | 3:D:774:ARG:HH22 | 1.64                     | 0.44              |
| 2:B:162:MET:HE1  | 2:B:198:TRP:CZ3  | 2.53                     | 0.44              |
| 1:C:361:LEU:HD12 | 1:C:361:LEU:HA   | 1.85                     | 0.44              |
| 1:C:523:ARG:O    | 1:C:527:ILE:HG22 | 2.17                     | 0.44              |
| 6:G:33:GLY:H     | 6:G:55:ALA:HB3   | 1.83                     | 0.44              |
| 4:I:66:LEU:CD2   | 5:J:110:TYR:HE1  | 2.25                     | 0.44              |
| 5:J:108:THR:C    | 5:J:125:THR:O    | 2.61                     | 0.44              |
| 1:A:209:MET:O    | 1:A:213:GLU:HG2  | 2.18                     | 0.43              |
| 2:B:329:THR:O    | 2:B:329:THR:HG23 | 2.18                     | 0.43              |
| 2:B:418:ILE:HG22 | 2:B:457:LYS:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:606:TRP:HE1  | 2:B:617:VAL:HG12  | 1.83                     | 0.43              |
| 1:C:354:MET:HB3  | 1:C:361:LEU:HD11  | 1.99                     | 0.43              |
| 3:D:109:ALA:HA   | 3:D:112:LEU:HD12  | 2.00                     | 0.43              |
| 3:D:605:ALA:O    | 3:D:609:LEU:HD23  | 2.18                     | 0.43              |
| 3:D:774:ARG:HH21 | 3:D:778:LEU:HD11  | 1.82                     | 0.43              |
| 6:G:123:ALA:HB3  | 6:G:156:TYR:CD1   | 2.53                     | 0.43              |
| 1:A:495:LYS:HA   | 2:B:193:ASN:HD21  | 1.83                     | 0.43              |
| 2:B:501:VAL:HG13 | 2:B:502:TYR:CD1   | 2.53                     | 0.43              |
| 1:C:68:LYS:HG3   | 1:C:73:GLN:HG3    | 1.99                     | 0.43              |
| 1:C:669:ASP:O    | 1:C:673:ARG:HG2   | 2.18                     | 0.43              |
| 1:C:794:ARG:NH1  | 1:C:794:ARG:HA    | 2.32                     | 0.43              |
| 3:D:102:ASP:O    | 3:D:103:THR:OG1   | 2.31                     | 0.43              |
| 3:D:365:ILE:HD12 | 3:D:373:TRP:HB3   | 2.00                     | 0.43              |
| 3:D:406:LEU:O    | 3:D:476:TYR:HA    | 2.18                     | 0.43              |
| 6:G:133:ILE:HD13 | 6:G:223:LYS:HA    | 2.01                     | 0.43              |
| 7:H:145:LYS:HB2  | 7:H:197:THR:HB    | 2.00                     | 0.43              |
| 8:K:49:PHE:HZ    | 8:K:54:MET:HE2    | 1.83                     | 0.43              |
| 1:A:174:ARG:O    | 1:A:178:LYS:HG3   | 2.18                     | 0.43              |
| 1:A:700:SER:O    | 1:A:704:ARG:N     | 2.43                     | 0.43              |
| 1:C:40:GLN:HG3   | 1:C:43:ARG:NH2    | 2.32                     | 0.43              |
| 3:D:780:ILE:O    | 3:D:783:LEU:HG    | 2.18                     | 0.43              |
| 5:F:26:SER:HA    | 5:F:27:PRO:HA     | 1.85                     | 0.43              |
| 5:F:109:TYR:O    | 5:F:124:GLY:HA2   | 2.18                     | 0.43              |
| 1:A:155:MET:O    | 1:A:159:ASN:N     | 2.52                     | 0.43              |
| 1:A:321:PHE:HA   | 1:A:324:VAL:HG22  | 2.01                     | 0.43              |
| 2:B:691:GLU:OE1  | 2:B:692:ARG:NH1   | 2.45                     | 0.43              |
| 1:C:70:ASN:OD1   | 1:C:71:ALA:N      | 2.50                     | 0.43              |
| 1:C:341:ASN:N    | 1:C:345:ASP:O     | 2.48                     | 0.43              |
| 1:C:683:THR:OG1  | 1:C:684:VAL:N     | 2.51                     | 0.43              |
| 3:D:99:PHE:CE1   | 3:D:112:LEU:HD21  | 2.53                     | 0.43              |
| 3:D:308:LEU:HA   | 3:D:312:SER:HA    | 1.99                     | 0.43              |
| 3:D:365:ILE:HG22 | 3:D:375:ARG:HA    | 1.99                     | 0.43              |
| 5:F:40:ILE:HB    | 5:F:96:LEU:HB3    | 2.00                     | 0.43              |
| 6:G:37:GLY:HA2   | 6:G:52:HIS:HA     | 2.00                     | 0.43              |
| 1:A:84:SER:O     | 1:A:306:ARG:NH1   | 2.51                     | 0.43              |
| 2:B:149:ALA:HB3  | 2:B:154:GLN:HE22  | 1.82                     | 0.43              |
| 1:C:408:PHE:HB3  | 1:C:459:CYS:SG    | 2.59                     | 0.43              |
| 3:D:348:ASN:HD21 | 12:D:1502:NAG:H62 | 1.83                     | 0.43              |
| 4:E:49:ILE:HG21  | 4:E:97:ASN:HB3    | 2.01                     | 0.43              |
| 6:G:132:PHE:HB3  | 6:G:151:LEU:HD22  | 2.00                     | 0.43              |
| 2:B:536:MET:SD   | 2:B:728:PHE:HB3   | 2.59                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:180:GLN:HG2  | 3:D:181:ASP:N     | 2.34                     | 0.43              |
| 3:D:695:ILE:HD11 | 3:D:702:MET:SD    | 2.57                     | 0.43              |
| 4:I:26:GLU:OE2   | 4:I:42:CYS:HB2    | 2.18                     | 0.43              |
| 1:A:29:ILE:HG12  | 1:A:60:LEU:HD12   | 2.00                     | 0.43              |
| 1:A:125:MET:HB3  | 1:A:128:TYR:CD2   | 2.53                     | 0.43              |
| 1:A:387:GLU:O    | 1:A:389:PRO:HD3   | 2.19                     | 0.43              |
| 2:B:42:HIS:CE1   | 2:B:76:ARG:HA     | 2.53                     | 0.43              |
| 2:B:283:ASP:OD1  | 2:B:283:ASP:N     | 2.51                     | 0.43              |
| 3:D:134:MET:HE2  | 3:D:137:LYS:HG2   | 2.00                     | 0.43              |
| 3:D:421:SER:HA   | 3:D:455:LYS:HD3   | 2.00                     | 0.43              |
| 3:D:428:THR:OG1  | 3:D:429:CYS:N     | 2.50                     | 0.43              |
| 3:D:486:HIS:CG   | 13:D:1504:7RC:O05 | 2.71                     | 0.43              |
| 9:L:55:TRP:HB2   | 9:L:68:ILE:HB     | 2.00                     | 0.43              |
| 1:A:731:TRP:HB3  | 1:A:736:LEU:CD2   | 2.46                     | 0.43              |
| 2:B:127:ILE:HG23 | 2:B:291:ARG:HB3   | 2.01                     | 0.43              |
| 1:C:34:SER:O     | 1:C:36:ARG:NH1    | 2.50                     | 0.43              |
| 1:C:109:TYR:CZ   | 3:D:110:GLN:HB3   | 2.53                     | 0.43              |
| 1:C:538:LEU:HD13 | 1:C:754:PHE:HD2   | 1.84                     | 0.43              |
| 3:D:89:MET:CE    | 3:D:119:THR:HG22  | 2.48                     | 0.43              |
| 7:H:196:VAL:HG23 | 7:H:196:VAL:O     | 2.18                     | 0.43              |
| 1:A:755:ARG:HH21 | 3:D:531:GLU:HB3   | 1.83                     | 0.43              |
| 1:C:79:CYS:HB3   | 1:C:83:ILE:HD12   | 2.00                     | 0.43              |
| 1:C:459:CYS:HB3  | 1:C:514:VAL:HG12  | 2.01                     | 0.43              |
| 3:D:151:GLU:HA   | 3:D:185:LYS:HG2   | 2.00                     | 0.43              |
| 4:E:65:LYS:NZ    | 5:F:123:GLY:O     | 2.51                     | 0.43              |
| 4:E:72:ILE:HD11  | 4:E:90:ILE:HG13   | 2.00                     | 0.43              |
| 4:E:114:TYR:O    | 4:E:132:GLY:HA2   | 2.19                     | 0.43              |
| 7:H:189:HIS:O    | 7:H:192:TYR:OH    | 2.24                     | 0.43              |
| 9:L:58:HIS:N     | 9:L:104:ALA:HB1   | 2.34                     | 0.43              |
| 1:A:77:SER:O     | 1:A:81:ASP:HB2    | 2.19                     | 0.43              |
| 2:B:98:LEU:HB3   | 2:B:124:ILE:HG13  | 2.00                     | 0.43              |
| 2:B:230:TYR:HD1  | 2:B:258:PRO:HG3   | 1.84                     | 0.43              |
| 2:B:274:SER:HB2  | 2:B:394:LYS:O     | 2.19                     | 0.43              |
| 1:C:522:GLU:H    | 1:C:522:GLU:CD    | 2.25                     | 0.43              |
| 3:D:40:ILE:HD12  | 3:D:71:VAL:HG23   | 2.01                     | 0.43              |
| 3:D:234:LYS:O    | 3:D:238:THR:HG23  | 2.19                     | 0.43              |
| 4:E:58:ILE:C     | 4:E:69:MET:HE1    | 2.43                     | 0.43              |
| 5:F:68:LYS:C     | 5:F:68:LYS:HD3    | 2.44                     | 0.43              |
| 4:I:112:ALA:HB3  | 4:I:114:TYR:HE1   | 1.83                     | 0.43              |
| 1:A:205:THR:HG22 | 1:A:238:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:470:MET:HE1  | 1:A:772:VAL:HG22  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:657:LEU:HD22 | 2:B:806:GLU:OE1  | 2.19                     | 0.42              |
| 1:C:295:LEU:HG   | 1:C:301:ILE:HD11 | 2.00                     | 0.42              |
| 3:D:126:ILE:HA   | 3:D:146:PHE:CE2  | 2.54                     | 0.42              |
| 4:E:61:PHE:CD1   | 4:E:62:PRO:HD2   | 2.54                     | 0.42              |
| 9:L:107:TYR:HB3  | 9:L:117:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:111:ALA:O    | 1:A:115:ARG:N    | 2.52                     | 0.42              |
| 1:A:354:MET:HG3  | 1:A:361:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:402:THR:OG1  | 1:A:403:ILE:N    | 2.51                     | 0.42              |
| 2:B:127:ILE:HA   | 2:B:147:PHE:CD2  | 2.54                     | 0.42              |
| 2:B:191:VAL:HA   | 2:B:198:TRP:CD1  | 2.53                     | 0.42              |
| 2:B:414:ALA:HB2  | 2:B:418:ILE:HD13 | 2.01                     | 0.42              |
| 2:B:466:LYS:HG2  | 2:B:469:ARG:HH22 | 1.84                     | 0.42              |
| 1:C:287:VAL:HG11 | 1:C:340:PHE:HE2  | 1.84                     | 0.42              |
| 1:C:351:TYR:O    | 1:C:367:TYR:HB3  | 2.19                     | 0.42              |
| 1:C:551:LEU:HB3  | 1:C:812:ASN:HB2  | 2.01                     | 0.42              |
| 1:C:624:PRO:HD2  | 3:D:607:TRP:HH2  | 1.84                     | 0.42              |
| 3:D:351:PHE:HA   | 3:D:357:GLN:HA   | 2.01                     | 0.42              |
| 6:G:99:ARG:HE    | 6:G:107:TYR:HB2  | 1.84                     | 0.42              |
| 8:K:23:LYS:HD3   | 8:K:23:LYS:HA    | 1.83                     | 0.42              |
| 8:K:31:LEU:HD21  | 8:K:107:LYS:HA   | 2.01                     | 0.42              |
| 2:B:231:CYS:O    | 2:B:261:VAL:HG22 | 2.20                     | 0.42              |
| 2:B:535:VAL:HA   | 2:B:728:PHE:O    | 2.18                     | 0.42              |
| 2:B:737:TYR:HA   | 2:B:797:THR:CG2  | 2.48                     | 0.42              |
| 4:E:59:ARG:HD3   | 4:E:114:TYR:CE1  | 2.55                     | 0.42              |
| 6:G:214:HIS:O    | 6:G:218:SER:HA   | 2.19                     | 0.42              |
| 7:H:18:THR:HG1   | 7:H:74:LYS:HE2   | 1.83                     | 0.42              |
| 7:H:36:TYR:CD1   | 7:H:46:LEU:HA    | 2.54                     | 0.42              |
| 1:A:209:MET:SD   | 1:A:212:ARG:NE   | 2.92                     | 0.42              |
| 1:A:220:ILE:HG13 | 1:A:248:LEU:O    | 2.19                     | 0.42              |
| 1:A:570:VAL:HG23 | 1:A:636:TRP:CZ2  | 2.54                     | 0.42              |
| 2:B:528:PHE:CD1  | 2:B:529:VAL:HG22 | 2.54                     | 0.42              |
| 1:C:55:SER:HA    | 1:C:293:HIS:CE1  | 2.54                     | 0.42              |
| 1:C:822:GLY:O    | 1:C:825:VAL:HB   | 2.19                     | 0.42              |
| 3:D:656:GLN:OE1  | 3:D:656:GLN:N    | 2.47                     | 0.42              |
| 6:G:149:VAL:HB   | 6:G:225:PHE:CE2  | 2.54                     | 0.42              |
| 6:G:149:VAL:HG11 | 6:G:193:SER:HB3  | 2.00                     | 0.42              |
| 4:I:52:ASP:OD1   | 4:I:52:ASP:N     | 2.51                     | 0.42              |
| 4:I:120:TYR:HD2  | 4:I:124:TYR:HB3  | 1.84                     | 0.42              |
| 5:J:58:TRP:O     | 5:J:70:LEU:N     | 2.50                     | 0.42              |
| 1:A:358:ASN:OD1  | 5:F:76:ASN:ND2   | 2.52                     | 0.42              |
| 1:A:527:ILE:HG13 | 1:A:528:GLU:N    | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:541:LEU:HD11 | 1:A:721:VAL:HG21 | 2.01                     | 0.42              |
| 2:B:377:LYS:HB3  | 2:B:384:SER:OG   | 2.19                     | 0.42              |
| 2:B:710:GLN:HG3  | 2:B:716:ALA:HB2  | 2.01                     | 0.42              |
| 1:C:72:ILE:HD12  | 3:D:321:CYS:O    | 2.20                     | 0.42              |
| 1:C:357:GLN:O    | 1:C:360:LYS:HG2  | 2.20                     | 0.42              |
| 3:D:169:PHE:HA   | 3:D:227:ILE:O    | 2.19                     | 0.42              |
| 1:A:117:PRO:HG2  | 1:A:321:PHE:HD2  | 1.84                     | 0.42              |
| 1:A:397:ARG:NH1  | 1:A:474:TYR:O    | 2.53                     | 0.42              |
| 1:A:514:VAL:O    | 1:A:514:VAL:HG13 | 2.20                     | 0.42              |
| 2:B:503:GLN:HE22 | 7:H:94:ALA:N     | 2.17                     | 0.42              |
| 1:C:167:VAL:O    | 1:C:196:GLN:HA   | 2.19                     | 0.42              |
| 1:C:436:CYS:HB2  | 1:C:455:CYS:HB2  | 1.91                     | 0.42              |
| 1:C:497:GLU:N    | 1:C:497:GLU:OE1  | 2.53                     | 0.42              |
| 1:C:540:ILE:HD12 | 1:C:730:ILE:HG13 | 2.00                     | 0.42              |
| 3:D:685:THR:HG22 | 3:D:706:MET:HE2  | 2.00                     | 0.42              |
| 5:F:62:LYS:HB2   | 5:F:65:GLN:CB    | 2.49                     | 0.42              |
| 6:G:134:PHE:CZ   | 6:G:148:VAL:HG13 | 2.54                     | 0.42              |
| 5:J:60:GLN:N     | 5:J:68:LYS:O     | 2.36                     | 0.42              |
| 1:A:698:GLU:OE1  | 1:A:698:GLU:N    | 2.47                     | 0.42              |
| 2:B:298:ILE:HA   | 2:B:341:VAL:HG11 | 2.02                     | 0.42              |
| 2:B:773:ARG:HH22 | 1:C:525:GLN:C    | 2.28                     | 0.42              |
| 1:C:79:CYS:O     | 1:C:308:CYS:HB2  | 2.19                     | 0.42              |
| 1:C:489:ARG:HH11 | 1:C:492:ASN:HA   | 1.85                     | 0.42              |
| 3:D:332:SER:O    | 3:D:335:LEU:HB2  | 2.20                     | 0.42              |
| 3:D:720:SER:HB3  | 3:D:725:LYS:HB2  | 2.01                     | 0.42              |
| 5:F:30:LEU:HD21  | 5:F:127:LEU:HD13 | 2.02                     | 0.42              |
| 7:H:121:SER:OG   | 7:H:124:GLN:OE1  | 2.33                     | 0.42              |
| 1:A:682:ALA:HA   | 1:A:706:MET:HE3  | 2.02                     | 0.42              |
| 2:B:730:TYR:HB3  | 2:B:735:LEU:CD2  | 2.50                     | 0.42              |
| 1:C:192:GLU:HG3  | 1:C:216:ALA:HB2  | 2.01                     | 0.42              |
| 3:D:408:ILE:HD13 | 3:D:465:LEU:HD11 | 2.01                     | 0.42              |
| 2:B:504:ARG:CZ   | 6:G:54:ALA:HB2   | 2.50                     | 0.42              |
| 2:B:561:MET:O    | 2:B:565:LEU:HG   | 2.20                     | 0.42              |
| 2:B:695:ARG:HG3  | 2:B:702:HIS:ND1  | 2.35                     | 0.42              |
| 1:C:36:ARG:O     | 1:C:39:GLU:HB2   | 2.19                     | 0.42              |
| 1:C:111:ALA:HB1  | 1:C:116:ILE:O    | 2.20                     | 0.42              |
| 1:C:113:PHE:CZ   | 3:D:78:PRO:HG3   | 2.54                     | 0.42              |
| 3:D:530:ILE:HG13 | 3:D:762:TYR:HB2  | 2.02                     | 0.42              |
| 6:G:140:GLN:NE2  | 6:G:227:ARG:HG3  | 2.35                     | 0.42              |
| 7:H:186:TYR:HA   | 7:H:192:TYR:OH   | 2.20                     | 0.42              |
| 7:H:190:LYS:HZ1  | 7:H:211:ARG:HE   | 1.66                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:HIS:HA   | 1:A:174:ARG:HD2  | 2.01                     | 0.42              |
| 1:A:228:ALA:HA   | 1:A:231:VAL:HG12 | 2.00                     | 0.42              |
| 1:A:443:SER:HB2  | 1:A:446:SER:HB3  | 2.02                     | 0.42              |
| 1:A:461:ASP:HA   | 1:A:464:ILE:HG22 | 2.01                     | 0.42              |
| 1:A:557:PRO:HG2  | 1:A:647:TYR:CZ   | 2.55                     | 0.42              |
| 1:A:683:THR:OG1  | 1:A:684:VAL:N    | 2.53                     | 0.42              |
| 2:B:191:VAL:HG22 | 2:B:198:TRP:CD1  | 2.55                     | 0.42              |
| 2:B:625:THR:HA   | 2:B:628:LYS:HG3  | 2.02                     | 0.42              |
| 1:C:408:PHE:CD2  | 1:C:516:PRO:HB3  | 2.55                     | 0.42              |
| 1:C:682:ALA:HB1  | 1:C:710:ASN:HA   | 2.00                     | 0.42              |
| 1:C:731:TRP:HB3  | 1:C:736:LEU:CD2  | 2.50                     | 0.42              |
| 3:D:285:TRP:N    | 3:D:375:ARG:HH22 | 2.18                     | 0.42              |
| 7:H:107:LYS:HA   | 7:H:107:LYS:HD2  | 1.90                     | 0.42              |
| 4:I:108:THR:HA   | 4:I:137:VAL:HG12 | 2.01                     | 0.42              |
| 8:K:56:TRP:CZ2   | 8:K:69:ALA:HB3   | 2.55                     | 0.42              |
| 1:A:27:VAL:HG11  | 1:A:292:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:181:GLU:O    | 1:A:184:LEU:HG   | 2.20                     | 0.41              |
| 1:A:521:ASN:ND2  | 3:D:782:GLN:HB2  | 2.35                     | 0.41              |
| 2:B:220:LYS:HE2  | 3:D:224:GLN:HA   | 2.01                     | 0.41              |
| 1:C:527:ILE:HG13 | 1:C:528:GLU:H    | 1.85                     | 0.41              |
| 1:C:554:PHE:CD2  | 1:C:816:VAL:HG22 | 2.53                     | 0.41              |
| 3:D:141:SER:O    | 3:D:142:MET:HE2  | 2.19                     | 0.41              |
| 1:A:105:THR:HB   | 1:A:106:PRO:HD3  | 2.01                     | 0.41              |
| 1:A:183:LEU:O    | 1:A:186:GLU:HG3  | 2.19                     | 0.41              |
| 1:A:634:MET:SD   | 2:B:609:TRP:CD1  | 3.13                     | 0.41              |
| 2:B:406:LEU:HD21 | 2:B:771:TRP:NE1  | 2.35                     | 0.41              |
| 2:B:571:ILE:HD12 | 2:B:571:ILE:HA   | 1.97                     | 0.41              |
| 2:B:670:PHE:HD1  | 2:B:682:PHE:CZ   | 2.37                     | 0.41              |
| 2:B:685:VAL:HG23 | 2:B:728:PHE:HZ   | 1.84                     | 0.41              |
| 1:C:121:LEU:HG   | 1:C:122:THR:HG23 | 2.02                     | 0.41              |
| 3:D:146:PHE:O    | 3:D:357:GLN:NE2  | 2.53                     | 0.41              |
| 3:D:532:THR:HA   | 3:D:733:ALA:HB3  | 2.02                     | 0.41              |
| 4:E:59:ARG:NH1   | 4:E:61:PHE:HB2   | 2.35                     | 0.41              |
| 6:G:100:ALA:HA   | 6:G:106:PRO:HB3  | 2.02                     | 0.41              |
| 6:G:129:PRO:HA   | 6:G:155:PHE:CG   | 2.55                     | 0.41              |
| 1:A:150:VAL:HG21 | 1:A:351:TYR:CD2  | 2.55                     | 0.41              |
| 1:A:519:ILE:HG23 | 1:A:529:PHE:HD2  | 1.85                     | 0.41              |
| 1:A:574:ALA:HB1  | 1:A:607:MET:HA   | 2.02                     | 0.41              |
| 1:A:810:PHE:O    | 1:A:810:PHE:CG   | 2.73                     | 0.41              |
| 2:B:374:LYS:NZ   | 2:B:377:LYS:HB2  | 2.36                     | 0.41              |
| 2:B:569:SER:O    | 2:B:573:VAL:HG13 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:86:GLN:HB3   | 1:C:304:PRO:HB2  | 2.02                     | 0.41              |
| 1:C:631:ILE:HA   | 1:C:634:MET:HG2  | 2.03                     | 0.41              |
| 3:D:77:ASP:OD2   | 3:D:80:SER:OG    | 2.26                     | 0.41              |
| 3:D:732:ASP:OD2  | 3:D:762:TYR:OH   | 2.32                     | 0.41              |
| 3:D:815:ILE:H    | 3:D:815:ILE:HD12 | 1.85                     | 0.41              |
| 8:K:78:THR:HB    | 8:K:90:ILE:HG21  | 2.02                     | 0.41              |
| 1:A:27:VAL:HG13  | 1:A:88:TYR:CD1   | 2.56                     | 0.41              |
| 2:B:89:LEU:HB3   | 2:B:95:ILE:HD11  | 2.02                     | 0.41              |
| 2:B:470:THR:O    | 2:B:472:LYS:NZ   | 2.54                     | 0.41              |
| 1:C:401:VAL:HG13 | 1:C:501:MET:CE   | 2.51                     | 0.41              |
| 1:C:548:ARG:NH2  | 1:C:807:THR:O    | 2.37                     | 0.41              |
| 3:D:718:LEU:HB2  | 3:D:739:MET:CE   | 2.50                     | 0.41              |
| 5:F:84:ARG:HH22  | 5:F:101:VAL:C    | 2.29                     | 0.41              |
| 7:H:125:LEU:HD23 | 7:H:183:LYS:HZ2  | 1.85                     | 0.41              |
| 1:A:505:LEU:HD22 | 1:A:513:ILE:HG12 | 2.00                     | 0.41              |
| 1:A:736:LEU:HD13 | 1:A:736:LEU:HA   | 1.82                     | 0.41              |
| 2:B:48:GLU:OE2   | 2:B:52:ARG:NE    | 2.51                     | 0.41              |
| 1:C:283:ASP:O    | 1:C:287:VAL:HG23 | 2.20                     | 0.41              |
| 3:D:84:ARG:HH21  | 3:D:92:ARG:HH22  | 1.68                     | 0.41              |
| 3:D:95:GLN:O     | 3:D:121:THR:HB   | 2.20                     | 0.41              |
| 3:D:290:PRO:HA   | 3:D:293:VAL:HG22 | 2.02                     | 0.41              |
| 6:G:18:LEU:HB3   | 6:G:84:ILE:HG23  | 2.03                     | 0.41              |
| 6:G:49:TRP:HH2   | 6:G:52:HIS:HB3   | 1.84                     | 0.41              |
| 7:H:61:ARG:HH22  | 7:H:81:GLU:CD    | 2.28                     | 0.41              |
| 7:H:142:ARG:HA   | 7:H:173:TYR:HE2  | 1.86                     | 0.41              |
| 7:H:151:ASP:HB2  | 7:H:189:HIS:CD2  | 2.56                     | 0.41              |
| 9:L:105:THR:HG23 | 9:L:107:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:817:PHE:O    | 1:A:821:ALA:N    | 2.47                     | 0.41              |
| 5:J:71:ILE:HD12  | 5:J:78:GLU:HB2   | 2.01                     | 0.41              |
| 8:K:92:ARG:NH2   | 8:K:94:ASN:OD1   | 2.40                     | 0.41              |
| 1:A:150:VAL:HG22 | 1:A:367:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:519:ILE:HG12 | 1:A:529:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:534:LYS:HB3  | 1:A:758:PHE:HD2  | 1.85                     | 0.41              |
| 1:A:670:PRO:HA   | 1:A:673:ARG:HG2  | 2.03                     | 0.41              |
| 2:B:526:VAL:HG21 | 2:B:780:LEU:HD21 | 2.02                     | 0.41              |
| 2:B:784:GLY:HA2  | 1:C:754:PHE:CE1  | 2.54                     | 0.41              |
| 1:C:47:ASN:C     | 1:C:51:LYS:HZ2   | 2.28                     | 0.41              |
| 1:C:68:LYS:HB3   | 1:C:73:GLN:HE21  | 1.85                     | 0.41              |
| 1:C:72:ILE:HG12  | 3:D:114:PHE:CE2  | 2.54                     | 0.41              |
| 1:C:412:LYS:HD3  | 1:C:412:LYS:HA   | 1.94                     | 0.41              |
| 3:D:47:GLU:O     | 3:D:51:LYS:HG2   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:637:PHE:O    | 3:D:641:ILE:HG12 | 2.21                     | 0.41              |
| 6:G:120:ARG:H    | 6:G:123:ALA:HB2  | 1.86                     | 0.41              |
| 7:H:142:ARG:NH1  | 7:H:143:GLU:HB2  | 2.36                     | 0.41              |
| 1:A:48:GLN:NE2   | 1:A:52:ARG:HD3   | 2.36                     | 0.41              |
| 1:A:831:ILE:HG13 | 1:A:834:GLU:OE1  | 2.21                     | 0.41              |
| 2:B:702:HIS:O    | 2:B:706:THR:HG23 | 2.20                     | 0.41              |
| 1:C:251:GLU:OE2  | 1:C:271:LEU:N    | 2.52                     | 0.41              |
| 1:C:495:LYS:NZ   | 1:C:497:GLU:HB3  | 2.36                     | 0.41              |
| 1:C:680:ILE:HG22 | 1:C:705:HIS:HE1  | 1.85                     | 0.41              |
| 3:D:536:VAL:HB   | 3:D:751:ILE:HD13 | 2.01                     | 0.41              |
| 9:L:36:GLY:HA2   | 9:L:97:ASN:HA    | 2.03                     | 0.41              |
| 1:A:425:THR:OG1  | 1:A:429:ASP:N    | 2.54                     | 0.41              |
| 1:A:540:ILE:CG2  | 1:A:728:ALA:HB1  | 2.51                     | 0.41              |
| 1:A:700:SER:HA   | 1:A:703:TYR:HB3  | 2.02                     | 0.41              |
| 1:A:732:ASP:OD1  | 1:A:733:SER:N    | 2.53                     | 0.41              |
| 2:B:177:PHE:O    | 2:B:180:TYR:HD1  | 2.04                     | 0.41              |
| 2:B:442:ILE:HG13 | 2:B:449:GLY:HA2  | 2.03                     | 0.41              |
| 2:B:504:ARG:NH2  | 6:G:54:ALA:HB2   | 2.36                     | 0.41              |
| 1:C:287:VAL:HG11 | 1:C:340:PHE:CE2  | 2.56                     | 0.41              |
| 1:C:338:VAL:HG22 | 1:C:346:ARG:CZ   | 2.51                     | 0.41              |
| 1:C:483:LYS:O    | 1:C:501:MET:HB2  | 2.21                     | 0.41              |
| 1:C:495:LYS:HD3  | 3:D:192:ASN:HA   | 2.01                     | 0.41              |
| 1:C:562:LEU:O    | 1:C:565:LEU:HG   | 2.21                     | 0.41              |
| 3:D:415:PRO:HD3  | 3:D:738:TYR:CG   | 2.55                     | 0.41              |
| 3:D:448:GLU:HG3  | 3:D:449:GLU:N    | 2.36                     | 0.41              |
| 3:D:564:VAL:O    | 3:D:568:ILE:HG23 | 2.21                     | 0.41              |
| 3:D:711:GLN:HG2  | 3:D:717:ALA:HB2  | 2.03                     | 0.41              |
| 6:G:34:VAL:HA    | 6:G:101:ALA:HA   | 2.02                     | 0.41              |
| 7:H:109:THR:HA   | 7:H:140:TYR:HD2  | 1.86                     | 0.41              |
| 1:A:295:LEU:HG   | 1:A:301:ILE:HD11 | 2.03                     | 0.41              |
| 1:A:465:LYS:HG2  | 1:A:784:PHE:CE2  | 2.56                     | 0.41              |
| 1:A:547:PRO:HB2  | 1:A:806:ALA:HA   | 2.03                     | 0.41              |
| 3:D:216:ILE:HA   | 3:D:219:GLN:NE2  | 2.36                     | 0.41              |
| 3:D:524:ASP:O    | 3:D:766:ILE:HG22 | 2.20                     | 0.41              |
| 4:E:74:TYR:O     | 4:E:76:GLY:N     | 2.54                     | 0.41              |
| 1:C:233:ARG:HG3  | 1:C:261:TYR:HB3  | 2.03                     | 0.40              |
| 1:C:457:GLY:H    | 1:C:460:ILE:HB   | 1.86                     | 0.40              |
| 1:C:614:LEU:HD12 | 1:C:636:TRP:CZ2  | 2.57                     | 0.40              |
| 1:C:685:LYS:HB3  | 1:C:686:GLN:CD   | 2.46                     | 0.40              |
| 3:D:109:ALA:O    | 3:D:112:LEU:HB2  | 2.21                     | 0.40              |
| 5:J:57:ASN:HB2   | 5:J:69:LEU:HD11  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:127:LEU:HD12 | 5:J:127:LEU:HA   | 1.88                     | 0.40              |
| 1:A:525:GLN:HE22 | 3:D:778:LEU:HD23 | 1.87                     | 0.40              |
| 1:A:552:ASP:OD1  | 1:A:553:SER:N    | 2.49                     | 0.40              |
| 2:B:514:ILE:HD13 | 1:C:531:LYS:NZ   | 2.36                     | 0.40              |
| 3:D:436:CYS:HB3  | 3:D:478:LEU:HD22 | 2.03                     | 0.40              |
| 6:G:39:ILE:HD12  | 6:G:39:ILE:HA    | 1.92                     | 0.40              |
| 7:H:61:ARG:HB2   | 7:H:76:ASN:HB2   | 2.03                     | 0.40              |
| 9:L:31:LEU:HD22  | 9:L:39:VAL:HG21  | 2.04                     | 0.40              |
| 2:B:631:VAL:HG11 | 1:C:619:ILE:HD11 | 2.03                     | 0.40              |
| 3:D:671:PHE:HA   | 3:D:683:PHE:CE2  | 2.56                     | 0.40              |
| 5:F:99:HIS:HA    | 5:F:100:PRO:HA   | 1.97                     | 0.40              |
| 7:H:196:VAL:O    | 7:H:204:PRO:HB3  | 2.21                     | 0.40              |
| 1:A:548:ARG:C    | 1:A:806:ALA:HB1  | 2.46                     | 0.40              |
| 1:A:722:ARG:HG2  | 1:A:746:LEU:HD21 | 2.02                     | 0.40              |
| 2:B:282:ASP:HB3  | 2:B:286:TYR:H    | 1.86                     | 0.40              |
| 2:B:730:TYR:HB3  | 2:B:735:LEU:HD21 | 2.03                     | 0.40              |
| 1:C:462:LEU:HD13 | 1:C:785:MET:HE1  | 2.03                     | 0.40              |
| 1:C:527:ILE:HD12 | 1:C:527:ILE:HA   | 1.98                     | 0.40              |
| 1:C:536:GLN:HG2  | 1:C:758:PHE:CE2  | 2.57                     | 0.40              |
| 3:D:357:GLN:OE1  | 3:D:357:GLN:N    | 2.43                     | 0.40              |
| 7:H:12:SER:HB3   | 7:H:107:LYS:HD3  | 2.04                     | 0.40              |
| 7:H:115:VAL:HG21 | 7:H:196:VAL:HG21 | 2.03                     | 0.40              |
| 8:K:53:THR:OG1   | 8:K:54:MET:N     | 2.54                     | 0.40              |
| 1:A:72:ILE:HG23  | 2:B:119:GLN:HE22 | 1.86                     | 0.40              |
| 1:A:150:VAL:HG12 | 1:A:154:MET:HE1  | 2.04                     | 0.40              |
| 1:A:167:VAL:HG21 | 1:A:177:GLN:HB3  | 2.03                     | 0.40              |
| 1:A:174:ARG:HA   | 1:A:177:GLN:HG2  | 2.02                     | 0.40              |
| 1:A:467:ALA:HA   | 1:A:472:PHE:CE1  | 2.56                     | 0.40              |
| 2:B:49:ARG:NH1   | 2:B:52:ARG:HD2   | 2.36                     | 0.40              |
| 1:C:115:ARG:HD2  | 1:C:115:ARG:HA   | 1.81                     | 0.40              |
| 1:C:277:GLU:N    | 1:C:277:GLU:OE1  | 2.54                     | 0.40              |
| 1:C:295:LEU:HD22 | 1:C:324:VAL:HG21 | 2.03                     | 0.40              |
| 1:C:533:PHE:CZ   | 1:C:758:PHE:HB3  | 2.56                     | 0.40              |
| 3:D:110:GLN:HE22 | 3:D:134:MET:HE1  | 1.85                     | 0.40              |
| 3:D:529:PHE:O    | 3:D:784:PHE:HZ   | 2.05                     | 0.40              |
| 3:D:706:MET:HB3  | 3:D:706:MET:HE3  | 1.92                     | 0.40              |
| 4:E:70:GLY:HA2   | 4:E:79:GLY:O     | 2.21                     | 0.40              |
| 5:F:58:TRP:CZ3   | 5:F:111:CYS:HB3  | 2.56                     | 0.40              |
| 5:F:62:LYS:HB2   | 5:F:65:GLN:HB3   | 2.03                     | 0.40              |
| 6:G:13:GLN:HG2   | 6:G:120:ARG:NH1  | 2.37                     | 0.40              |
| 7:H:6:GLN:CD     | 7:H:100:GLY:H    | 2.28                     | 0.40              |

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| Atom-1          | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 5:J:23:LEU:HD13 | 5:J:42:CYS:SG | 2.61                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 796/938 (85%)   | 758 (95%)  | 37 (5%)  | 1 (0%)   | 48          | 82  |
| 1   | C     | 796/938 (85%)   | 758 (95%)  | 36 (4%)  | 2 (0%)   | 36          | 71  |
| 2   | B     | 788/1464 (54%)  | 743 (94%)  | 44 (6%)  | 1 (0%)   | 48          | 82  |
| 3   | D     | 788/1482 (53%)  | 730 (93%)  | 57 (7%)  | 1 (0%)   | 48          | 82  |
| 4   | E     | 116/140 (83%)   | 104 (90%)  | 9 (8%)   | 3 (3%)   | 4           | 26  |
| 4   | I     | 116/140 (83%)   | 109 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 5   | F     | 108/131 (82%)   | 96 (89%)   | 12 (11%) | 0        | 100         | 100 |
| 5   | J     | 108/131 (82%)   | 92 (85%)   | 14 (13%) | 2 (2%)   | 6           | 32  |
| 6   | G     | 225/227 (99%)   | 189 (84%)  | 35 (16%) | 1 (0%)   | 30          | 66  |
| 7   | H     | 210/212 (99%)   | 204 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 8   | K     | 112/248 (45%)   | 106 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 9   | L     | 104/265 (39%)   | 89 (86%)   | 15 (14%) | 0        | 100         | 100 |
| All | All   | 4267/6316 (68%) | 3978 (93%) | 278 (6%) | 11 (0%)  | 37          | 71  |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 659 | VAL  |
| 1   | C     | 545 | GLU  |
| 4   | E     | 53  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | G     | 225 | PHE  |
| 1   | A     | 811 | GLU  |
| 4   | E     | 51  | SER  |
| 5   | J     | 108 | THR  |
| 5   | J     | 109 | TYR  |
| 3   | D     | 661 | ASP  |
| 1   | C     | 664 | ILE  |
| 4   | E     | 105 | SER  |

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 689/806 (86%)   | 689 (100%)  | 0        | 100         | 100 |
| 1   | C     | 690/806 (86%)   | 690 (100%)  | 0        | 100         | 100 |
| 2   | B     | 695/1308 (53%)  | 695 (100%)  | 0        | 100         | 100 |
| 3   | D     | 691/1299 (53%)  | 691 (100%)  | 0        | 100         | 100 |
| 4   | E     | 104/119 (87%)   | 103 (99%)   | 1 (1%)   | 68          | 75  |
| 4   | I     | 104/119 (87%)   | 104 (100%)  | 0        | 100         | 100 |
| 5   | F     | 90/104 (86%)    | 90 (100%)   | 0        | 100         | 100 |
| 5   | J     | 89/104 (86%)    | 88 (99%)    | 1 (1%)   | 65          | 73  |
| 6   | G     | 181/181 (100%)  | 181 (100%)  | 0        | 100         | 100 |
| 7   | H     | 169/169 (100%)  | 169 (100%)  | 0        | 100         | 100 |
| 8   | K     | 95/205 (46%)    | 95 (100%)   | 0        | 100         | 100 |
| 9   | L     | 91/221 (41%)    | 91 (100%)   | 0        | 100         | 100 |
| All | All   | 3688/5441 (68%) | 3686 (100%) | 2 (0%)   | 87          | 88  |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 51  | SER  |
| 5   | J     | 110 | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 177 | GLN  |
| 1   | A     | 293 | HIS  |
| 1   | A     | 427 | ASN  |
| 1   | A     | 536 | GLN  |
| 2   | B     | 35  | ASN  |
| 2   | B     | 42  | HIS  |
| 2   | B     | 111 | GLN  |
| 2   | B     | 168 | HIS  |
| 2   | B     | 216 | GLN  |
| 2   | B     | 503 | GLN  |
| 2   | B     | 648 | ASN  |
| 2   | B     | 697 | ASN  |
| 2   | B     | 839 | HIS  |
| 1   | C     | 67  | HIS  |
| 1   | C     | 177 | GLN  |
| 1   | C     | 293 | HIS  |
| 1   | C     | 525 | GLN  |
| 3   | D     | 159 | ASN  |
| 3   | D     | 217 | GLN  |
| 3   | D     | 348 | ASN  |
| 3   | D     | 401 | GLN  |
| 5   | F     | 61  | GLN  |
| 5   | F     | 112 | GLN  |
| 6   | G     | 13  | GLN  |
| 6   | G     | 79  | GLN  |
| 6   | G     | 171 | GLN  |
| 6   | G     | 226 | ASN  |
| 7   | H     | 158 | ASN  |
| 7   | H     | 160 | GLN  |
| 7   | H     | 189 | HIS  |
| 4   | I     | 23  | GLN  |
| 4   | I     | 102 | GLN  |
| 5   | J     | 57  | ASN  |
| 5   | J     | 65  | GLN  |
| 9   | L     | 75  | GLN  |

### 5.3.3 RNA ⓘ

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](#)

8 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 10  | NAG  | M     | 1   | 10,1 | 14,14,15     | 0.30 | 0           | 17,19,21    | 0.42 | 0           |
| 10  | NAG  | M     | 2   | 10   | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.42 | 0           |
| 10  | MAN  | M     | 3   | 10   | 11,11,12     | 0.79 | 0           | 15,15,17    | 1.35 | 2 (13%)     |
| 11  | NAG  | N     | 1   | 11,2 | 14,14,15     | 0.63 | 1 (7%)      | 17,19,21    | 0.67 | 0           |
| 11  | NAG  | N     | 2   | 11   | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.48 | 0           |
| 10  | NAG  | O     | 1   | 10,1 | 14,14,15     | 0.25 | 0           | 17,19,21    | 0.41 | 0           |
| 10  | NAG  | O     | 2   | 10   | 14,14,15     | 0.21 | 0           | 17,19,21    | 0.48 | 0           |
| 10  | MAN  | O     | 3   | 10   | 11,11,12     | 0.81 | 0           | 15,15,17    | 1.11 | 2 (13%)     |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 10  | NAG  | M     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | M     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | MAN  | M     | 3   | 10   | -       | 2/2/19/22 | 1/1/1/1 |
| 11  | NAG  | N     | 1   | 11,2 | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | N     | 2   | 11   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | O     | 1   | 10,1 | -       | 1/6/23/26 | 0/1/1/1 |
| 10  | NAG  | O     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | MAN  | O     | 3   | 10   | -       | 2/2/19/22 | 1/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11  | N     | 1   | NAG  | O5-C1 | -2.23 | 1.39        | 1.43     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 10  | M     | 3   | MAN  | C1-O5-C5 | 4.21  | 117.83      | 112.19   |
| 10  | O     | 3   | MAN  | C1-O5-C5 | 3.12  | 116.36      | 112.19   |
| 10  | M     | 3   | MAN  | O2-C2-C3 | -2.18 | 105.64      | 110.15   |
| 10  | O     | 3   | MAN  | O2-C2-C3 | -2.06 | 105.88      | 110.15   |

There are no chirality outliers.

All (15) torsion outliers are listed below:

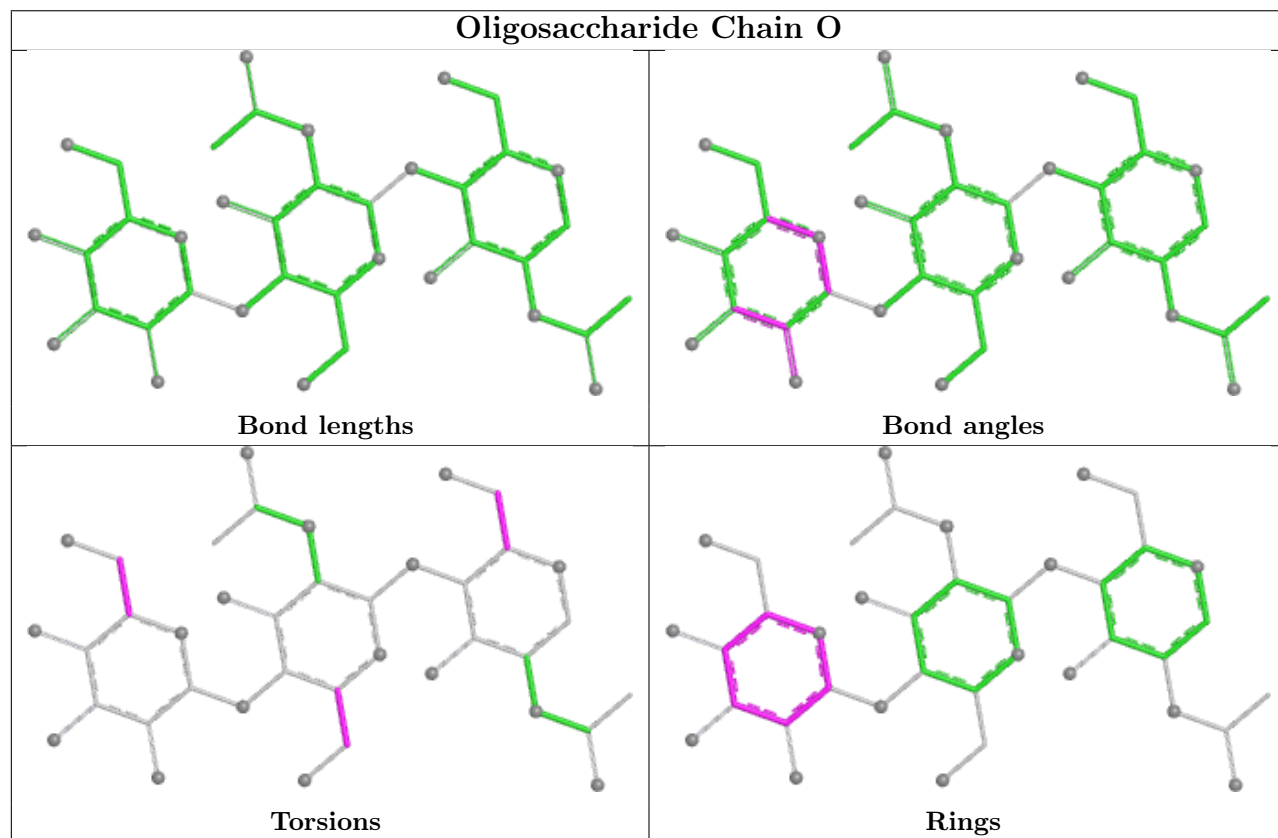
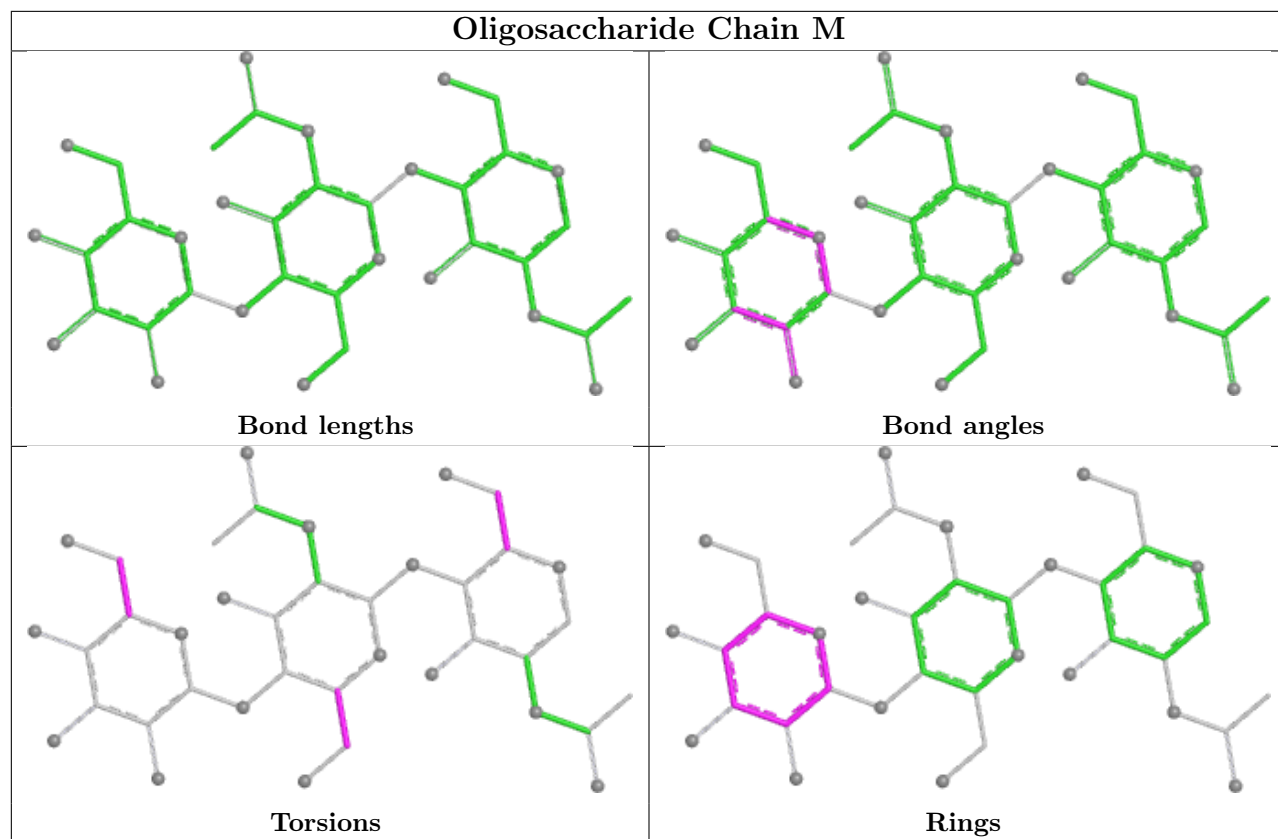
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 10  | O     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | M     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | M     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | O     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | O     | 3   | MAN  | O5-C5-C6-O6 |
| 10  | M     | 3   | MAN  | C4-C5-C6-O6 |
| 10  | M     | 3   | MAN  | O5-C5-C6-O6 |
| 10  | M     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | M     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | O     | 3   | MAN  | C4-C5-C6-O6 |
| 11  | N     | 1   | NAG  | C4-C5-C6-O6 |
| 11  | N     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | O     | 1   | NAG  | O5-C5-C6-O6 |
| 11  | N     | 1   | NAG  | O5-C5-C6-O6 |
| 11  | N     | 2   | NAG  | O5-C5-C6-O6 |

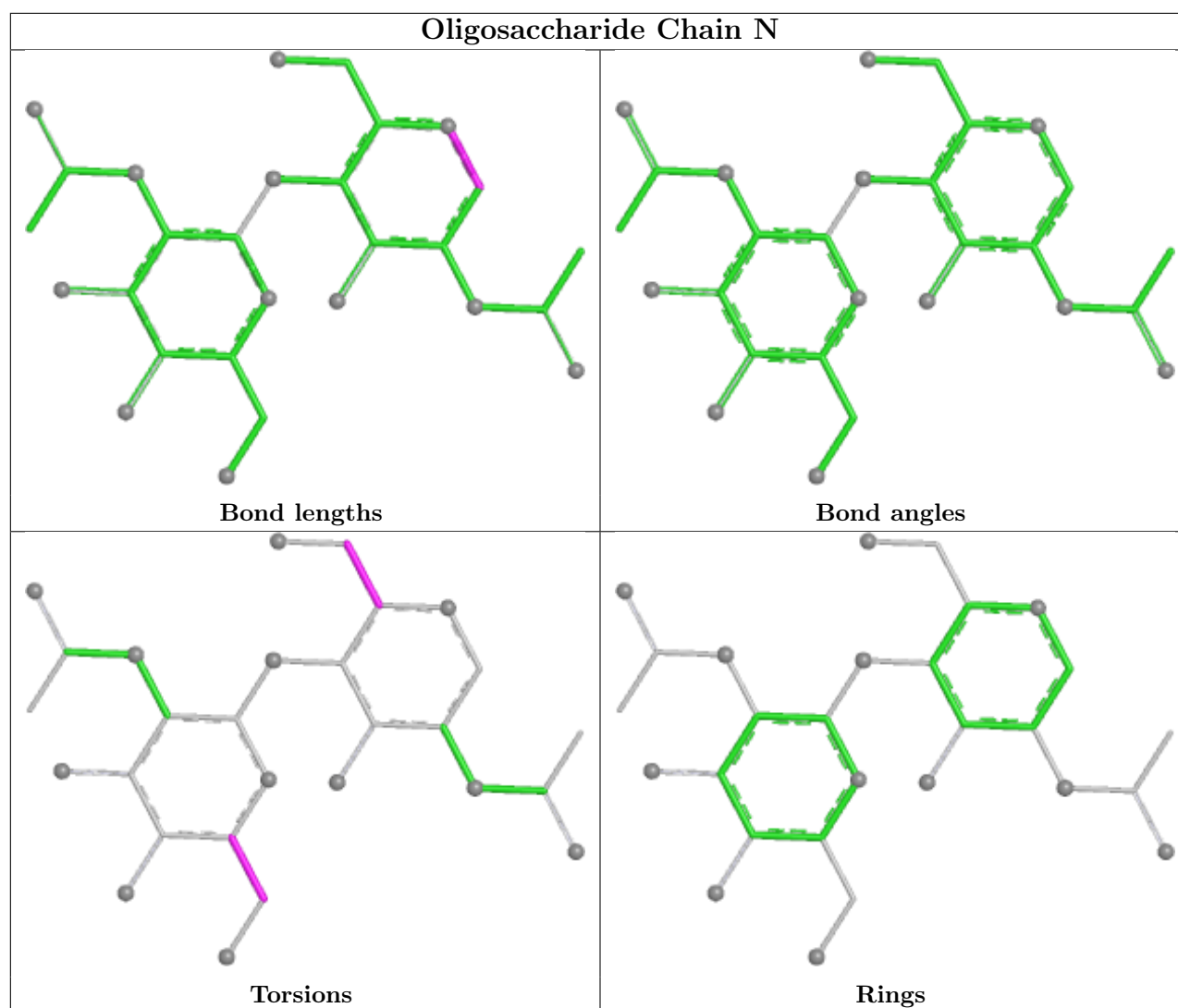
All (2) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 10  | O     | 3   | MAN  | C1-C2-C3-C4-C5-O5 |
| 10  | M     | 3   | MAN  | C1-C2-C3-C4-C5-O5 |

No monomer is involved in short contacts.

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





## 5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 12  | NAG  | A     | 1006 | 1    | 14,14,15     | 0.26 | 0           | 17,19,21    | 0.48 | 0           |
| 12  | NAG  | C     | 1001 | 1    | 14,14,15     | 0.29 | 0           | 17,19,21    | 0.36 | 0           |
| 12  | NAG  | C     | 1006 | 1    | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.40 | 0           |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | NAG  | B     | 1503 | 2    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.66 | 1 (5%)   |
| 12  | NAG  | C     | 1003 | 1    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.49 | 0        |
| 12  | NAG  | A     | 1001 | 1    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.40 | 0        |
| 13  | 7RC  | B     | 1504 | -    | 16,16,16     | 1.88 | 1 (6%)   | 18,22,22    | 1.91 | 3 (16%)  |
| 12  | NAG  | C     | 1005 | 1    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.38 | 0        |
| 13  | 7RC  | D     | 1504 | -    | 16,16,16     | 1.87 | 1 (6%)   | 18,22,22    | 1.71 | 5 (27%)  |
| 12  | NAG  | B     | 1501 | 2    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.45 | 0        |
| 12  | NAG  | D     | 1503 | 3    | 14,14,15     | 0.43 | 0        | 17,19,21    | 1.16 | 2 (11%)  |
| 12  | NAG  | C     | 1002 | 1    | 14,14,15     | 0.43 | 0        | 17,19,21    | 0.39 | 0        |
| 12  | NAG  | A     | 1007 | 1    | 14,14,15     | 0.41 | 0        | 17,19,21    | 1.15 | 2 (11%)  |
| 12  | NAG  | B     | 1502 | 2    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.48 | 0        |
| 12  | NAG  | A     | 1002 | 1    | 14,14,15     | 0.42 | 0        | 17,19,21    | 1.15 | 2 (11%)  |
| 12  | NAG  | A     | 1005 | 1    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.44 | 0        |
| 12  | NAG  | C     | 1004 | 1    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.44 | 0        |
| 12  | NAG  | D     | 1501 | 3    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.44 | 0        |
| 12  | NAG  | A     | 1004 | 1    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.43 | 0        |
| 12  | NAG  | A     | 1003 | 1    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.45 | 0        |
| 12  | NAG  | D     | 1502 | 3    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.42 | 0        |
| 12  | NAG  | C     | 1007 | 1    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.39 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 12  | NAG  | A     | 1006 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 12  | NAG  | C     | 1001 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 12  | NAG  | C     | 1006 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 12  | NAG  | B     | 1503 | 2    | -       | 0/6/23/26  | 0/1/1/1 |
| 12  | NAG  | C     | 1003 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 12  | NAG  | A     | 1001 | 1    | -       | 3/6/23/26  | 0/1/1/1 |
| 13  | 7RC  | B     | 1504 | -    | -       | 4/11/21/21 | 0/1/1/1 |
| 12  | NAG  | C     | 1005 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 13  | 7RC  | D     | 1504 | -    | -       | 0/11/21/21 | 0/1/1/1 |
| 12  | NAG  | B     | 1501 | 2    | -       | 2/6/23/26  | 0/1/1/1 |
| 12  | NAG  | D     | 1503 | 3    | -       | 0/6/23/26  | 0/1/1/1 |
| 12  | NAG  | C     | 1002 | 1    | -       | 0/6/23/26  | 0/1/1/1 |
| 12  | NAG  | A     | 1007 | 1    | -       | 0/6/23/26  | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 12  | NAG  | B     | 1502 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | A     | 1002 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | NAG  | A     | 1005 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | C     | 1004 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 12  | NAG  | D     | 1501 | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 12  | NAG  | A     | 1004 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | A     | 1003 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | D     | 1502 | 3    | -       | 3/6/23/26 | 0/1/1/1 |
| 12  | NAG  | C     | 1007 | 1    | -       | 4/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 13  | B     | 1504 | 7RC  | P01-C07 | 6.47 | 1.85        | 1.78     |
| 13  | D     | 1504 | 7RC  | P01-C07 | 6.42 | 1.85        | 1.78     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | B     | 1504 | 7RC  | P01-C07-C06 | -5.70 | 107.92      | 114.94   |
| 13  | D     | 1504 | 7RC  | P01-C07-C06 | -4.25 | 109.71      | 114.94   |
| 13  | D     | 1504 | 7RC  | C03-N01-C02 | 2.60  | 113.86      | 109.53   |
| 13  | B     | 1504 | 7RC  | C04-N01-C02 | -2.38 | 105.90      | 111.69   |
| 12  | A     | 1007 | NAG  | C8-C7-N2    | 2.37  | 120.05      | 116.12   |
| 12  | A     | 1002 | NAG  | C8-C7-N2    | 2.35  | 120.02      | 116.12   |
| 12  | D     | 1503 | NAG  | C8-C7-N2    | 2.35  | 120.01      | 116.12   |
| 13  | B     | 1504 | 7RC  | O01-C08-C01 | 2.26  | 121.16      | 113.51   |
| 13  | D     | 1504 | 7RC  | O01-C08-C01 | 2.25  | 121.14      | 113.51   |
| 12  | B     | 1503 | NAG  | C1-O5-C5    | 2.20  | 115.14      | 112.19   |
| 13  | D     | 1504 | 7RC  | C06-C04-N01 | -2.15 | 107.88      | 113.93   |
| 12  | D     | 1503 | NAG  | C2-N2-C7    | -2.15 | 120.01      | 122.90   |
| 12  | A     | 1002 | NAG  | C2-N2-C7    | -2.14 | 120.03      | 122.90   |
| 13  | D     | 1504 | 7RC  | C04-N01-C02 | -2.12 | 106.54      | 111.69   |
| 12  | A     | 1007 | NAG  | C2-N2-C7    | -2.11 | 120.07      | 122.90   |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | B     | 1504 | 7RC  | C06-C07-P01-O03 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | B     | 1504 | 7RC  | C06-C07-P01-O04 |
| 12  | A     | 1006 | NAG  | O5-C5-C6-O6     |
| 12  | A     | 1005 | NAG  | C4-C5-C6-O6     |
| 12  | B     | 1502 | NAG  | O5-C5-C6-O6     |
| 12  | D     | 1502 | NAG  | O5-C5-C6-O6     |
| 12  | B     | 1502 | NAG  | C4-C5-C6-O6     |
| 12  | A     | 1001 | NAG  | O5-C5-C6-O6     |
| 12  | A     | 1004 | NAG  | O5-C5-C6-O6     |
| 12  | C     | 1001 | NAG  | O5-C5-C6-O6     |
| 12  | C     | 1007 | NAG  | O5-C5-C6-O6     |
| 12  | C     | 1001 | NAG  | C4-C5-C6-O6     |
| 12  | A     | 1006 | NAG  | C4-C5-C6-O6     |
| 12  | A     | 1005 | NAG  | O5-C5-C6-O6     |
| 12  | C     | 1003 | NAG  | C4-C5-C6-O6     |
| 12  | C     | 1006 | NAG  | O5-C5-C6-O6     |
| 12  | B     | 1501 | NAG  | C4-C5-C6-O6     |
| 12  | C     | 1006 | NAG  | C4-C5-C6-O6     |
| 12  | C     | 1007 | NAG  | C8-C7-N2-C2     |
| 12  | C     | 1007 | NAG  | O7-C7-N2-C2     |
| 12  | B     | 1501 | NAG  | O5-C5-C6-O6     |
| 12  | D     | 1501 | NAG  | O5-C5-C6-O6     |
| 12  | C     | 1007 | NAG  | C4-C5-C6-O6     |
| 12  | D     | 1502 | NAG  | C4-C5-C6-O6     |
| 12  | C     | 1003 | NAG  | O5-C5-C6-O6     |
| 12  | A     | 1001 | NAG  | C4-C5-C6-O6     |
| 12  | A     | 1004 | NAG  | C4-C5-C6-O6     |
| 13  | B     | 1504 | 7RC  | C06-C07-P01-O02 |
| 12  | C     | 1004 | NAG  | O5-C5-C6-O6     |
| 13  | B     | 1504 | 7RC  | C04-C06-C07-P01 |
| 12  | A     | 1003 | NAG  | C4-C5-C6-O6     |
| 12  | C     | 1005 | NAG  | C4-C5-C6-O6     |
| 12  | A     | 1003 | NAG  | O5-C5-C6-O6     |
| 12  | A     | 1001 | NAG  | C1-C2-N2-C7     |
| 12  | D     | 1502 | NAG  | C1-C2-N2-C7     |
| 12  | C     | 1005 | NAG  | O5-C5-C6-O6     |

There are no ring outliers.

5 monomers are involved in 16 short contacts:

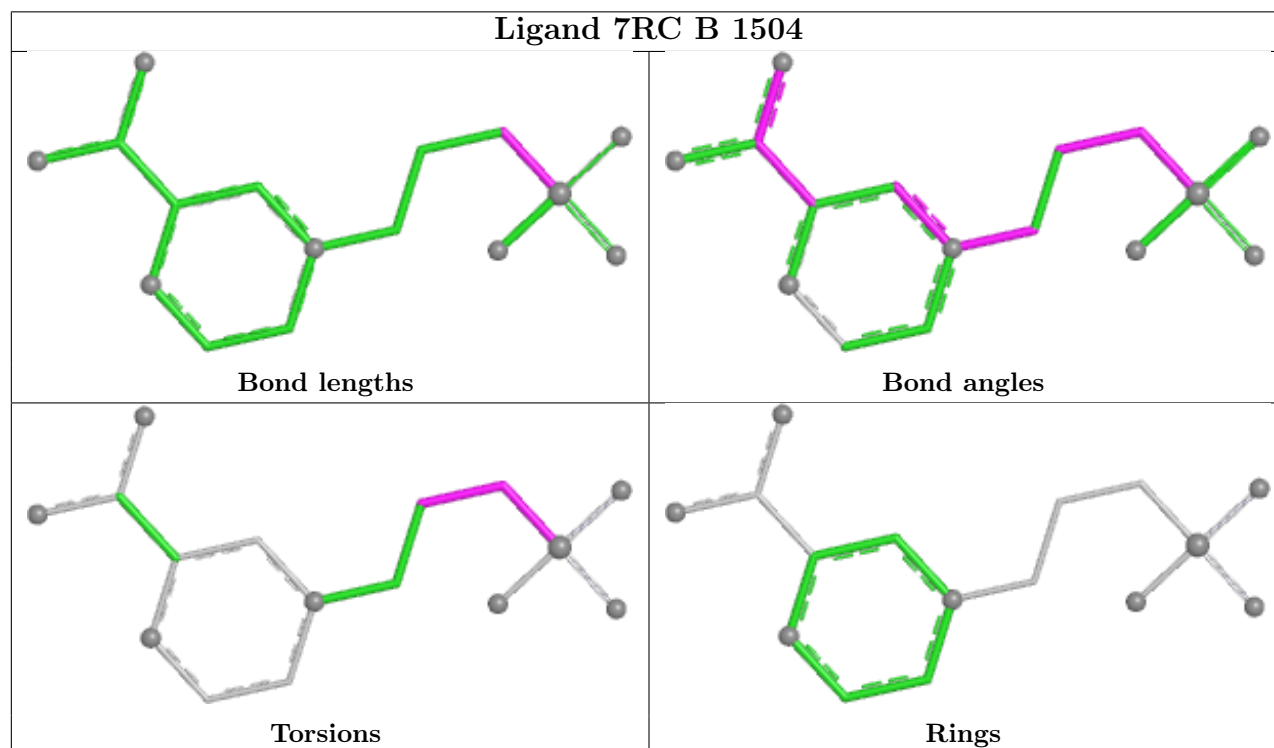
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 12  | B     | 1503 | NAG  | 1       | 0            |
| 13  | B     | 1504 | 7RC  | 7       | 0            |

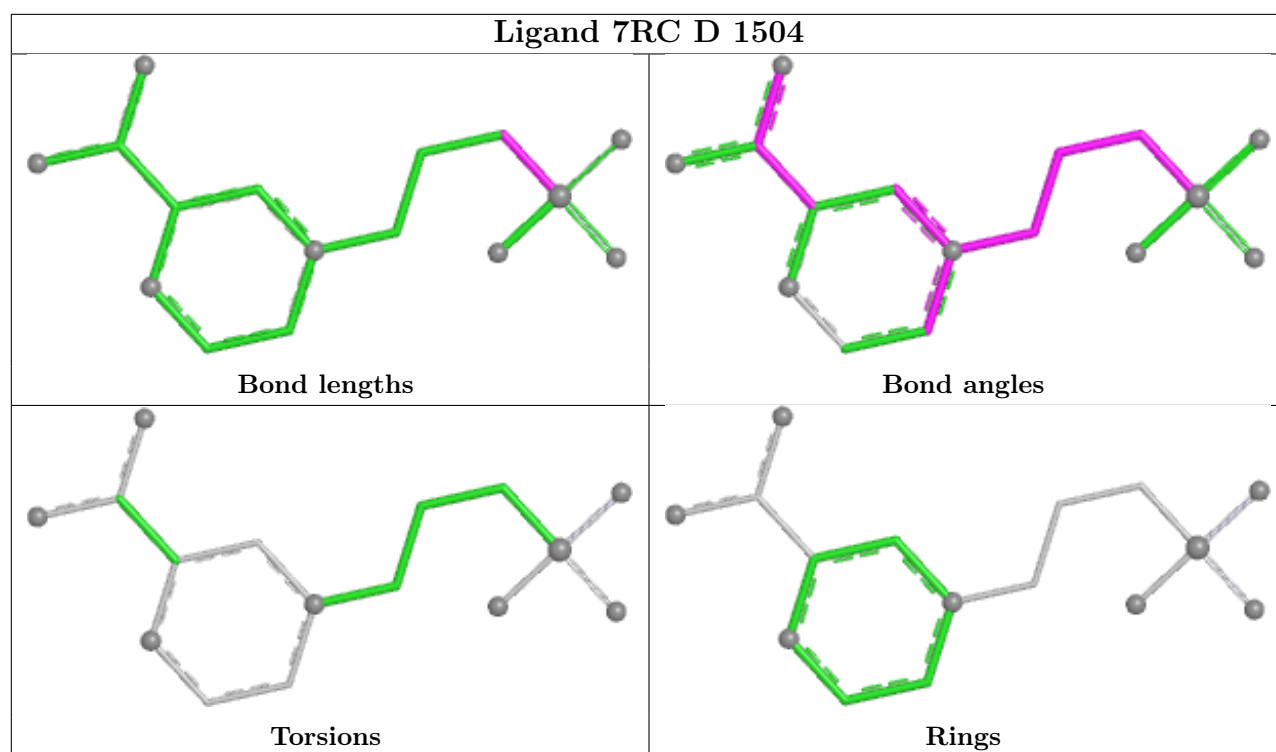
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 13  | D     | 1504 | 7RC  | 6       | 0            |
| 12  | C     | 1002 | NAG  | 1       | 0            |
| 12  | D     | 1502 | NAG  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.

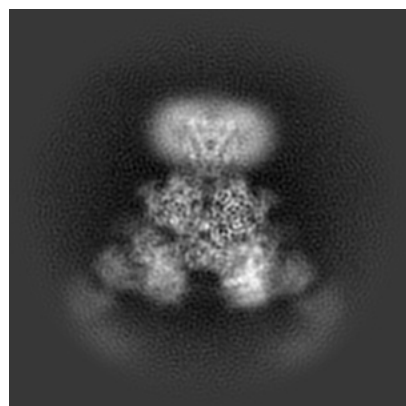
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38451. These allow visual inspection of the internal detail of the map and identification of artifacts.

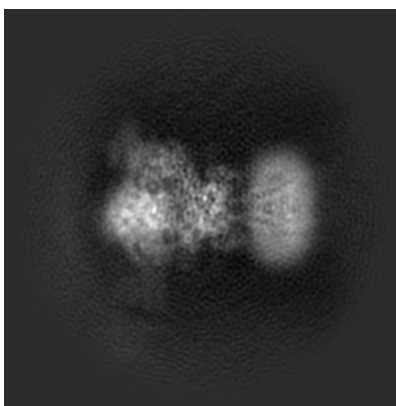
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

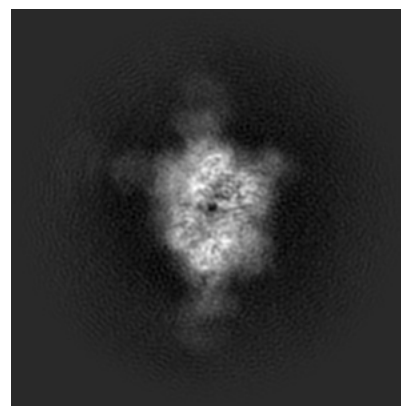
#### 6.1.1 Primary map



X

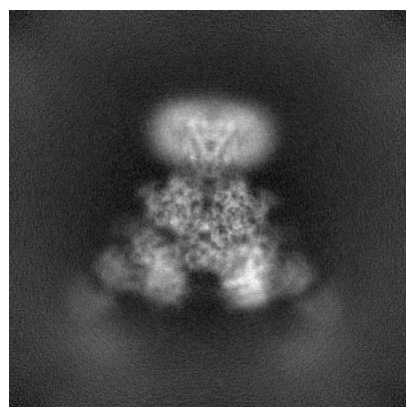


Y

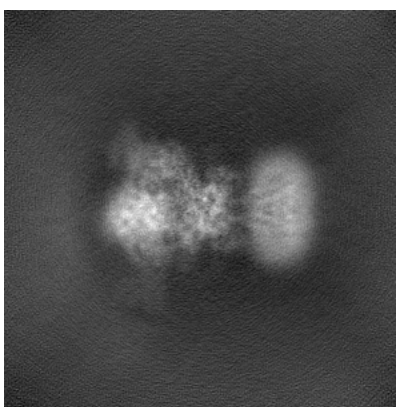


Z

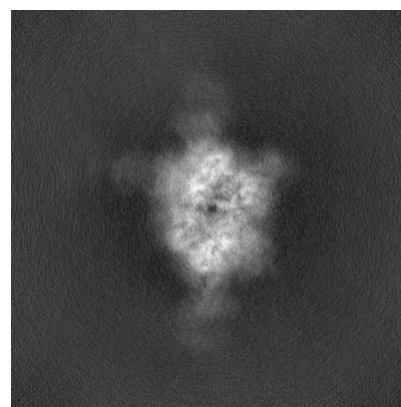
#### 6.1.2 Raw map



X



Y

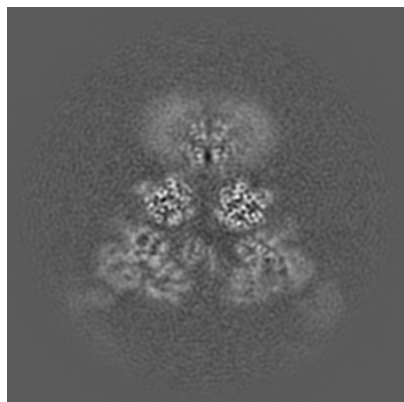


Z

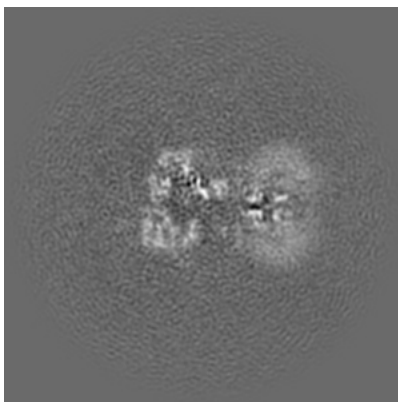
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

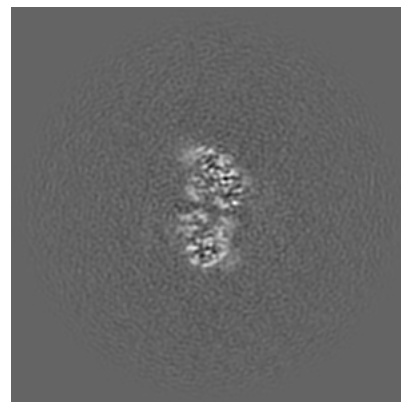
### 6.2.1 Primary map



X Index: 160

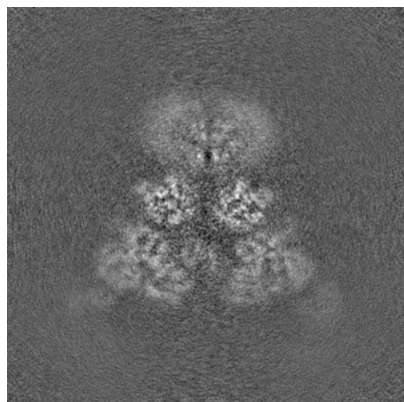


Y Index: 160

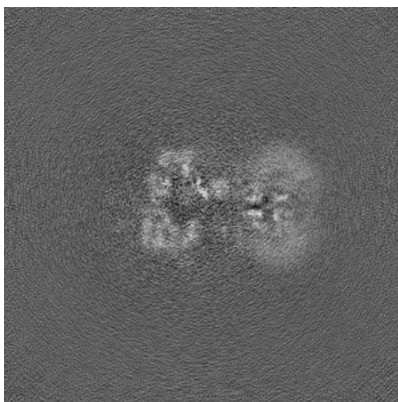


Z Index: 160

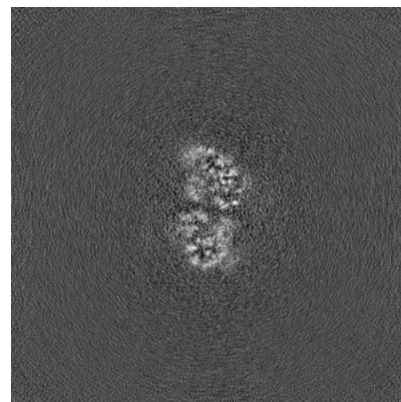
### 6.2.2 Raw map



X Index: 160



Y Index: 160



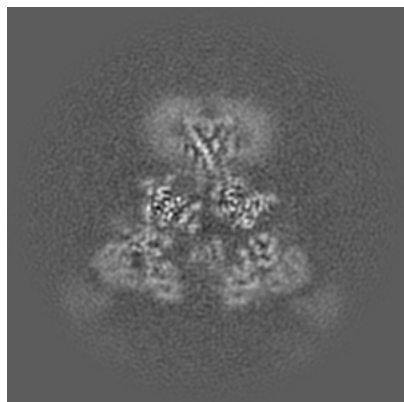
Z Index: 160

The images above show central slices of the map in three orthogonal directions.

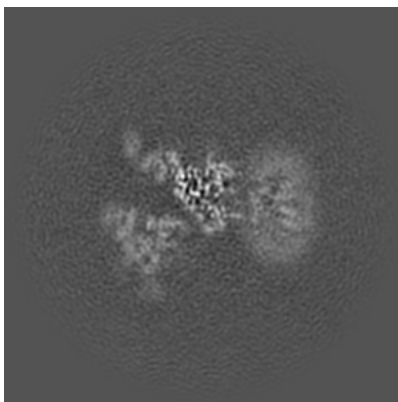


## 6.3 Largest variance slices [i](#)

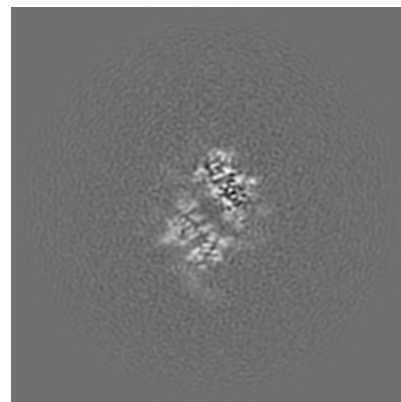
### 6.3.1 Primary map



X Index: 154

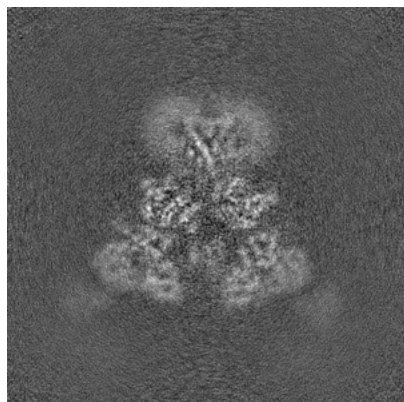


Y Index: 176

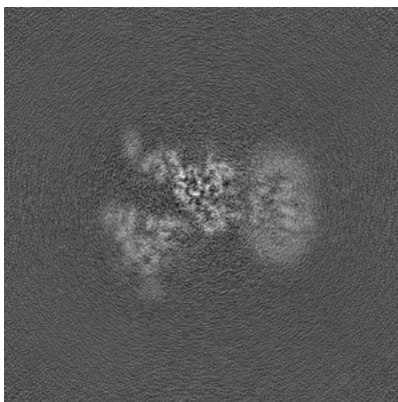


Z Index: 151

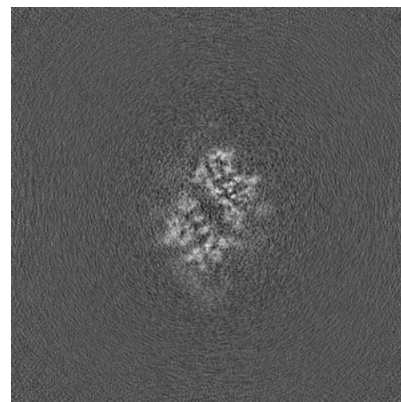
### 6.3.2 Raw map



X Index: 155



Y Index: 176



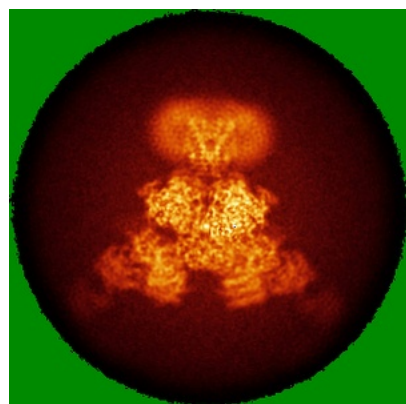
Z Index: 150

The images above show the largest variance slices of the map in three orthogonal directions.

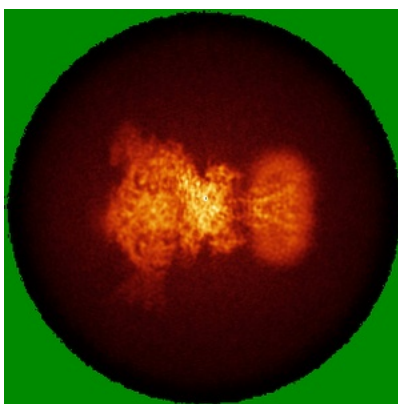


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

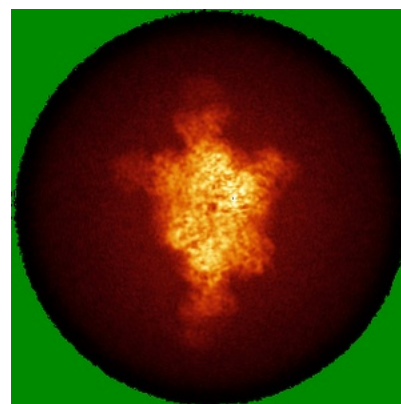
### 6.4.1 Primary map



X

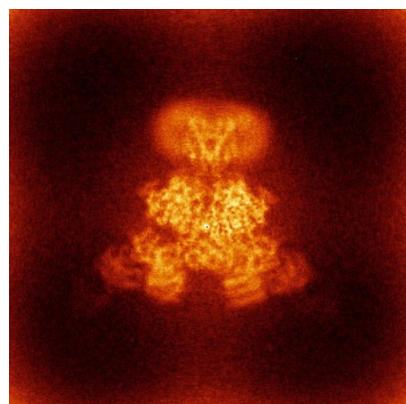


Y

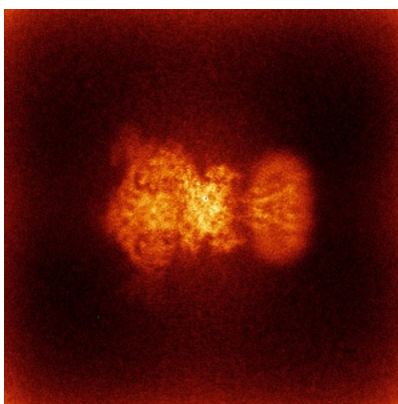


Z

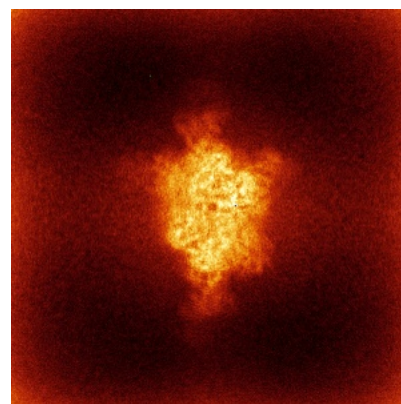
### 6.4.2 Raw map



X



Y

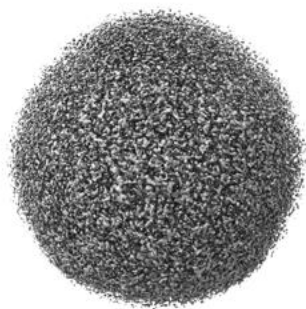


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



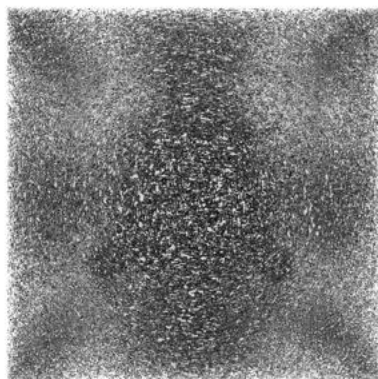
Y



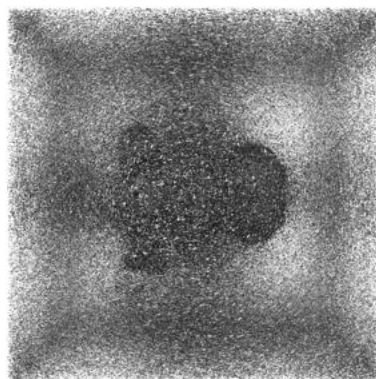
Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

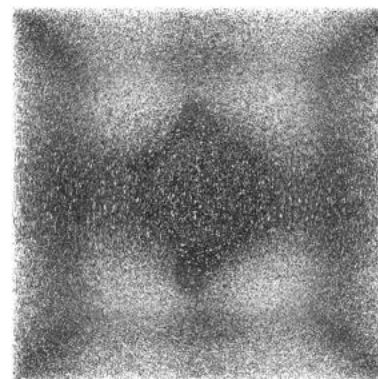
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

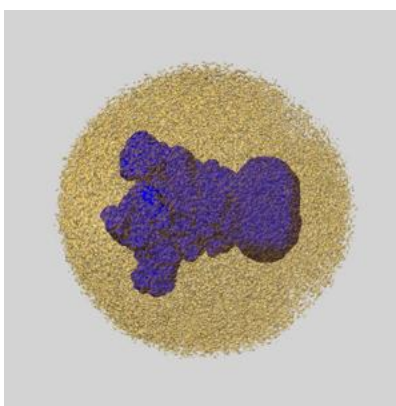
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

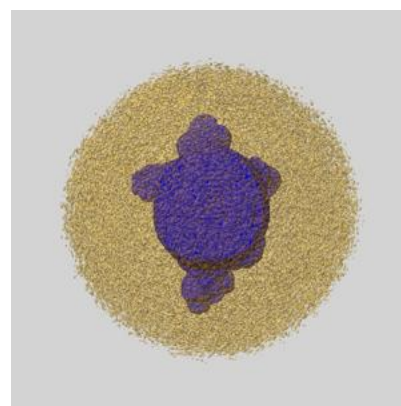
### 6.6.1 emd\_38451\_msk\_1.map [i](#)



X



Y

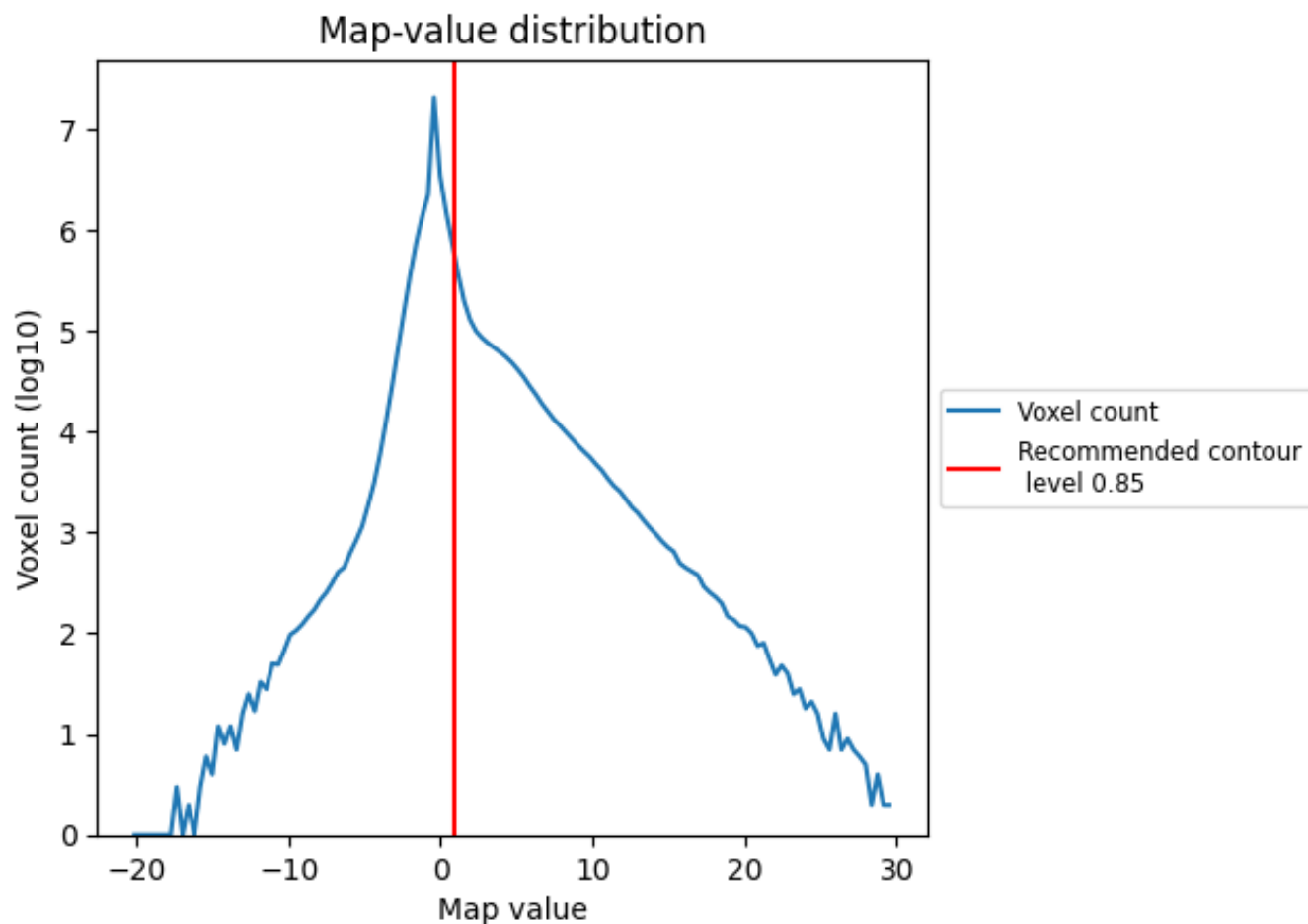


Z

## 7 Map analysis [i](#)

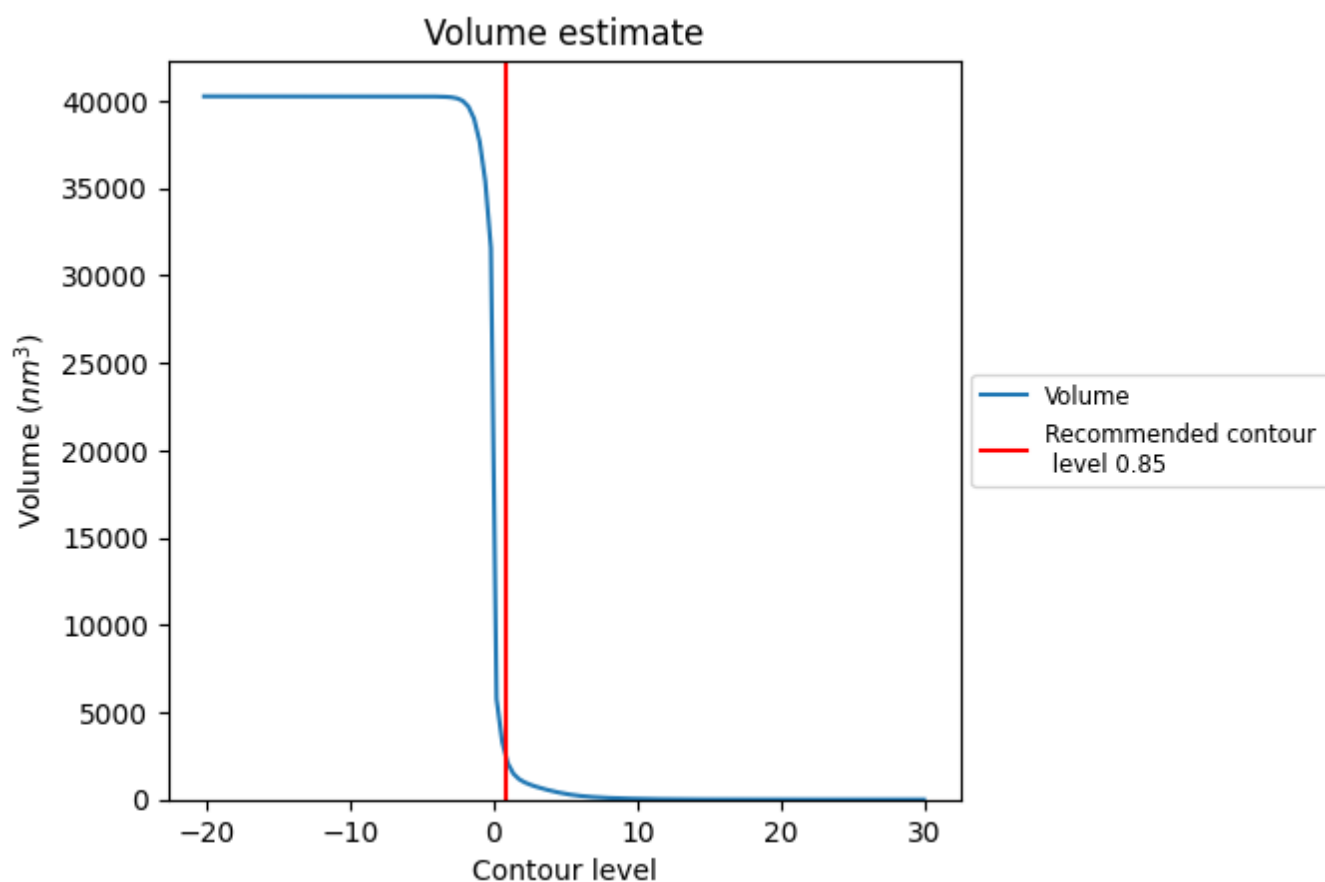
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

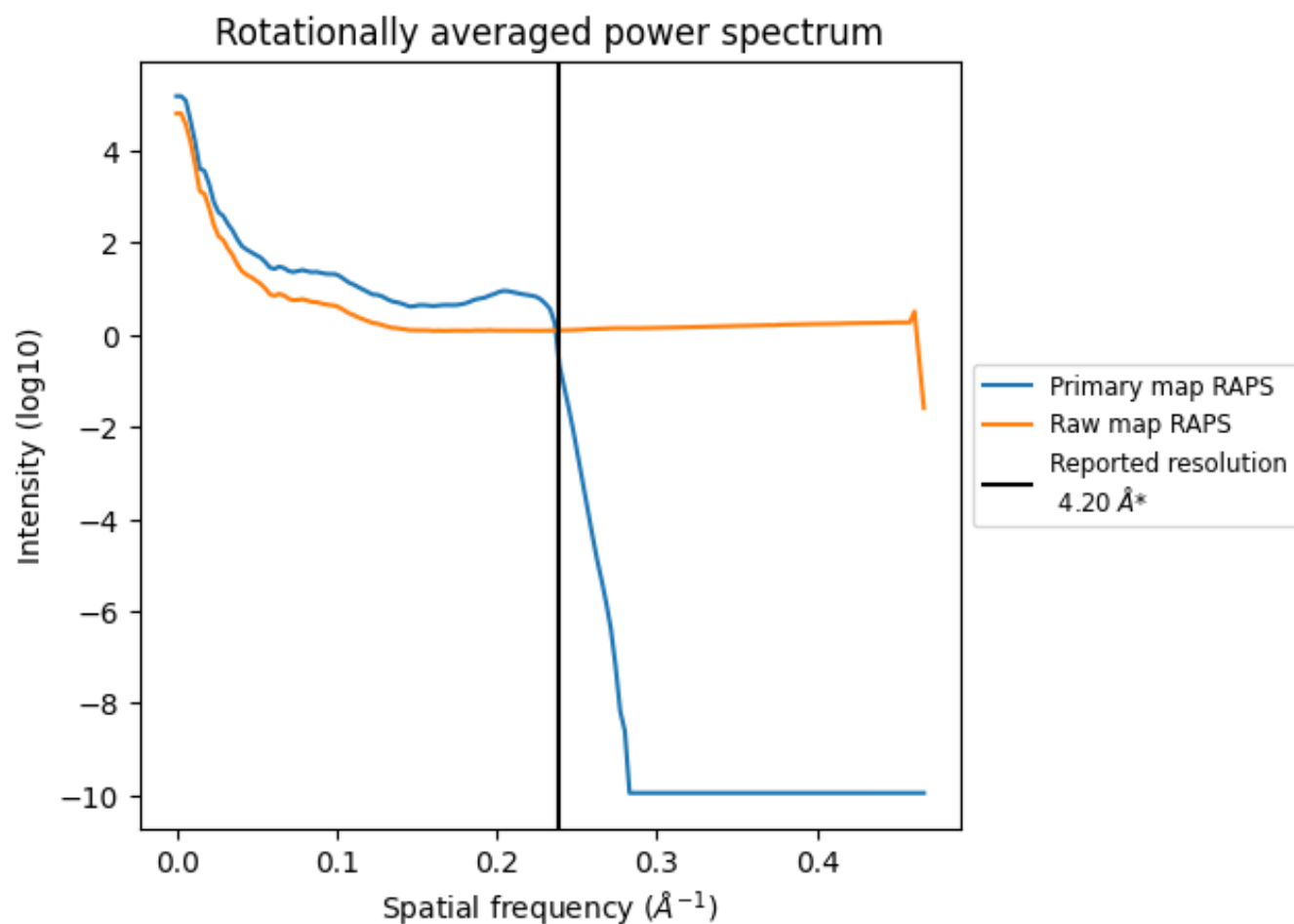
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2547  $\text{nm}^3$ ; this corresponds to an approximate mass of 2300 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



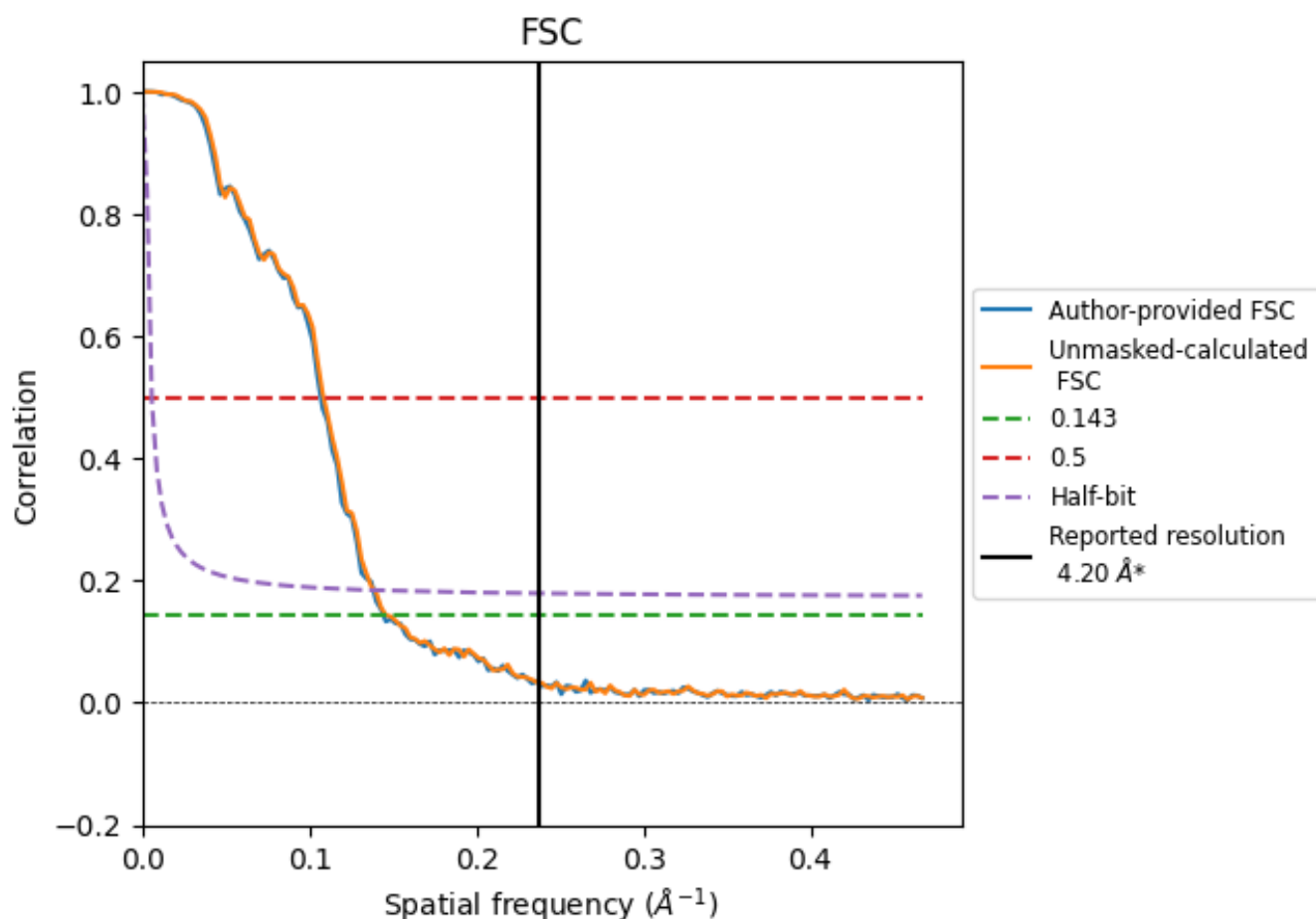
\*Reported resolution corresponds to spatial frequency of 0.238  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.20                               | -    | -        |
| Author-provided FSC curve | 6.93                               | 9.35 | 7.23     |
| Unmasked-calculated*      | 6.85                               | 9.22 | 7.19     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.93 differs from the reported value 4.2 by more than 10 %

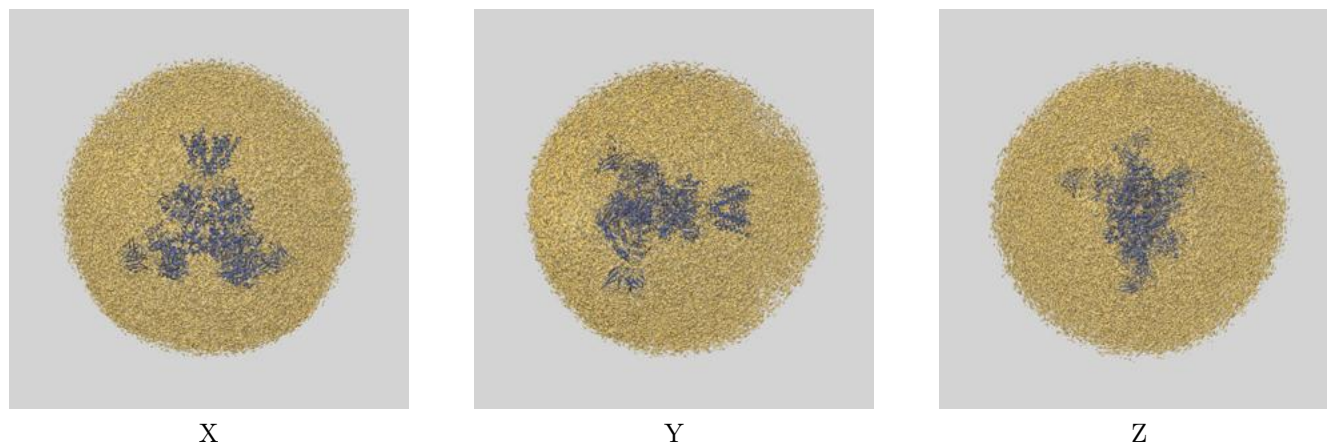
The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.85 differs from the reported value 4.2 by more than 10 %



## 9 Map-model fit [i](#)

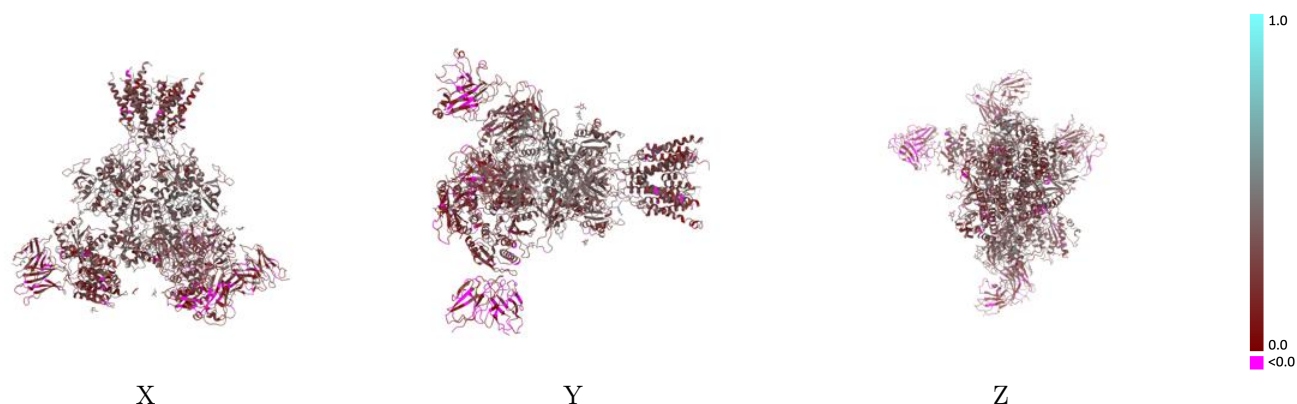
This section contains information regarding the fit between EMDB map EMD-38451 and PDB model 8XLK. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



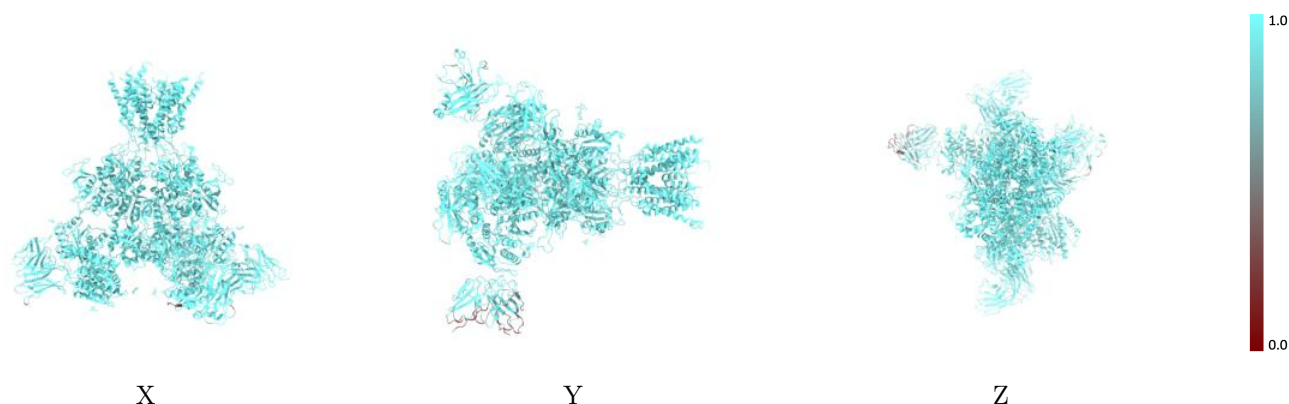
The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



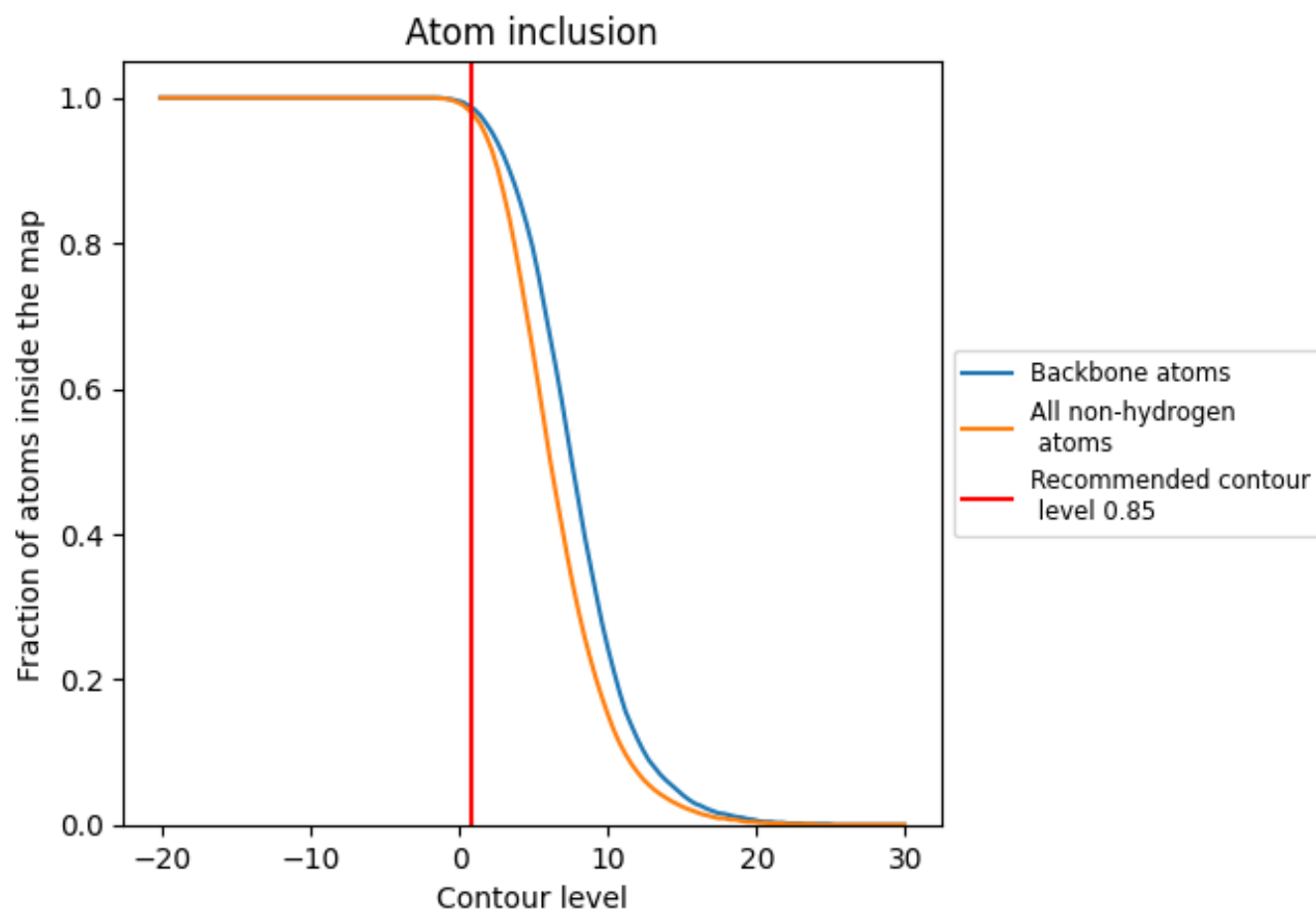
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9790 | <div></div> 0.2780 |
| A     | <div></div> 0.9950 | <div></div> 0.3110 |
| B     | <div></div> 0.9930 | <div></div> 0.3300 |
| C     | <div></div> 0.9930 | <div></div> 0.3080 |
| D     | <div></div> 0.9920 | <div></div> 0.2890 |
| E     | <div></div> 0.9760 | <div></div> 0.1930 |
| F     | <div></div> 0.9990 | <div></div> 0.1970 |
| G     | <div></div> 0.9530 | <div></div> 0.2290 |
| H     | <div></div> 0.9860 | <div></div> 0.2520 |
| I     | <div></div> 0.9880 | <div></div> 0.1660 |
| J     | <div></div> 0.9980 | <div></div> 0.2190 |
| K     | <div></div> 0.7550 | <div></div> 0.0500 |
| L     | <div></div> 0.7600 | <div></div> 0.0320 |
| M     | <div></div> 1.0000 | <div></div> 0.3810 |
| N     | <div></div> 0.9290 | <div></div> 0.3400 |
| O     | <div></div> 1.0000 | <div></div> 0.3680 |

