



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:11 PM UTC

PDB ID : 7V5M / pdb\_00007v5m  
EMDB ID : EMD-31727  
Title : 20S+monoUb-CyclinB1-NT (S2)  
Authors : Xu, C.; Cong, Y.  
Deposited on : 2021-08-17  
Resolution : 3.88 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  
MolProbity : 4-5-2 with Phenix2.0  
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

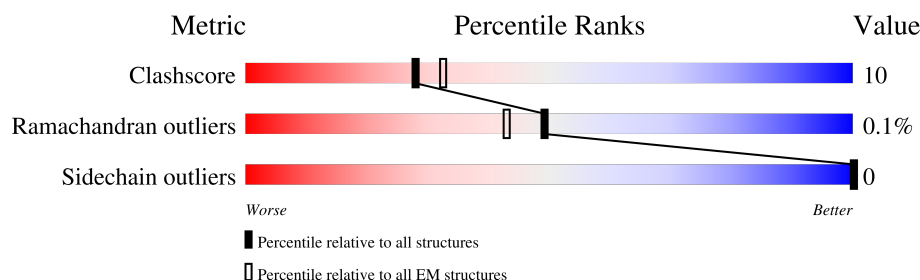
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.88 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |
| Sidechain outliers    | 223484                      | 23102                       |

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     | 246    | <div> <div>98%</div> <div>80% 17% .</div> </div>  |
| 1   | O     | 246    | <div> <div>94%</div> <div>82% 15% .</div> </div>  |
| 2   | B     | 234    | <div> <div>98%</div> <div>79% 19% .</div> </div>  |
| 2   | P     | 234    | <div> <div>97%</div> <div>78% 20% .</div> </div>  |
| 3   | C     | 261    | <div> <div>95%</div> <div>78% 16% 5%</div> </div> |
| 3   | Q     | 261    | <div> <div>91%</div> <div>78% 16% 5%</div> </div> |
| 4   | D     | 248    | <div> <div>94%</div> <div>77% 16% 6%</div> </div> |
| 4   | R     | 248    | <div> <div>79%</div> <div>77% 16% 6%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 241    |                  |
| 5   | S     | 241    |                  |
| 6   | F     | 263    |                  |
| 6   | T     | 263    |                  |
| 7   | G     | 255    |                  |
| 7   | U     | 255    |                  |
| 8   | H     | 205    |                  |
| 8   | V     | 205    |                  |
| 9   | I     | 234    |                  |
| 9   | W     | 234    |                  |
| 10  | J     | 205    |                  |
| 10  | X     | 205    |                  |
| 11  | K     | 201    |                  |
| 11  | Y     | 201    |                  |
| 12  | L     | 204    |                  |
| 12  | Z     | 204    |                  |
| 13  | M     | 213    |                  |
| 13  | a     | 213    |                  |
| 14  | N     | 219    |                  |
| 14  | b     | 219    |                  |

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 45340 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 Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1734  | 1104 | 304 | 314 | 12 |         |       |
| 1   | O     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1734  | 1104 | 304 | 314 | 12 |         |       |

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1662  | 1080 | 288 | 288 | 6 |         |       |
| 2   | P     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1662  | 1080 | 288 | 288 | 6 |         |       |

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 247      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1786  | 1143 | 320 | 313 | 10 |         |       |
| 3   | Q     | 247      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1786  | 1143 | 320 | 313 | 10 |         |       |

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | D     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1633  | 1038 | 306 | 284 | 5 |         |       |
| 4   | R     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1633  | 1038 | 306 | 284 | 5 |         |       |

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 233      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1659  | 1056 | 287 | 305 | 11 |         |       |
| 5   | S     | 233      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1659  | 1056 | 287 | 305 | 11 |         |       |

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | F     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1087 | 315 | 293 | 9 |         |       |
| 6   | T     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1087 | 315 | 293 | 9 |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | G     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1760  | 1131 | 308 | 311 | 10 |         |       |
| 7   | U     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1760  | 1131 | 308 | 311 | 10 |         |       |

- Molecule 8 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | H     | 202      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1465  | 926 | 256 | 271 | 12 |         |       |
| 8   | V     | 202      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1465  | 926 | 256 | 271 | 12 |         |       |

- Molecule 9 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | I     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1576  | 1003 | 272 | 292 | 9 |         |       |
| 9   | W     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1576  | 1003 | 272 | 292 | 9 |         |       |

- Molecule 10 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10  | J     | 204      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1534  | 987 | 262 | 267 | 18 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10  | X     | 204      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1534  | 987 | 262 | 267 | 18 |         |       |

- Molecule 11 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 973 | 259 | 266 | 8 |         |       |
| 11  | Y     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 973 | 259 | 266 | 8 |         |       |

- Molecule 12 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1500  | 954 | 270 | 267 | 9 |         |       |
| 12  | Z     | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1500  | 954 | 270 | 267 | 9 |         |       |

- Molecule 13 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | M     | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1583  | 1016 | 279 | 278 | 10 |         |       |
| 13  | a     | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1583  | 1016 | 279 | 278 | 10 |         |       |

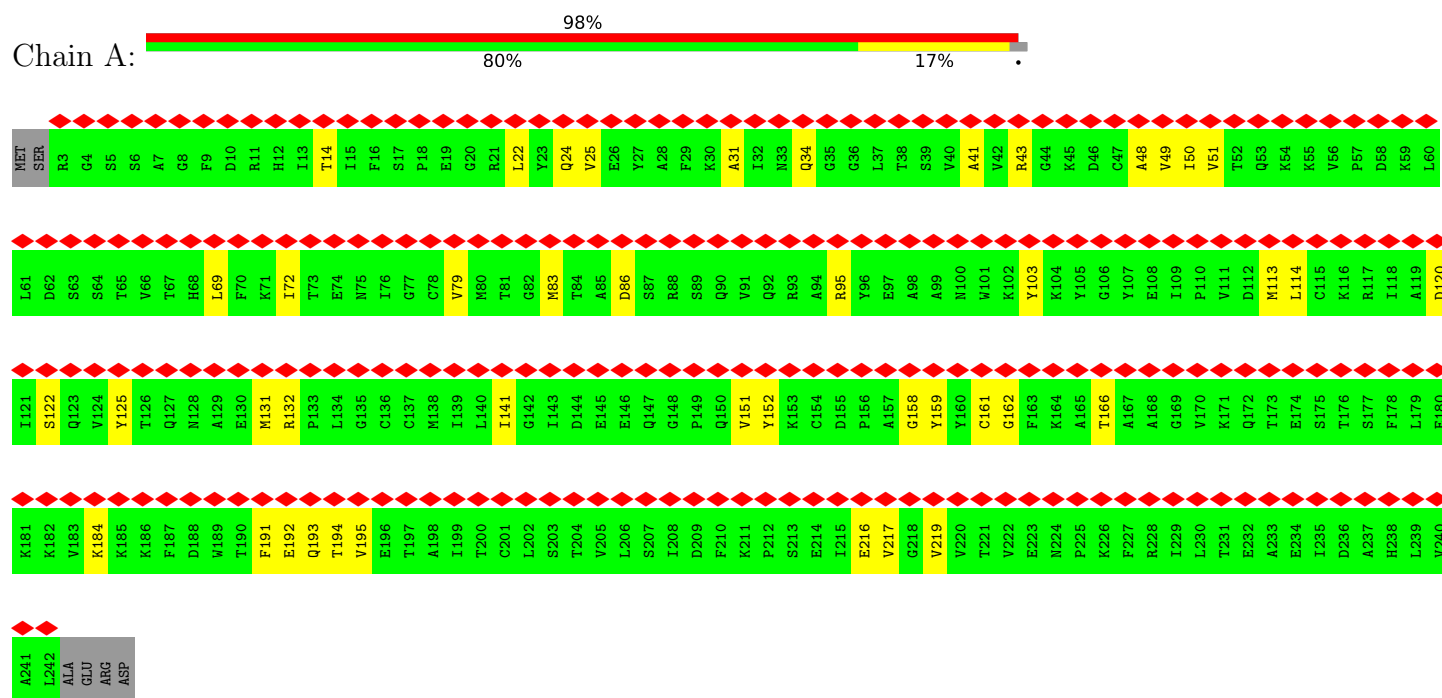
- Molecule 14 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14  | N     | 212      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1568  | 998 | 279 | 280 | 11 |         |       |
| 14  | b     | 212      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1568  | 998 | 279 | 280 | 11 |         |       |

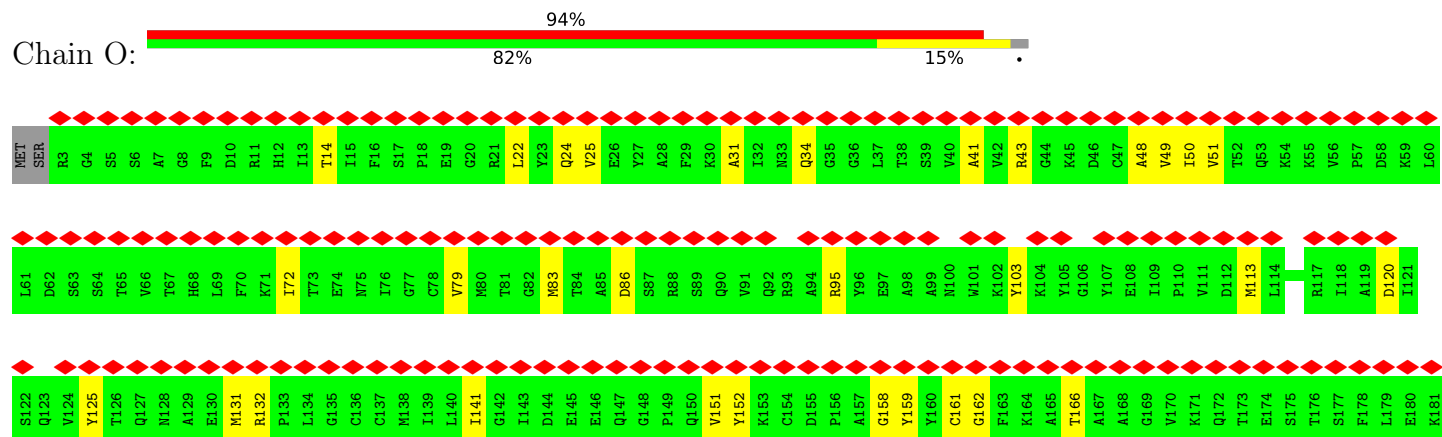
### 3 Residue-property plots

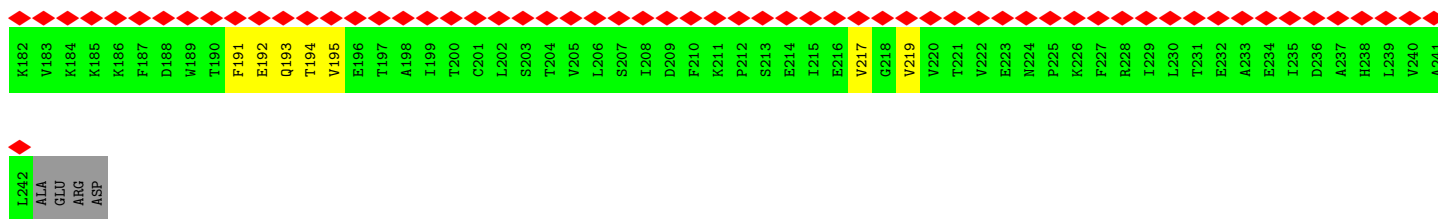
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Proteasome subunit alpha type-6

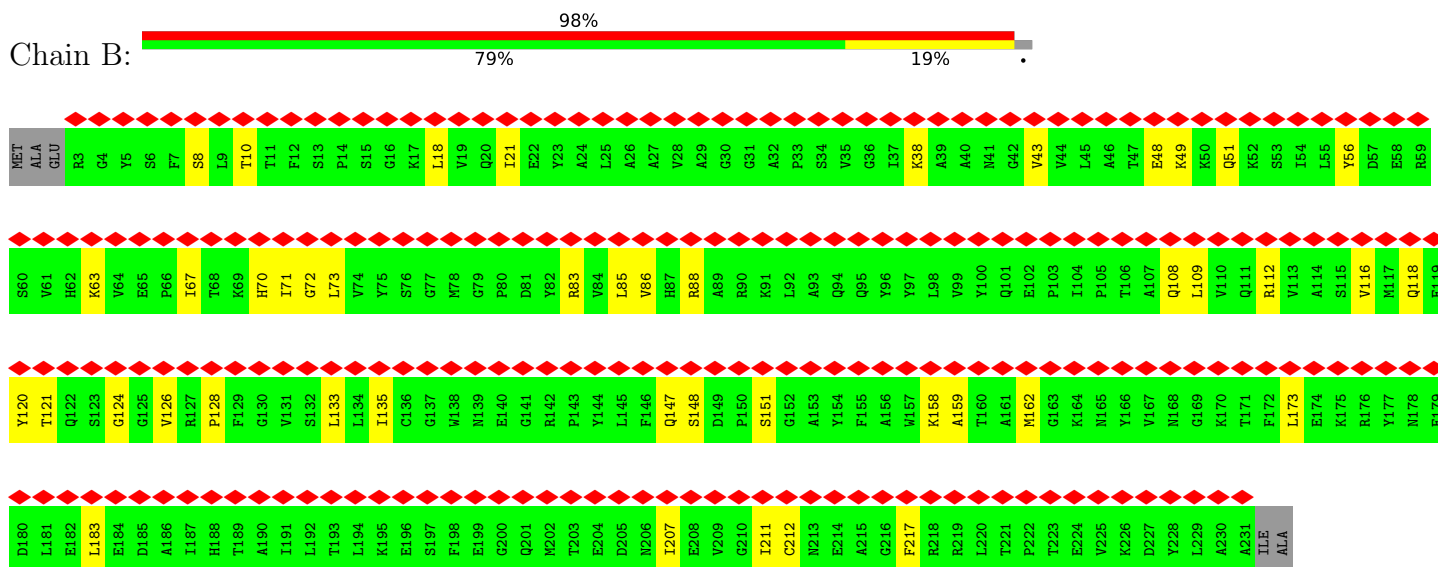


#### • Molecule 1: Proteasome subunit alpha type-6

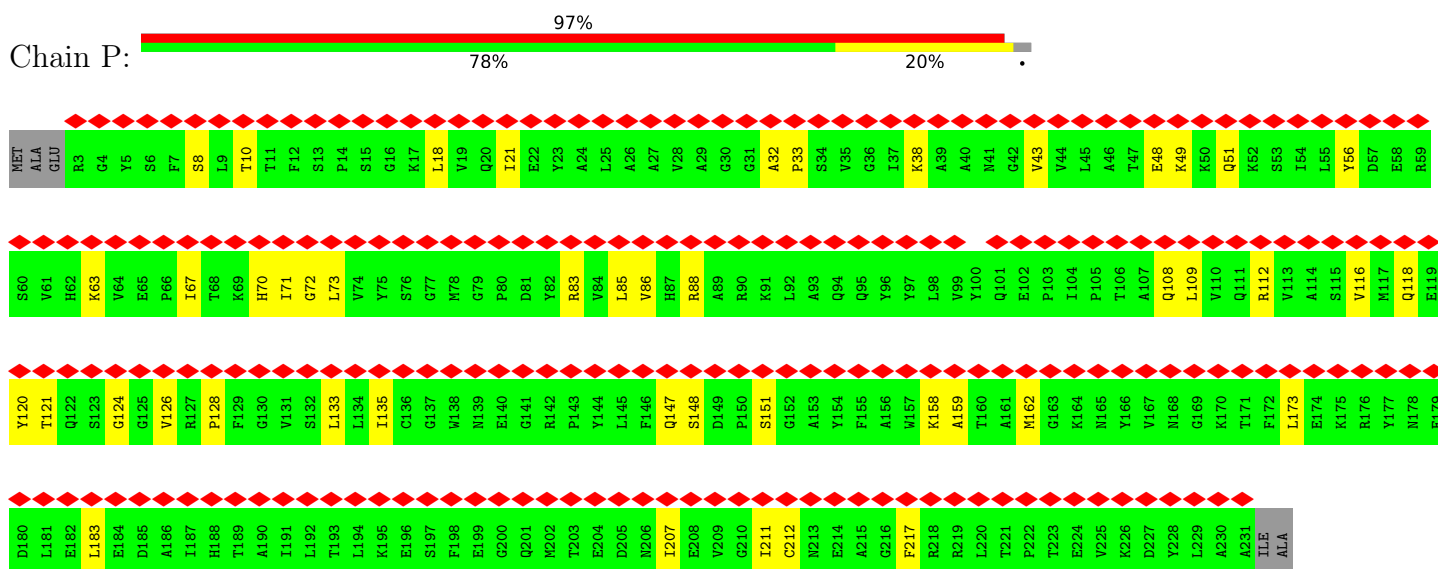




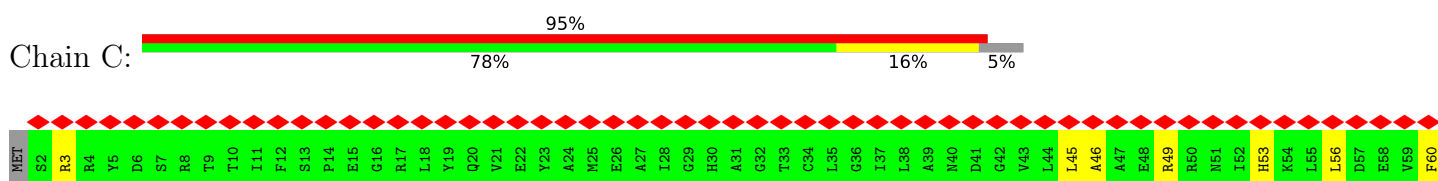
• Molecule 2: Proteasome subunit alpha type-2

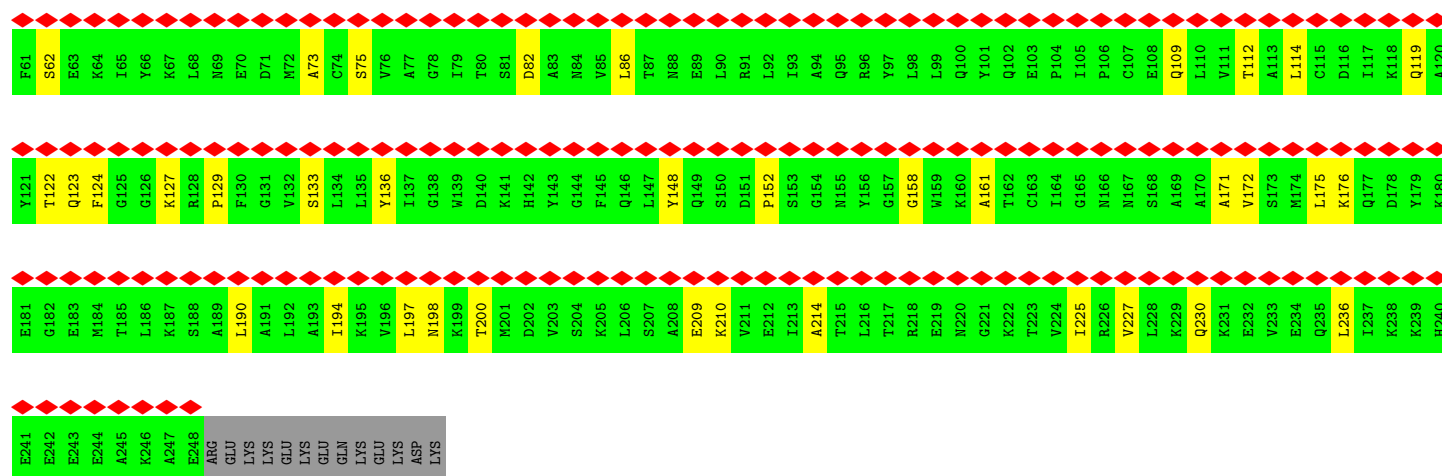


• Molecule 2: Proteasome subunit alpha type-2

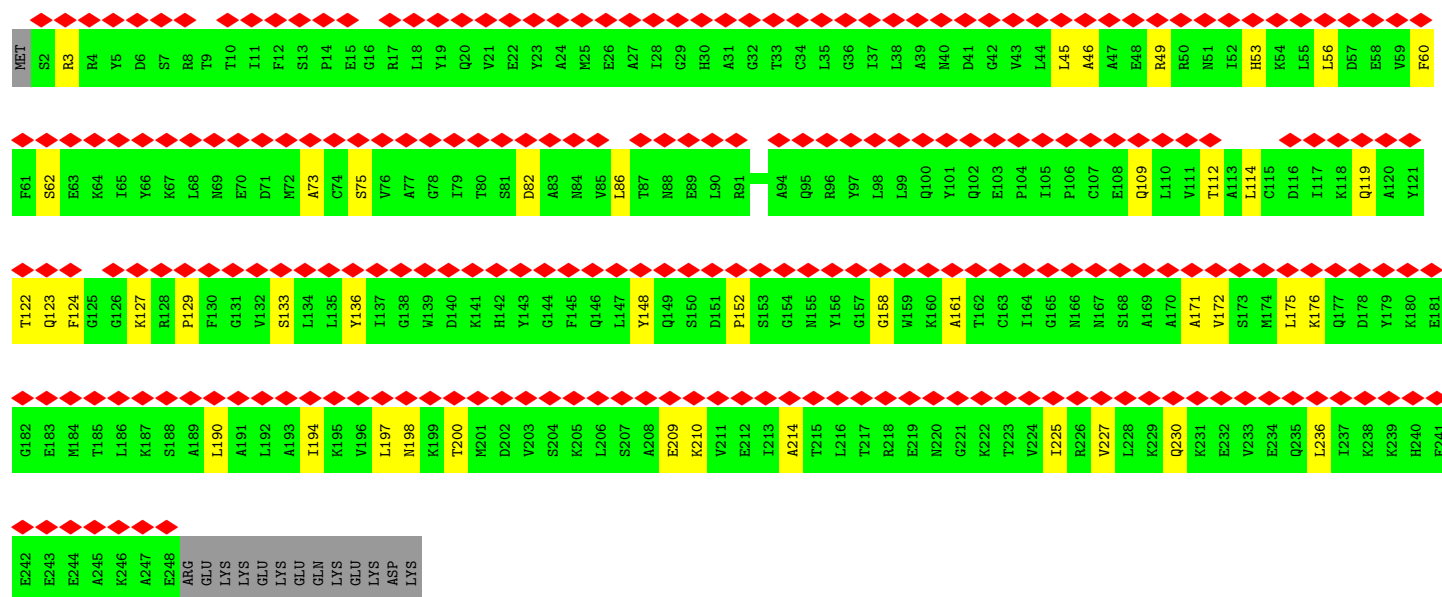
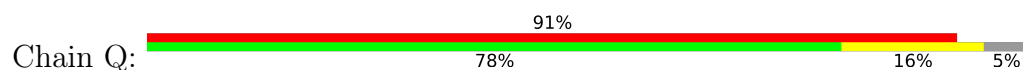


• Molecule 3: Proteasome subunit alpha type-4

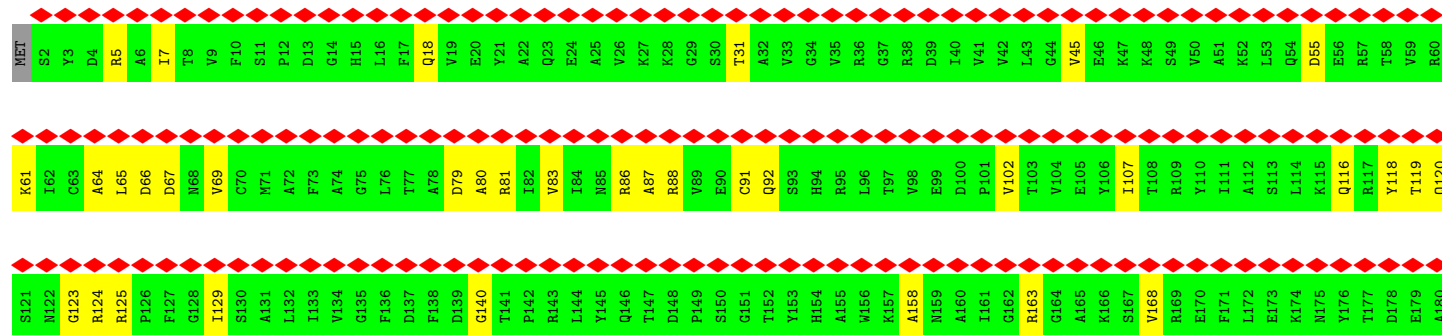
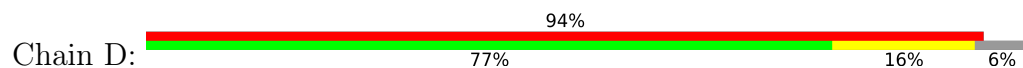


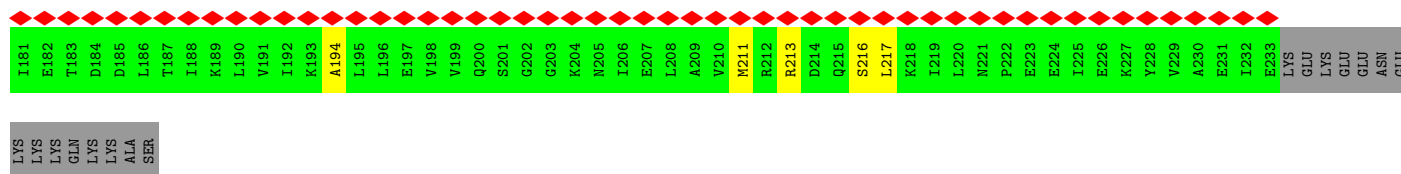


• Molecule 3: Proteasome subunit alpha type-4

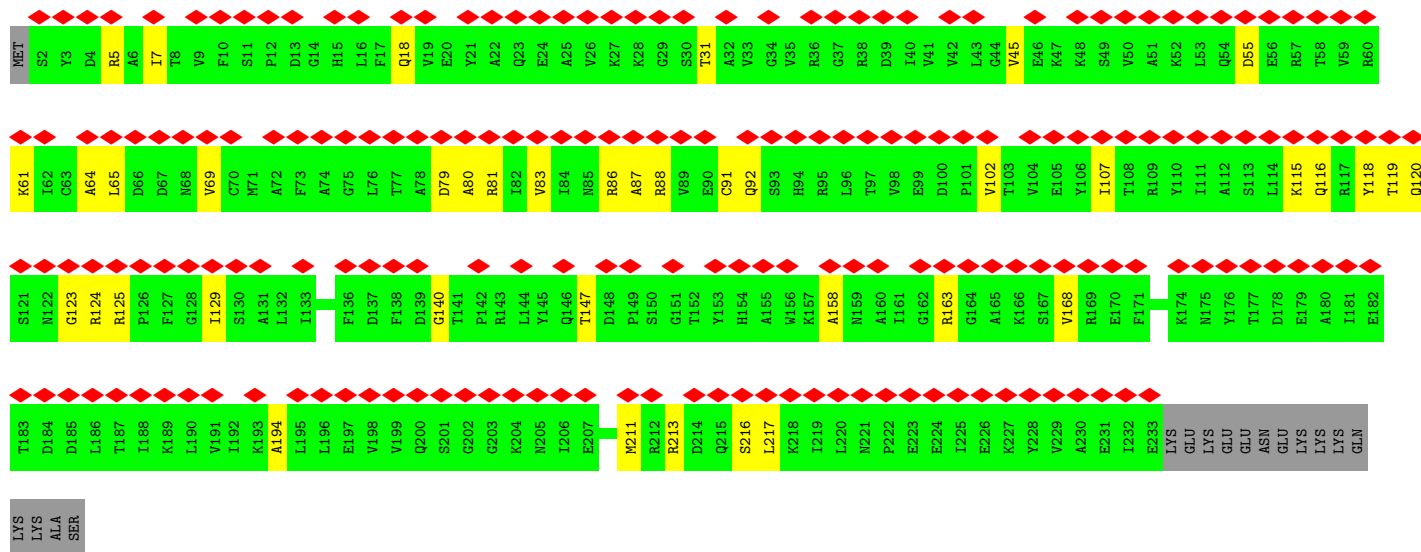
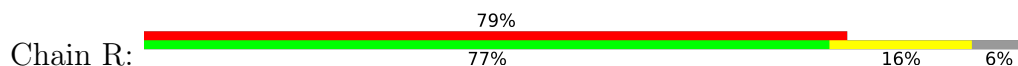


• Molecule 4: Proteasome subunit alpha type-7

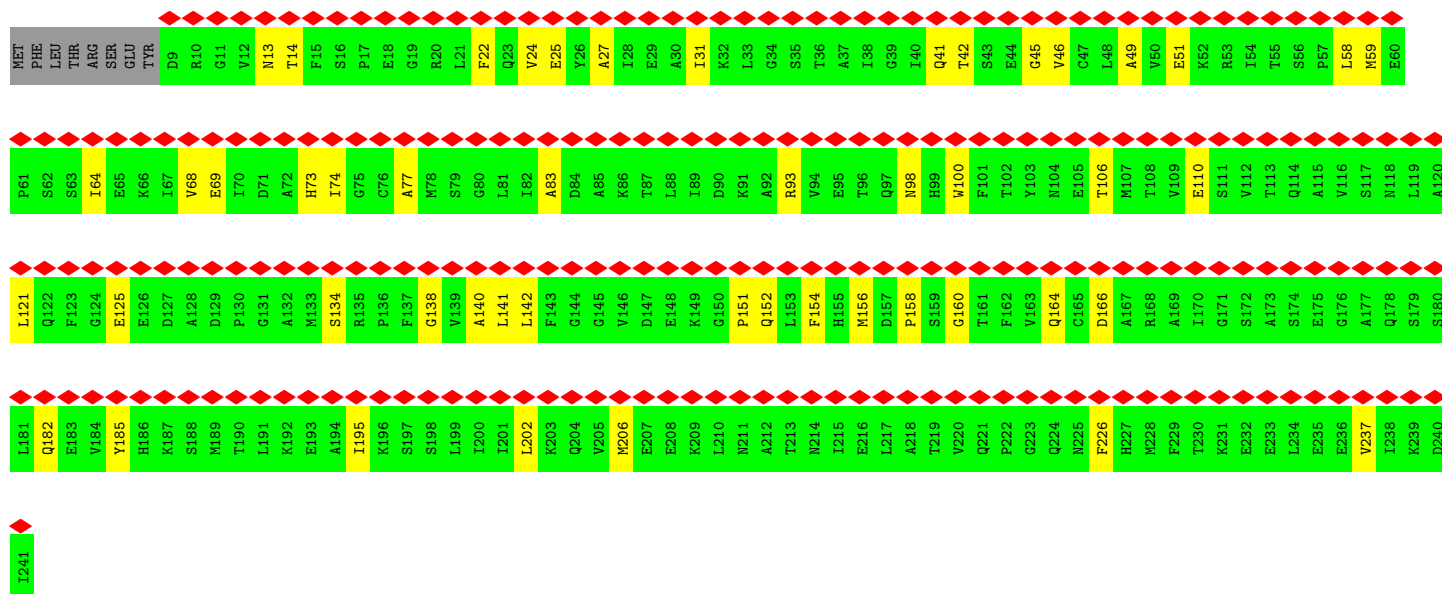
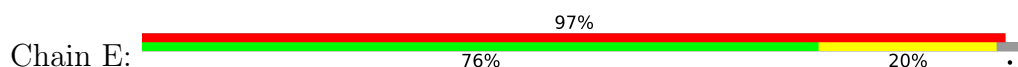




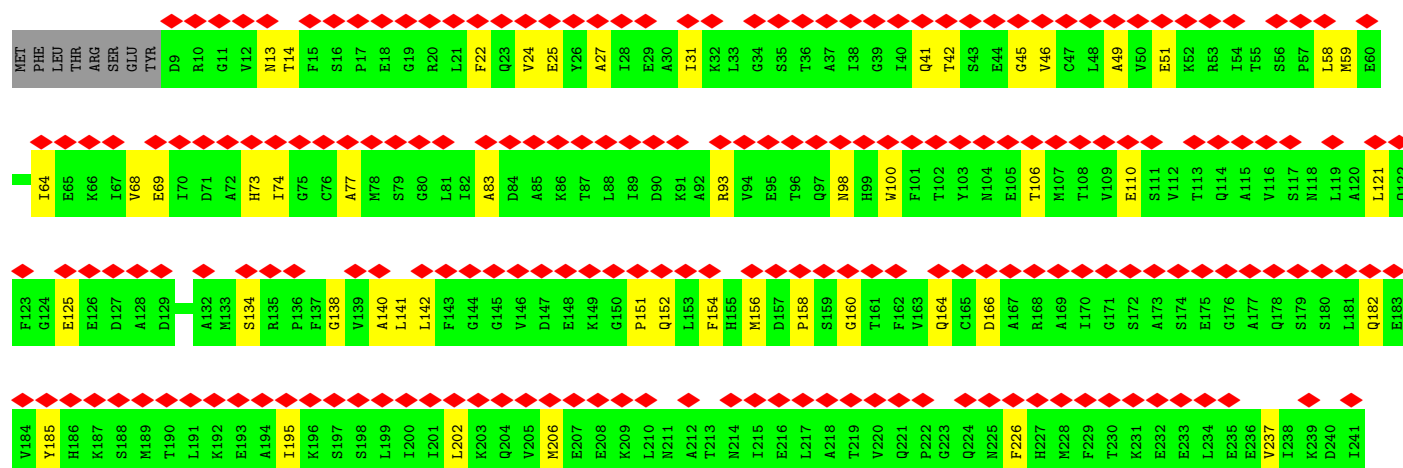
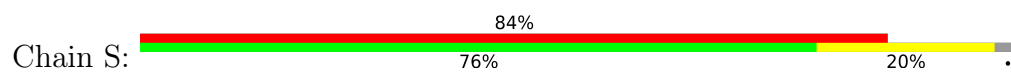
• Molecule 4: Proteasome subunit alpha type-7



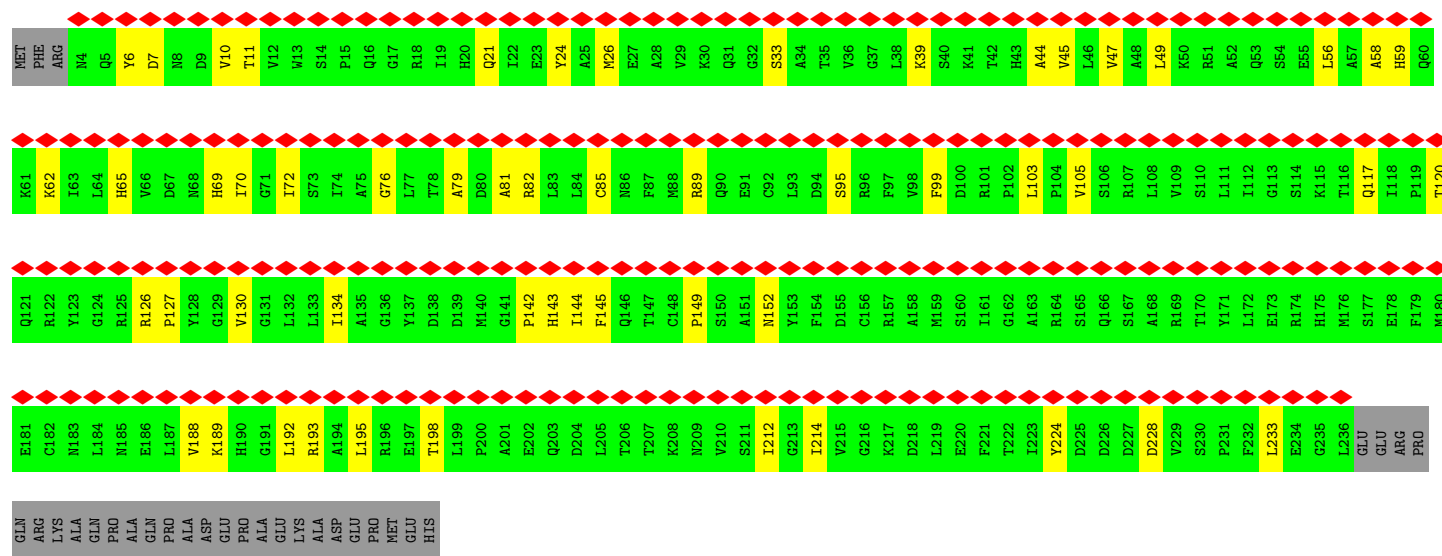
• Molecule 5: Proteasome subunit alpha type-5



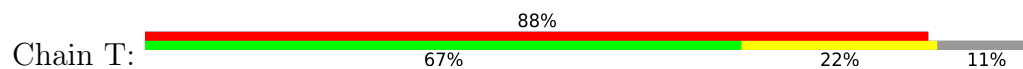
• Molecule 5: Proteasome subunit alpha type-5



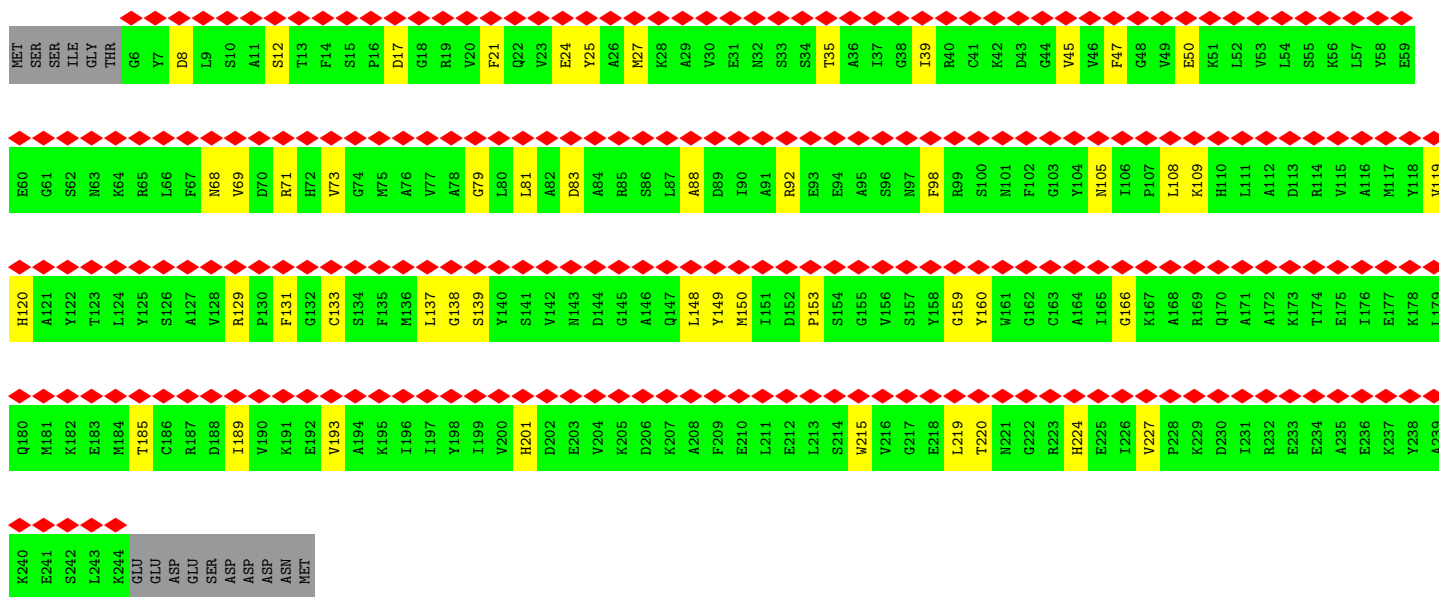
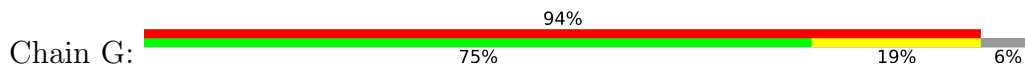
• Molecule 6: Proteasome subunit alpha type-1



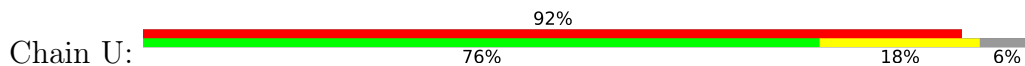
• Molecule 6: Proteasome subunit alpha type-1

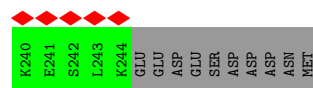


- Molecule 7: Proteasome subunit alpha type-3

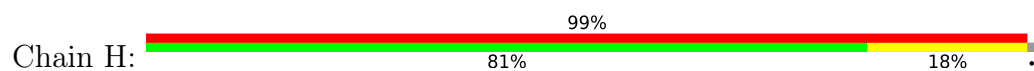


- Molecule 7: Proteasome subunit alpha type-3

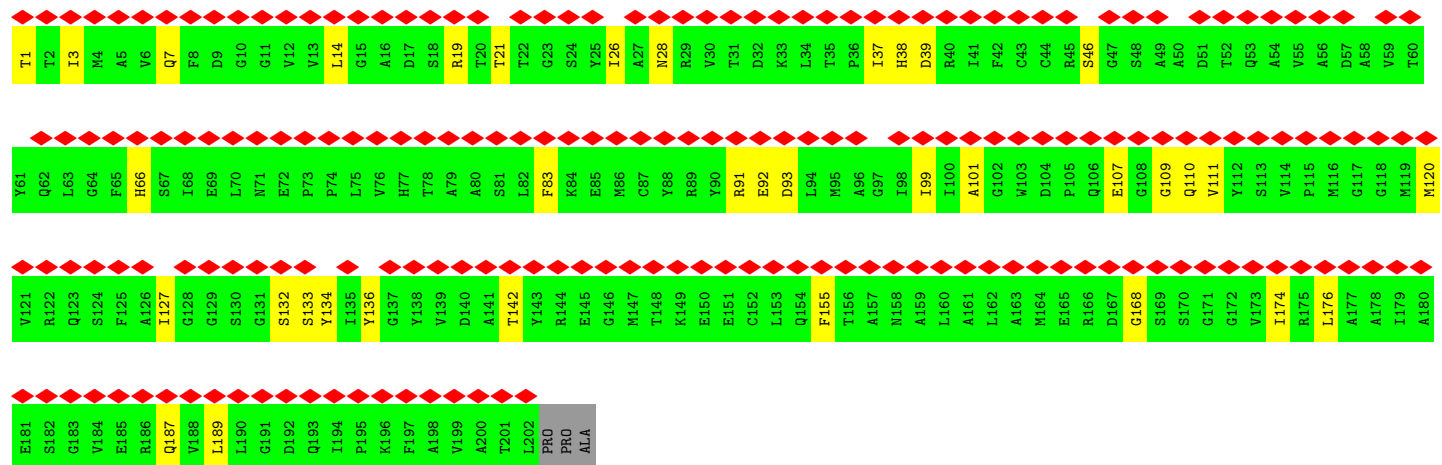
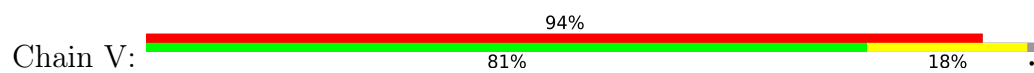




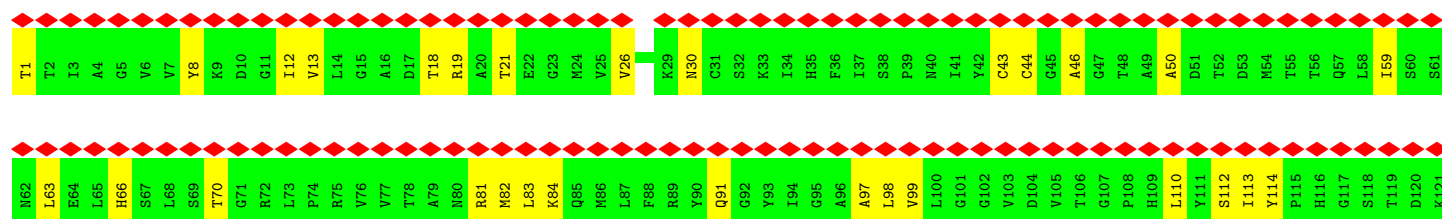
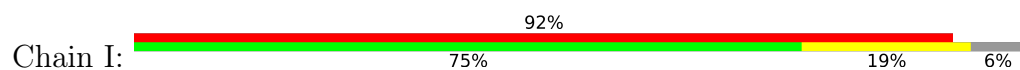
• Molecule 8: Proteasome subunit beta type-6

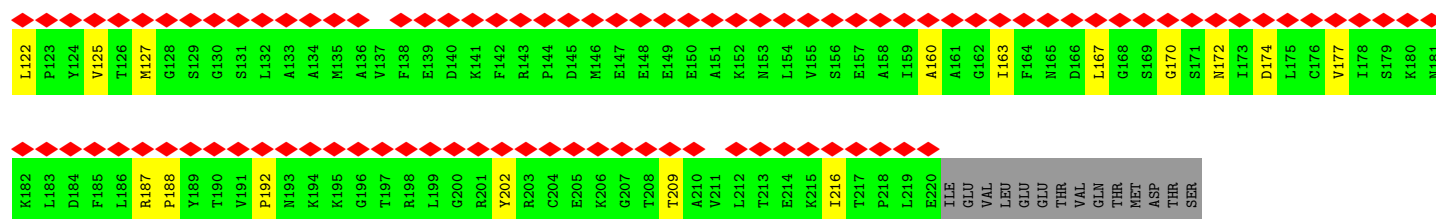


• Molecule 8: Proteasome subunit beta type-6



• Molecule 9: Proteasome subunit beta type-7



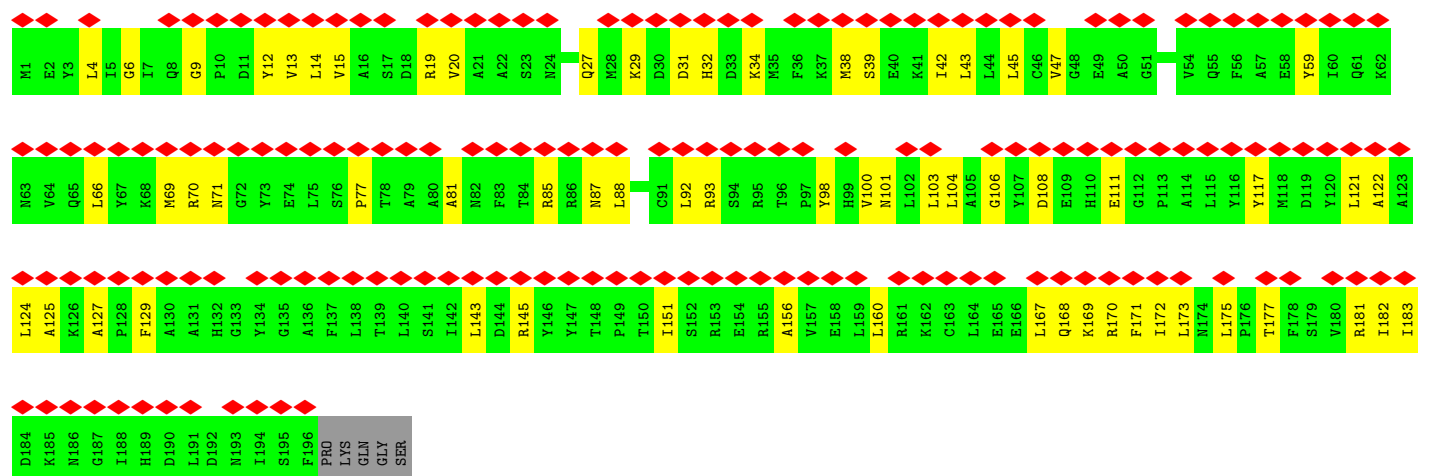




• Molecule 11: Proteasome subunit beta type-2



• Molecule 11: Proteasome subunit beta type-2



Chain L:

98%

71%

27%

•

T1 T2 T3 L4 A5 F6 K7 F8 R9 H10 G11 V12 I13 V14 A15 A16 A17 D17 S18 R19 A20 T21 A22 G23 A24 Y25 L26 A27 S28 Q29 Q30 T30 V31 K32 K33 V34 I35 E36 I37 N38 P39 Y40 L41 L42 G43 T44 M45 A46 G47 G48 A49 A50 C51 D52 C53 S53 F54 W55 E56 R57 L58 L59 A60

R61 R62 R63 R64 R65 R66 R67 R68 R69 R70 R71 K71 E72 R73 I74 R75 V76 V77 A78 R79 S80 R81 L82 L83 A84 R85 R86 R87 Y88 Q89 Y90 K91 G92 M93 G94 L95 S96 M97 G98 T99 M100 L101 C102 G103 W104 D105 K106 R107 G108 P109 G110 L111 Y112 Y113 V114 D115 S116 E117 G118 M119 R120

I121 I122 A124 T125 F126 S127 V128 S130 G131 S132 V133 Y134 A135 Y136 G137 V138 M139 D140 R141 G142 Y143 I144 Y145 D146 L147 E148 V149 E150 Q151 A152 Y153 D154 L155 A156 R157 R158 A159 I160 Y161 G162 A163 T164 Y165 R166 D167 A168 Y169 S170 G171 G172 A173 V174 M175 L176 Y177 H178 V179 R180

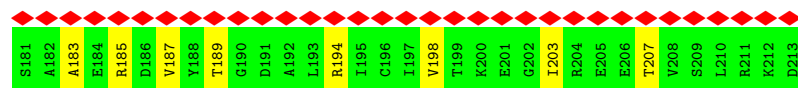
E181 D182 G183 W184 I185 R186 V187 S188 D189 N191 V192 A193 D194 L195 H196 E197 K198 Y199 S200 GLY SER THR PRO

Chain Z:

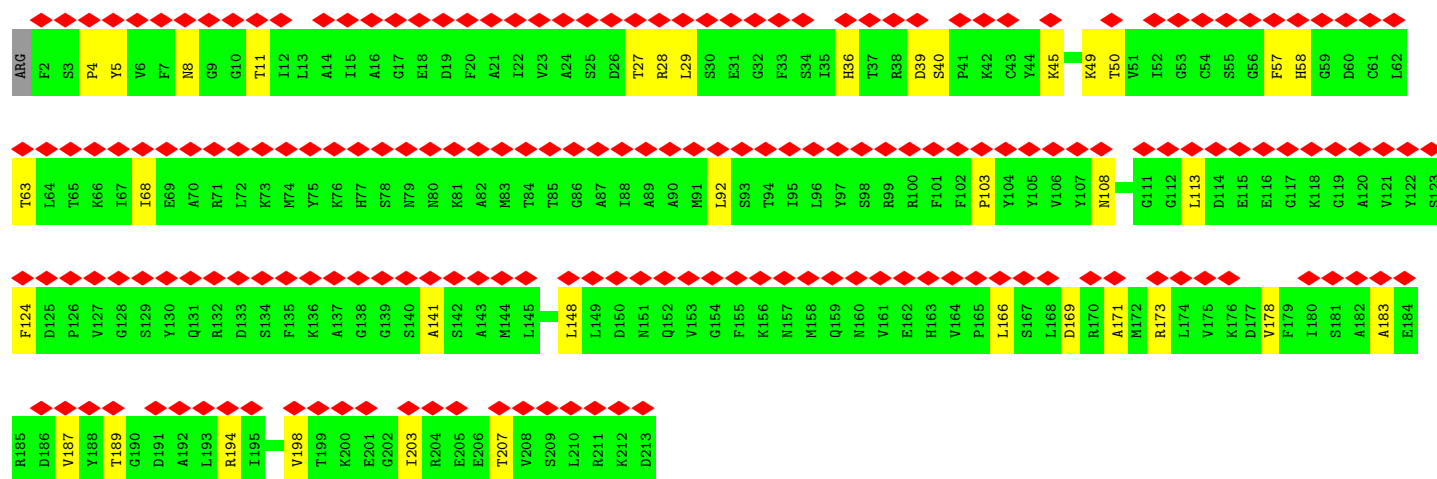
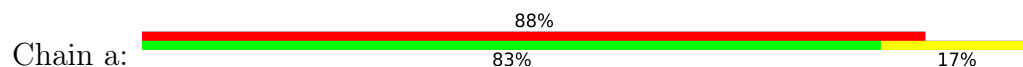
| Amino Acid | Percentage |
|------------|------------|
| T1         | 73%        |
| T2         | 73%        |
| T3         | 73%        |
| L4         | 73%        |
| A5         | 73%        |
| F6         | 73%        |
| K7         | 73%        |
| E8         | 73%        |
| R9         | 73%        |
| H10        | 73%        |
| G11        | 73%        |
| V12        | 73%        |
| I13        | 73%        |
| V14        | 73%        |
| A15        | 73%        |
| A16        | 73%        |
| D17        | 73%        |
| S18        | 73%        |
| R19        | 73%        |
| A20        | 73%        |
| T21        | 73%        |
| A22        | 73%        |
| Q23        | 73%        |
| A24        | 73%        |
| Y25        | 73%        |
| L26        | 73%        |
| A27        | 73%        |
| S28        | 73%        |
| Q29        | 73%        |
| T30        | 73%        |
| V31        | 73%        |
| K32        | 73%        |
| K33        | 73%        |
| V34        | 73%        |
| T35        | 73%        |
| E36        | 73%        |
| T37        | 73%        |
| N38        | 73%        |
| P39        | 73%        |
| Y40        | 73%        |
| L41        | 73%        |
| L42        | 73%        |
| G43        | 73%        |
| T44        | 73%        |
| M45        | 73%        |
| A46        | 73%        |
| G47        | 73%        |
| G48        | 73%        |
| A49        | 73%        |
| A50        | 73%        |
| D51        | 73%        |
| C52        | 73%        |
| S53        | 73%        |
| F54        | 73%        |
| W55        | 73%        |
| E56        | 73%        |
| R57        | 73%        |
| L58        | 73%        |
| L59        | 73%        |
| A60        | 73%        |

Chain M:

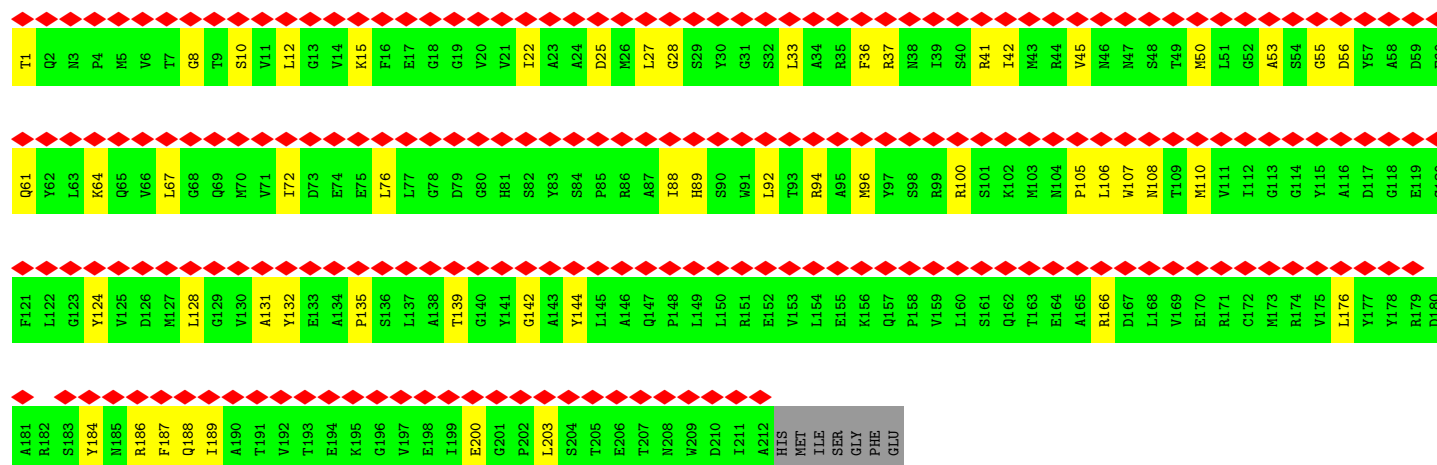
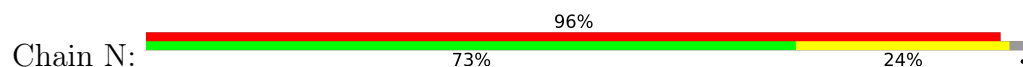
| ARG  | F2 | S3 | P4 | Y5 | V6 | F7 | N8 | G9 | G10 | T11 | I12 | L13 | A14 | I15 | A16 | G17 | E18 | D19 | F20 | A21 | T22 | T27 | R28 | L29 | S30 | E31 | C32 | F33 | S34 | I35 | H36 | T37 | R38 | D39 | S40 | P41 | K42 | C43 | Y44 | K45 | L46 | T47 | D48 | K49 | T50 | U51 | L52 | G53 | C54 | S55 | G56 | F57 | H58 | G59 | D60 |
|------|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C61  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L62  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| T63  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L64  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| T65  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| K66  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L67  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| T68  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| E69  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| A70  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| R71  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L72  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| K73  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| M74  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Y75  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| K76  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| H77  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| S78  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| M79  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| N80  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| R81  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| A82  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| M83  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| T84  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| T85  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| G86  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| A87  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| T88  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| A89  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| A90  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| N91  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L92  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| S93  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| T94  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| I95  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L96  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Y97  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| S98  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| R99  |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| R100 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| F101 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| F102 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| P103 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Y104 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Y105 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| V106 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Y107 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| N108 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| I109 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| I110 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| G111 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| G112 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L113 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| D114 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| E115 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| X116 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| G117 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| K118 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| G119 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| A120 |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |



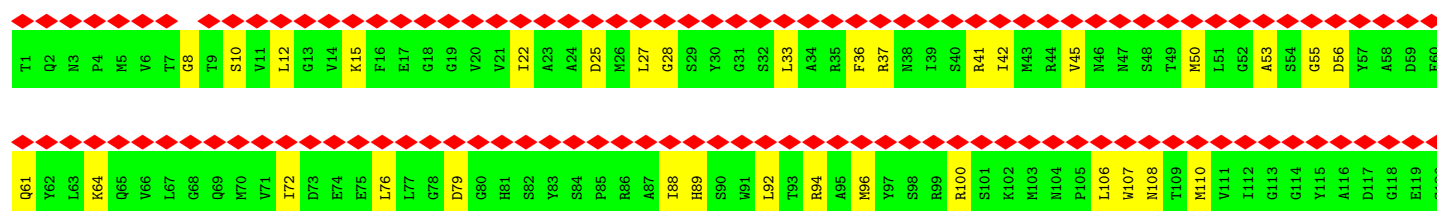
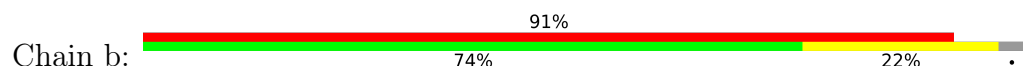
• Molecule 13: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit beta type-4



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A181 | A182 | A183 | Y184 | M185 | R186 | F187 | Q188 | I189 | A190 | T191 | V192 | T193 | E194 | K195 | G196 | V197 | E198 | I199 | E200 | G201 | P202 | L203 | N208 | W209 | D210 | I211 | A212 | HIS | MET | ILE | SER | GLY | PHE | GLU | F121 | L122 | G123 | Y124 | V125 | D126 | M127 | L128 | G129 | A130 | A131 | Y132 | E133 | A134 | P135 | S136 | L137 | A138 | T139 | G140 | Y141 | G142 | A143 | Y144 | L145 | A146 | Q147 | P148 | L149 | L150 | R151 | E152 | V153 | L154 | E155 | K156 | Q157 | P158 | V159 | L160 | S161 | Q162 | T163 | E164 | A165 | R166 | D167 | L168 | V169 | E170 | R171 | C172 | M173 | R174 | V175 | L176 | Y177 | Y178 | R179 | D180 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 179590                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 38                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.137                                   | Depositor |
| Minimum map value                    | -0.074                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.027                                   | Depositor |
| Map size (Å)                         | 219.648, 219.648, 219.648               | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.858, 0.858, 0.858                     | Depositor |

## 5 Model quality [i](#)

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

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     | 0.15         | 0/1763  | 0.42        | 0/2393  |
| 1   | O     | 0.14         | 0/1763  | 0.41        | 0/2393  |
| 2   | B     | 0.12         | 0/1701  | 0.37        | 0/2318  |
| 2   | P     | 0.12         | 0/1701  | 0.37        | 0/2318  |
| 3   | C     | 0.12         | 0/1815  | 0.38        | 0/2466  |
| 3   | Q     | 0.12         | 0/1815  | 0.38        | 0/2466  |
| 4   | D     | 0.14         | 0/1657  | 0.43        | 0/2261  |
| 4   | R     | 0.14         | 0/1657  | 0.43        | 0/2261  |
| 5   | E     | 0.12         | 0/1685  | 0.39        | 0/2290  |
| 5   | S     | 0.12         | 0/1685  | 0.39        | 0/2290  |
| 6   | F     | 0.13         | 0/1738  | 0.39        | 0/2364  |
| 6   | T     | 0.13         | 0/1738  | 0.39        | 0/2364  |
| 7   | G     | 0.11         | 0/1795  | 0.38        | 0/2434  |
| 7   | U     | 0.11         | 0/1795  | 0.38        | 0/2434  |
| 8   | H     | 0.12         | 0/1491  | 0.36        | 0/2021  |
| 8   | V     | 0.12         | 0/1491  | 0.36        | 0/2021  |
| 9   | I     | 0.13         | 0/1603  | 0.41        | 0/2180  |
| 9   | W     | 0.13         | 0/1603  | 0.41        | 0/2180  |
| 10  | J     | 0.14         | 0/1563  | 0.43        | 0/2113  |
| 10  | X     | 0.14         | 0/1563  | 0.43        | 0/2113  |
| 11  | K     | 0.14         | 0/1538  | 0.48        | 0/2088  |
| 11  | Y     | 0.14         | 0/1538  | 0.47        | 0/2088  |
| 12  | L     | 0.13         | 0/1531  | 0.42        | 0/2076  |
| 12  | Z     | 0.13         | 0/1531  | 0.42        | 0/2076  |
| 13  | M     | 0.13         | 0/1613  | 0.40        | 0/2178  |
| 13  | a     | 0.13         | 0/1613  | 0.40        | 0/2178  |
| 14  | N     | 0.13         | 0/1598  | 0.42        | 0/2170  |
| 14  | b     | 0.13         | 0/1598  | 0.42        | 0/2170  |
| All | All   | 0.13         | 0/46182 | 0.41        | 0/62704 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1734  | 0        | 1652     | 27      | 0            |
| 1   | O     | 1734  | 0        | 1652     | 24      | 0            |
| 2   | B     | 1662  | 0        | 1590     | 30      | 0            |
| 2   | P     | 1662  | 0        | 1590     | 31      | 0            |
| 3   | C     | 1786  | 0        | 1717     | 26      | 0            |
| 3   | Q     | 1786  | 0        | 1717     | 26      | 0            |
| 4   | D     | 1633  | 0        | 1518     | 31      | 0            |
| 4   | R     | 1633  | 0        | 1518     | 31      | 0            |
| 5   | E     | 1659  | 0        | 1589     | 37      | 0            |
| 5   | S     | 1659  | 0        | 1589     | 36      | 0            |
| 6   | F     | 1704  | 0        | 1638     | 43      | 0            |
| 6   | T     | 1704  | 0        | 1638     | 46      | 0            |
| 7   | G     | 1760  | 0        | 1680     | 33      | 0            |
| 7   | U     | 1760  | 0        | 1680     | 30      | 0            |
| 8   | H     | 1465  | 0        | 1419     | 23      | 0            |
| 8   | V     | 1465  | 0        | 1419     | 23      | 0            |
| 9   | I     | 1576  | 0        | 1558     | 38      | 0            |
| 9   | W     | 1576  | 0        | 1558     | 43      | 0            |
| 10  | J     | 1534  | 0        | 1539     | 43      | 0            |
| 10  | X     | 1534  | 0        | 1539     | 41      | 0            |
| 11  | K     | 1506  | 0        | 1475     | 55      | 0            |
| 11  | Y     | 1506  | 0        | 1475     | 59      | 0            |
| 12  | L     | 1500  | 0        | 1441     | 41      | 0            |
| 12  | Z     | 1500  | 0        | 1441     | 39      | 0            |
| 13  | M     | 1583  | 0        | 1579     | 31      | 0            |
| 13  | a     | 1583  | 0        | 1579     | 28      | 0            |
| 14  | N     | 1568  | 0        | 1513     | 38      | 0            |
| 14  | b     | 1568  | 0        | 1513     | 36      | 0            |
| All | All   | 45340 | 0        | 43816    | 856     | 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 10.

All (856) 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) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:187:ARG:HB3  | 9:I:188:PRO:HD3  | 1.32                     | 1.11              |
| 9:W:187:ARG:HB3  | 9:W:188:PRO:HD3  | 1.32                     | 1.07              |
| 5:E:121:LEU:HD12 | 6:F:79:ALA:HB3   | 1.63                     | 0.80              |
| 5:S:121:LEU:HD12 | 6:T:79:ALA:HB3   | 1.63                     | 0.80              |
| 4:D:211:MET:HB2  | 4:D:217:LEU:HD12 | 1.66                     | 0.78              |
| 4:R:211:MET:HB2  | 4:R:217:LEU:HD12 | 1.65                     | 0.78              |
| 7:G:35:THR:HA    | 7:G:166:GLY:HA3  | 1.68                     | 0.75              |
| 12:Z:97:MET:HG2  | 12:Z:98:GLY:H    | 1.52                     | 0.75              |
| 7:U:35:THR:HA    | 7:U:166:GLY:HA3  | 1.68                     | 0.74              |
| 4:D:140:GLY:O    | 4:D:213:ARG:NH1  | 2.21                     | 0.73              |
| 12:L:97:MET:HG2  | 12:L:98:GLY:H    | 1.52                     | 0.73              |
| 9:W:187:ARG:HB3  | 9:W:188:PRO:CD   | 2.17                     | 0.73              |
| 12:L:97:MET:HB3  | 12:L:116:SER:HB3 | 1.72                     | 0.71              |
| 4:R:140:GLY:O    | 4:R:213:ARG:NH1  | 2.22                     | 0.71              |
| 11:Y:19:ARG:HB3  | 11:Y:31:ASP:HA   | 1.72                     | 0.71              |
| 11:K:19:ARG:HB3  | 11:K:31:ASP:HA   | 1.72                     | 0.70              |
| 9:I:187:ARG:HB3  | 9:I:188:PRO:CD   | 2.17                     | 0.70              |
| 12:Z:97:MET:HB3  | 12:Z:116:SER:HB3 | 1.72                     | 0.70              |
| 14:b:56:ASP:O    | 14:b:108:ASN:ND2 | 2.24                     | 0.69              |
| 2:B:159:ALA:HB1  | 2:B:173:LEU:HD23 | 1.75                     | 0.68              |
| 12:L:14:VAL:HG21 | 12:L:42:LEU:HD11 | 1.75                     | 0.68              |
| 14:N:56:ASP:O    | 14:N:108:ASN:ND2 | 2.24                     | 0.68              |
| 10:X:29:ILE:HG22 | 10:X:30:GLN:H    | 1.58                     | 0.68              |
| 12:Z:14:VAL:HG21 | 12:Z:42:LEU:HD11 | 1.75                     | 0.68              |
| 10:J:29:ILE:HG22 | 10:J:30:GLN:H    | 1.58                     | 0.68              |
| 1:A:41:ALA:HB3   | 1:A:166:THR:HB   | 1.77                     | 0.67              |
| 1:A:49:VAL:HG11  | 1:A:195:VAL:HA   | 1.76                     | 0.67              |
| 9:I:110:LEU:HD21 | 9:I:125:VAL:HG22 | 1.77                     | 0.67              |
| 9:W:163:ILE:HG12 | 9:W:170:GLY:HA2  | 1.76                     | 0.67              |
| 1:O:41:ALA:HB3   | 1:O:166:THR:HB   | 1.76                     | 0.67              |
| 2:P:159:ALA:HB1  | 2:P:173:LEU:HD23 | 1.75                     | 0.67              |
| 2:P:85:LEU:HD21  | 2:P:133:LEU:HD11 | 1.78                     | 0.66              |
| 6:F:44:ALA:HB2   | 6:F:142:PRO:HB3  | 1.78                     | 0.66              |
| 1:O:49:VAL:HG11  | 1:O:195:VAL:HA   | 1.76                     | 0.66              |
| 3:Q:112:THR:HG23 | 4:R:81:ARG:HD2   | 1.78                     | 0.66              |
| 6:T:44:ALA:HB2   | 6:T:142:PRO:HB3  | 1.78                     | 0.66              |
| 9:I:163:ILE:HG12 | 9:I:170:GLY:HA2  | 1.76                     | 0.66              |
| 2:B:85:LEU:HD21  | 2:B:133:LEU:HD11 | 1.78                     | 0.65              |
| 9:W:110:LEU:HD21 | 9:W:125:VAL:HG22 | 1.77                     | 0.65              |
| 6:F:72:ILE:HG22  | 6:F:134:ILE:HG12 | 1.79                     | 0.65              |
| 11:K:27:GLN:NE2  | 11:Y:169:LYS:O   | 2.28                     | 0.65              |
| 6:T:72:ILE:HG22  | 6:T:134:ILE:HG12 | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:T:81:ALA:HB2    | 6:T:130:VAL:HG21  | 1.79                     | 0.65              |
| 8:H:7:GLN:NE2     | 8:H:109:GLY:O     | 2.29                     | 0.64              |
| 9:I:187:ARG:CB    | 9:I:188:PRO:HD3   | 2.17                     | 0.64              |
| 6:F:95:SER:HB3    | 6:F:103:LEU:HD12  | 1.78                     | 0.64              |
| 10:J:104:THR:HG23 | 10:J:106:PRO:HD3  | 1.80                     | 0.64              |
| 3:C:112:THR:HG23  | 4:D:81:ARG:HD2    | 1.78                     | 0.64              |
| 4:R:86:ARG:NH1    | 4:R:118:TYR:OH    | 2.27                     | 0.64              |
| 6:T:95:SER:HB3    | 6:T:103:LEU:HD12  | 1.78                     | 0.64              |
| 8:V:7:GLN:NE2     | 8:V:109:GLY:O     | 2.29                     | 0.64              |
| 6:F:81:ALA:HB2    | 6:F:130:VAL:HG21  | 1.79                     | 0.64              |
| 8:H:107:GLU:OE1   | 8:H:110:GLN:NE2   | 2.31                     | 0.64              |
| 4:D:5:ARG:O       | 4:D:123:GLY:N     | 2.30                     | 0.63              |
| 4:D:86:ARG:NH1    | 4:D:118:TYR:OH    | 2.27                     | 0.63              |
| 8:V:14:LEU:HD21   | 8:V:101:ALA:HB3   | 1.80                     | 0.63              |
| 13:M:49:LYS:O     | 13:M:50:THR:OG1   | 2.16                     | 0.63              |
| 8:V:120:MET:O     | 14:b:61:GLN:NE2   | 2.27                     | 0.63              |
| 10:X:34:VAL:HG12  | 10:X:35:THR:HG23  | 1.80                     | 0.63              |
| 3:C:194:ILE:O     | 3:C:198:ASN:ND2   | 2.32                     | 0.63              |
| 10:J:34:VAL:HG12  | 10:J:35:THR:HG23  | 1.80                     | 0.63              |
| 9:I:21:THR:HG22   | 9:I:26:VAL:HA     | 1.80                     | 0.63              |
| 3:Q:194:ILE:O     | 3:Q:198:ASN:ND2   | 2.31                     | 0.63              |
| 9:W:187:ARG:CB    | 9:W:188:PRO:HD3   | 2.17                     | 0.63              |
| 10:X:25:ARG:HH11  | 10:X:37:ASP:HA    | 1.64                     | 0.63              |
| 10:X:104:THR:HG23 | 10:X:106:PRO:HD3  | 1.80                     | 0.63              |
| 5:S:13:ASN:HB3    | 6:T:126:ARG:HB3   | 1.81                     | 0.63              |
| 13:M:45:LYS:HE3   | 13:M:203:ILE:HD12 | 1.80                     | 0.63              |
| 2:P:147:GLN:NE2   | 2:P:162:MET:SD    | 2.72                     | 0.63              |
| 8:H:120:MET:O     | 14:N:61:GLN:NE2   | 2.27                     | 0.62              |
| 9:W:21:THR:HG22   | 9:W:26:VAL:HA     | 1.80                     | 0.62              |
| 13:a:45:LYS:HE3   | 13:a:203:ILE:HD12 | 1.80                     | 0.62              |
| 11:K:169:LYS:O    | 11:Y:27:GLN:NE2   | 2.32                     | 0.62              |
| 10:X:3:MET:HE1    | 10:X:105:GLU:HG3  | 1.81                     | 0.62              |
| 7:G:24:GLU:HA     | 7:G:27:MET:HE3    | 1.81                     | 0.62              |
| 2:B:147:GLN:NE2   | 2:B:162:MET:SD    | 2.72                     | 0.62              |
| 7:G:50:GLU:OE2    | 7:G:201:HIS:ND1   | 2.33                     | 0.62              |
| 8:V:107:GLU:OE1   | 8:V:110:GLN:NE2   | 2.31                     | 0.62              |
| 7:U:50:GLU:OE2    | 7:U:201:HIS:ND1   | 2.33                     | 0.62              |
| 3:C:136:TYR:HB2   | 3:C:148:TYR:HB2   | 1.82                     | 0.62              |
| 8:H:14:LEU:HD21   | 8:H:101:ALA:HB3   | 1.80                     | 0.62              |
| 2:P:51:GLN:HB3    | 2:P:56:TYR:HD2    | 1.64                     | 0.62              |
| 14:N:61:GLN:HA    | 14:N:64:LYS:HD3   | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:120:ASP:OD1   | 2:P:83:ARG:NH1    | 2.33                     | 0.62              |
| 13:a:49:LYS:O     | 13:a:50:THR:OG1   | 2.16                     | 0.62              |
| 5:E:164:GLN:HB3   | 6:F:58:ALA:HB3    | 1.82                     | 0.62              |
| 10:J:25:ARG:HH11  | 10:J:37:ASP:HA    | 1.64                     | 0.61              |
| 12:L:18:SER:HB2   | 12:L:173:ALA:H    | 1.65                     | 0.61              |
| 3:Q:136:TYR:HB2   | 3:Q:148:TYR:HB2   | 1.82                     | 0.61              |
| 10:J:3:MET:HE1    | 10:J:105:GLU:HG3  | 1.81                     | 0.61              |
| 7:U:24:GLU:HA     | 7:U:27:MET:HE3    | 1.81                     | 0.61              |
| 1:A:120:ASP:OD1   | 2:B:83:ARG:NH1    | 2.33                     | 0.61              |
| 12:Z:18:SER:HB2   | 12:Z:173:ALA:H    | 1.66                     | 0.61              |
| 14:b:61:GLN:HA    | 14:b:64:LYS:HD3   | 1.81                     | 0.61              |
| 2:B:51:GLN:HB3    | 2:B:56:TYR:HD2    | 1.64                     | 0.60              |
| 5:E:13:ASN:HB3    | 6:F:126:ARG:HB3   | 1.81                     | 0.60              |
| 11:Y:29:LYS:HB2   | 12:Z:121:ILE:HD12 | 1.83                     | 0.60              |
| 2:B:108:GLN:HB3   | 2:B:112:ARG:HH12  | 1.66                     | 0.60              |
| 9:W:44:CYS:HB2    | 9:W:99:VAL:HB     | 1.82                     | 0.60              |
| 9:I:63:LEU:HA     | 9:I:66:HIS:HB3    | 1.84                     | 0.60              |
| 11:K:29:LYS:HD2   | 12:L:121:ILE:HB   | 1.82                     | 0.60              |
| 9:W:63:LEU:HA     | 9:W:66:HIS:HB3    | 1.84                     | 0.60              |
| 14:b:22:ILE:HG12  | 14:b:50:MET:HE2   | 1.83                     | 0.60              |
| 14:N:22:ILE:HG12  | 14:N:50:MET:HE2   | 1.83                     | 0.60              |
| 11:Y:29:LYS:HD2   | 12:Z:121:ILE:HB   | 1.82                     | 0.60              |
| 13:M:148:LEU:HD23 | 13:M:178:VAL:HG23 | 1.84                     | 0.60              |
| 10:X:47:ARG:NH2   | 10:X:191:LYS:O    | 2.35                     | 0.60              |
| 5:S:164:GLN:HB3   | 6:T:58:ALA:HB3    | 1.82                     | 0.60              |
| 2:B:48:GLU:O      | 2:B:63:LYS:NZ     | 2.35                     | 0.59              |
| 9:I:81:ARG:HA     | 9:I:84:LYS:HG2    | 1.83                     | 0.59              |
| 2:P:48:GLU:O      | 2:P:63:LYS:NZ     | 2.35                     | 0.59              |
| 6:T:76:GLY:HA3    | 6:T:130:VAL:HA    | 1.84                     | 0.59              |
| 11:K:29:LYS:HB2   | 12:L:121:ILE:HD12 | 1.83                     | 0.59              |
| 1:A:31:ALA:HB1    | 1:A:83:MET:HE3    | 1.84                     | 0.59              |
| 9:I:44:CYS:HB2    | 9:I:99:VAL:HB     | 1.82                     | 0.59              |
| 4:R:5:ARG:O       | 4:R:123:GLY:N     | 2.30                     | 0.59              |
| 9:W:81:ARG:HA     | 9:W:84:LYS:HG2    | 1.83                     | 0.59              |
| 13:a:148:LEU:HD23 | 13:a:178:VAL:HG23 | 1.84                     | 0.59              |
| 10:J:47:ARG:NH2   | 10:J:191:LYS:O    | 2.35                     | 0.59              |
| 6:T:49:LEU:HG     | 6:T:195:LEU:HD11  | 1.85                     | 0.59              |
| 2:P:108:GLN:HB3   | 2:P:112:ARG:HH12  | 1.66                     | 0.59              |
| 11:Y:85:ARG:HD2   | 11:Y:124:LEU:HB2  | 1.85                     | 0.59              |
| 12:L:14:VAL:HB    | 12:L:177:TYR:HB2  | 1.85                     | 0.58              |
| 13:M:169:ASP:HB3  | 13:M:173:ARG:HH22 | 1.68                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:113:MET:HE3   | 9:I:70:THR:HA     | 1.84                     | 0.58              |
| 6:T:39:LYS:HD3    | 6:T:144:ILE:HG12  | 1.84                     | 0.58              |
| 1:O:31:ALA:HB1    | 1:O:83:MET:HE3    | 1.84                     | 0.58              |
| 7:U:79:GLY:HA3    | 7:U:133:CYS:HA    | 1.85                     | 0.58              |
| 6:F:39:LYS:HD3    | 6:F:144:ILE:HG12  | 1.84                     | 0.58              |
| 6:F:76:GLY:HA3    | 6:F:130:VAL:HA    | 1.84                     | 0.58              |
| 1:O:113:MET:HE3   | 9:W:70:THR:HA     | 1.84                     | 0.58              |
| 11:K:85:ARG:HD2   | 11:K:124:LEU:HB2  | 1.85                     | 0.58              |
| 13:a:169:ASP:HB3  | 13:a:173:ARG:HH22 | 1.68                     | 0.58              |
| 13:M:198:VAL:HG22 | 13:M:203:ILE:HG12 | 1.86                     | 0.58              |
| 5:S:24:VAL:HG13   | 5:S:158:PRO:HB2   | 1.84                     | 0.58              |
| 5:S:51:GLU:HG3    | 5:S:206:MET:HE3   | 1.86                     | 0.58              |
| 2:B:67:ILE:HG21   | 2:B:109:LEU:HD11  | 1.85                     | 0.58              |
| 3:C:190:LEU:HD23  | 3:C:236:LEU:HD11  | 1.86                     | 0.58              |
| 6:F:49:LEU:HG     | 6:F:195:LEU:HD11  | 1.85                     | 0.58              |
| 2:P:67:ILE:HG21   | 2:P:109:LEU:HD11  | 1.85                     | 0.58              |
| 10:X:14:LYS:HE3   | 10:X:120:ILE:HG12 | 1.86                     | 0.58              |
| 14:N:33:LEU:HD13  | 8:V:134:TYR:CZ    | 2.39                     | 0.58              |
| 7:G:79:GLY:HA3    | 7:G:133:CYS:HA    | 1.85                     | 0.57              |
| 5:S:41:GLN:NE2    | 5:S:151:PRO:O     | 2.37                     | 0.57              |
| 13:a:27:THR:HB    | 13:a:39:ASP:HA    | 1.86                     | 0.57              |
| 5:E:24:VAL:HG13   | 5:E:158:PRO:HB2   | 1.84                     | 0.57              |
| 1:A:43:ARG:HA     | 1:A:48:ALA:HA     | 1.87                     | 0.57              |
| 3:C:133:SER:HB2   | 3:C:152:PRO:HD3   | 1.87                     | 0.57              |
| 5:E:14:THR:HG23   | 6:F:21:GLN:HE22   | 1.70                     | 0.57              |
| 13:M:27:THR:HB    | 13:M:39:ASP:HA    | 1.86                     | 0.57              |
| 6:T:39:LYS:HB3    | 6:T:144:ILE:HD11  | 1.87                     | 0.57              |
| 5:E:51:GLU:HG3    | 5:E:206:MET:HE3   | 1.86                     | 0.57              |
| 10:J:14:LYS:HE3   | 10:J:120:ILE:HG12 | 1.86                     | 0.57              |
| 1:O:43:ARG:HA     | 1:O:48:ALA:HA     | 1.87                     | 0.57              |
| 12:Z:14:VAL:HB    | 12:Z:177:TYR:HB2  | 1.85                     | 0.57              |
| 1:A:34:GLN:NE2    | 7:G:17:ASP:O      | 2.38                     | 0.57              |
| 2:P:21:ILE:HG21   | 2:P:151:SER:HB3   | 1.87                     | 0.57              |
| 3:Q:190:LEU:HD23  | 3:Q:236:LEU:HD11  | 1.86                     | 0.57              |
| 6:F:39:LYS:HB3    | 6:F:144:ILE:HD11  | 1.86                     | 0.57              |
| 5:E:41:GLN:NE2    | 5:E:151:PRO:O     | 2.37                     | 0.57              |
| 1:A:141:ILE:HG22  | 1:A:151:VAL:HG22  | 1.86                     | 0.57              |
| 10:J:125:LEU:HD12 | 10:J:126:ILE:HG23 | 1.86                     | 0.56              |
| 1:O:34:GLN:NE2    | 7:U:17:ASP:O      | 2.38                     | 0.56              |
| 3:Q:209:GLU:OE2   | 3:Q:230:GLN:NE2   | 2.38                     | 0.56              |
| 12:Z:59:LEU:HD22  | 12:Z:83:LEU:HB2   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:64:ALA:H      | 4:D:88:ARG:HH21   | 1.53                     | 0.56              |
| 1:O:141:ILE:HG22  | 1:O:151:VAL:HG22  | 1.86                     | 0.56              |
| 5:E:41:GLN:N      | 5:E:166:ASP:O     | 2.32                     | 0.56              |
| 11:K:27:GLN:O     | 11:Y:170:ARG:NH1  | 2.34                     | 0.56              |
| 12:L:19:ARG:O     | 12:L:33:LYS:NZ    | 2.32                     | 0.56              |
| 10:X:125:LEU:HD12 | 10:X:126:ILE:HG23 | 1.86                     | 0.56              |
| 5:E:31:ILE:HD13   | 5:E:140:ALA:HB2   | 1.87                     | 0.56              |
| 13:a:198:VAL:HG22 | 13:a:203:ILE:HG12 | 1.86                     | 0.56              |
| 5:S:31:ILE:HD13   | 5:S:140:ALA:HB2   | 1.88                     | 0.56              |
| 8:V:38:HIS:CD2    | 8:V:39:ASP:H      | 2.24                     | 0.56              |
| 5:S:14:THR:HG23   | 6:T:21:GLN:HE22   | 1.70                     | 0.56              |
| 2:B:21:ILE:HG21   | 2:B:151:SER:HB3   | 1.87                     | 0.56              |
| 5:S:41:GLN:N      | 5:S:166:ASP:O     | 2.32                     | 0.56              |
| 3:C:45:LEU:HD13   | 3:C:75:SER:HB2    | 1.88                     | 0.56              |
| 3:C:209:GLU:OE2   | 3:C:230:GLN:NE2   | 2.38                     | 0.56              |
| 4:D:80:ALA:HA     | 4:D:129:ILE:HD13  | 1.88                     | 0.56              |
| 3:Q:133:SER:HB2   | 3:Q:152:PRO:HD3   | 1.87                     | 0.56              |
| 12:L:59:LEU:HD22  | 12:L:83:LEU:HB2   | 1.87                     | 0.55              |
| 14:b:189:ILE:HD12 | 14:b:203:LEU:HD22 | 1.88                     | 0.55              |
| 6:F:117:GLN:HE22  | 7:G:83:ASP:HA     | 1.72                     | 0.55              |
| 11:K:170:ARG:NH1  | 11:Y:27:GLN:O     | 2.36                     | 0.55              |
| 12:L:34:VAL:HG22  | 12:L:44:THR:HG22  | 1.89                     | 0.55              |
| 8:H:38:HIS:CD2    | 8:H:39:ASP:H      | 2.24                     | 0.55              |
| 3:Q:45:LEU:HD13   | 3:Q:75:SER:HB2    | 1.88                     | 0.55              |
| 4:R:64:ALA:H      | 4:R:88:ARG:HH21   | 1.54                     | 0.55              |
| 6:T:117:GLN:HE22  | 7:U:83:ASP:HA     | 1.72                     | 0.55              |
| 8:V:93:ASP:OD2    | 9:W:91:GLN:NE2    | 2.40                     | 0.55              |
| 4:D:7:ILE:HG22    | 4:D:18:GLN:HG3    | 1.88                     | 0.55              |
| 14:N:8:GLY:N      | 14:N:55:GLY:O     | 2.38                     | 0.55              |
| 12:L:4:LEU:HB3    | 12:L:15:ALA:HB3   | 1.89                     | 0.55              |
| 4:R:80:ALA:HA     | 4:R:129:ILE:HD13  | 1.88                     | 0.55              |
| 8:V:3:ILE:HD12    | 8:V:99:ILE:HG22   | 1.89                     | 0.55              |
| 8:H:134:TYR:CZ    | 14:b:33:LEU:HD13  | 2.41                     | 0.54              |
| 9:I:216:ILE:HG12  | 10:J:195:THR:HG22 | 1.89                     | 0.54              |
| 14:N:189:ILE:HD12 | 14:N:203:LEU:HD22 | 1.88                     | 0.54              |
| 8:H:93:ASP:OD2    | 9:I:91:GLN:NE2    | 2.40                     | 0.54              |
| 11:Y:171:PHE:CE2  | 11:Y:173:LEU:HB2  | 2.42                     | 0.54              |
| 9:I:160:ALA:HA    | 9:I:163:ILE:HD12  | 1.90                     | 0.54              |
| 11:K:171:PHE:CE2  | 11:K:173:LEU:HB2  | 2.42                     | 0.54              |
| 12:L:98:GLY:HA2   | 12:L:115:ASP:HA   | 1.89                     | 0.54              |
| 10:X:9:ALA:HA     | 10:X:139:GLY:HA3  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:69:GLU:O     | 5:E:93:ARG:NE     | 2.41                     | 0.54              |
| 11:K:43:LEU:HD11 | 11:K:181:ARG:HD2  | 1.90                     | 0.54              |
| 11:Y:43:LEU:HD11 | 11:Y:181:ARG:HD2  | 1.90                     | 0.54              |
| 12:Z:34:VAL:HG22 | 12:Z:44:THR:HG22  | 1.89                     | 0.54              |
| 4:D:88:ARG:NH1   | 11:K:69:MET:O     | 2.41                     | 0.54              |
| 4:R:88:ARG:NH1   | 11:Y:69:MET:O     | 2.41                     | 0.54              |
| 9:W:216:ILE:HG12 | 10:X:195:THR:HG22 | 1.89                     | 0.54              |
| 11:Y:39:SER:HB2  | 11:Y:42:ILE:HG12  | 1.90                     | 0.54              |
| 4:D:69:VAL:HG11  | 4:D:107:ILE:HG21  | 1.90                     | 0.54              |
| 4:R:7:ILE:HG22   | 4:R:18:GLN:HG3    | 1.89                     | 0.54              |
| 5:S:100:TRP:O    | 12:Z:57:ARG:NH2   | 2.41                     | 0.54              |
| 9:W:160:ALA:HA   | 9:W:163:ILE:HD12  | 1.90                     | 0.54              |
| 10:X:122:SER:HB2 | 10:X:136:VAL:HB   | 1.90                     | 0.54              |
| 12:Z:4:LEU:HB3   | 12:Z:15:ALA:HB3   | 1.89                     | 0.54              |
| 8:H:3:ILE:HD12   | 8:H:99:ILE:HG22   | 1.89                     | 0.54              |
| 4:D:158:ALA:HB3  | 5:E:58:LEU:HD13   | 1.90                     | 0.53              |
| 10:J:9:ALA:HA    | 10:J:139:GLY:HA3  | 1.89                     | 0.53              |
| 10:J:143:GLU:HA  | 10:J:146:TYR:HD2  | 1.73                     | 0.53              |
| 14:N:89:HIS:HE1  | 14:N:131:ALA:HB1  | 1.72                     | 0.53              |
| 14:b:8:GLY:N     | 14:b:55:GLY:O     | 2.37                     | 0.53              |
| 14:b:89:HIS:HE1  | 14:b:131:ALA:HB1  | 1.72                     | 0.53              |
| 7:G:108:LEU:HD11 | 7:G:137:LEU:HB3   | 1.90                     | 0.53              |
| 8:H:174:ILE:HB   | 8:H:189:LEU:HB2   | 1.91                     | 0.53              |
| 10:J:9:ALA:HB1   | 10:J:145:MET:HE1  | 1.91                     | 0.53              |
| 10:J:52:LEU:HB2  | 10:J:59:VAL:HG13  | 1.91                     | 0.53              |
| 6:T:47:VAL:HG12  | 6:T:195:LEU:HD22  | 1.90                     | 0.53              |
| 11:K:39:SER:HB2  | 11:K:42:ILE:HG12  | 1.90                     | 0.53              |
| 12:L:4:LEU:N     | 12:L:15:ALA:O     | 2.40                     | 0.53              |
| 5:E:100:TRP:O    | 12:L:57:ARG:NH2   | 2.41                     | 0.53              |
| 9:I:30:ASN:O     | 9:I:187:ARG:NH2   | 2.40                     | 0.53              |
| 10:J:122:SER:HB2 | 10:J:136:VAL:HB   | 1.90                     | 0.53              |
| 5:S:77:ALA:HB3   | 5:S:142:LEU:HB2   | 1.90                     | 0.53              |
| 10:X:143:GLU:HA  | 10:X:146:TYR:HD2  | 1.73                     | 0.53              |
| 12:Z:127:SER:O   | 12:Z:136:TYR:OH   | 2.23                     | 0.53              |
| 1:A:125:TYR:HA   | 1:A:131:MET:HG3   | 1.90                     | 0.53              |
| 11:Y:6:GLY:HA2   | 11:Y:15:VAL:HA    | 1.90                     | 0.53              |
| 12:Z:98:GLY:HA2  | 12:Z:115:ASP:HA   | 1.89                     | 0.53              |
| 6:F:143:HIS:HB3  | 6:F:145:PHE:CD2   | 2.44                     | 0.53              |
| 3:Q:73:ALA:HB2   | 3:Q:225:ILE:HD13  | 1.91                     | 0.53              |
| 4:R:69:VAL:HG11  | 4:R:107:ILE:HG21  | 1.90                     | 0.53              |
| 12:Z:4:LEU:N     | 12:Z:15:ALA:O     | 2.40                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:a:63:THR:HG23 | 14:b:94:ARG:HH12  | 1.74                     | 0.53              |
| 5:E:77:ALA:HB3   | 5:E:142:LEU:HB2   | 1.90                     | 0.53              |
| 6:F:82:ARG:HA    | 6:F:85:CYS:HB3    | 1.91                     | 0.53              |
| 9:W:30:ASN:O     | 9:W:187:ARG:NH2   | 2.40                     | 0.53              |
| 5:S:69:GLU:O     | 5:S:93:ARG:NE     | 2.41                     | 0.53              |
| 14:N:28:GLY:N    | 14:N:36:PHE:O     | 2.42                     | 0.53              |
| 1:O:125:TYR:HA   | 1:O:131:MET:HG3   | 1.90                     | 0.53              |
| 4:R:116:GLN:O    | 4:R:119:THR:OG1   | 2.23                     | 0.53              |
| 6:T:11:THR:HA    | 7:U:129:ARG:HD3   | 1.91                     | 0.53              |
| 10:X:48:LEU:HD21 | 10:X:86:LEU:HD22  | 1.90                     | 0.53              |
| 14:b:28:GLY:N    | 14:b:36:PHE:O     | 2.42                     | 0.53              |
| 6:F:47:VAL:HG12  | 6:F:195:LEU:HD22  | 1.90                     | 0.52              |
| 10:J:48:LEU:HD21 | 10:J:86:LEU:HD22  | 1.90                     | 0.52              |
| 11:K:6:GLY:HA2   | 11:K:15:VAL:HA    | 1.90                     | 0.52              |
| 11:K:98:TYR:HB3  | 11:K:100:VAL:HG22 | 1.91                     | 0.52              |
| 6:T:143:HIS:HB3  | 6:T:145:PHE:CD2   | 2.44                     | 0.52              |
| 7:U:108:LEU:HD11 | 7:U:137:LEU:HB3   | 1.90                     | 0.52              |
| 10:X:52:LEU:HB2  | 10:X:59:VAL:HG13  | 1.91                     | 0.52              |
| 4:D:116:GLN:O    | 4:D:119:THR:OG1   | 2.23                     | 0.52              |
| 6:T:195:LEU:O    | 6:T:198:THR:OG1   | 2.25                     | 0.52              |
| 11:Y:34:LYS:HD3  | 11:Y:47:VAL:HG12  | 1.91                     | 0.52              |
| 3:Q:124:PHE:HB3  | 4:R:124:ARG:HG2   | 1.92                     | 0.52              |
| 6:T:7:ASP:HB2    | 6:T:24:TYR:HE2    | 1.74                     | 0.52              |
| 10:X:9:ALA:HB1   | 10:X:145:MET:HE1  | 1.90                     | 0.52              |
| 6:F:7:ASP:HB2    | 6:F:24:TYR:HE2    | 1.74                     | 0.52              |
| 6:F:33:SER:HB2   | 6:F:62:LYS:HE2    | 1.92                     | 0.52              |
| 7:G:109:LYS:HA   | 7:G:149:TYR:HE2   | 1.75                     | 0.52              |
| 4:R:158:ALA:HB3  | 5:S:58:LEU:HD13   | 1.90                     | 0.52              |
| 13:M:63:THR:HG23 | 14:N:94:ARG:HH12  | 1.74                     | 0.52              |
| 1:O:192:GLU:OE1  | 1:O:193:GLN:NE2   | 2.43                     | 0.52              |
| 6:F:11:THR:HA    | 7:G:129:ARG:HD3   | 1.91                     | 0.52              |
| 6:T:33:SER:HB2   | 6:T:62:LYS:HE2    | 1.92                     | 0.52              |
| 8:V:21:THR:HG22  | 8:V:26:ILE:HG12   | 1.92                     | 0.52              |
| 8:V:174:ILE:HB   | 8:V:189:LEU:HB2   | 1.91                     | 0.52              |
| 11:Y:98:TYR:HB3  | 11:Y:100:VAL:HG22 | 1.92                     | 0.52              |
| 3:C:73:ALA:HB2   | 3:C:225:ILE:HD13  | 1.91                     | 0.51              |
| 11:K:4:LEU:HD22  | 11:K:45:LEU:HD23  | 1.92                     | 0.51              |
| 6:T:82:ARG:HA    | 6:T:85:CYS:HB3    | 1.91                     | 0.51              |
| 9:W:50:ALA:HB2   | 10:X:128:CYS:HB2  | 1.93                     | 0.51              |
| 12:Z:6:PHE:HB3   | 12:Z:139:MET:HE3  | 1.92                     | 0.51              |
| 1:A:51:VAL:HG22  | 1:A:217:VAL:HG22  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:212:CYS:HB2  | 2:B:217:PHE:HD1  | 1.75                     | 0.51              |
| 8:H:91:ARG:NH1   | 8:H:92:GLU:OE2   | 2.43                     | 0.51              |
| 7:U:109:LYS:HA   | 7:U:149:TYR:HE2  | 1.75                     | 0.51              |
| 8:V:127:ILE:HD12 | 8:V:132:SER:HB2  | 1.92                     | 0.51              |
| 1:A:192:GLU:OE1  | 1:A:193:GLN:NE2  | 2.43                     | 0.51              |
| 11:K:34:LYS:HD3  | 11:K:47:VAL:HG12 | 1.91                     | 0.51              |
| 2:B:83:ARG:HA    | 2:B:86:VAL:HG12  | 1.93                     | 0.51              |
| 13:M:187:VAL:HB  | 9:W:167:LEU:HB3  | 1.93                     | 0.51              |
| 2:B:183:LEU:HD21 | 2:B:211:ILE:HD12 | 1.93                     | 0.51              |
| 8:H:37:ILE:HG13  | 8:H:83:PHE:HZ    | 1.75                     | 0.51              |
| 3:Q:46:ALA:HB1   | 3:Q:197:LEU:HD11 | 1.93                     | 0.51              |
| 6:T:224:TYR:HD1  | 6:T:228:ASP:HB3  | 1.76                     | 0.51              |
| 3:C:124:PHE:HB3  | 4:D:124:ARG:HG2  | 1.92                     | 0.51              |
| 6:F:152:ASN:HB2  | 7:G:81:LEU:HD23  | 1.92                     | 0.51              |
| 8:H:28:ASN:ND2   | 9:I:122:LEU:HD11 | 2.25                     | 0.51              |
| 8:V:28:ASN:ND2   | 9:W:122:LEU:HD11 | 2.25                     | 0.51              |
| 8:V:91:ARG:NH1   | 8:V:92:GLU:OE2   | 2.43                     | 0.51              |
| 10:X:35:THR:HG22 | 11:Y:127:ALA:HB2 | 1.92                     | 0.51              |
| 3:C:46:ALA:HB1   | 3:C:197:LEU:HD11 | 1.93                     | 0.51              |
| 8:H:127:ILE:HD12 | 8:H:132:SER:HB2  | 1.92                     | 0.51              |
| 12:L:6:PHE:HB3   | 12:L:139:MET:HE3 | 1.92                     | 0.51              |
| 1:O:51:VAL:HG22  | 1:O:217:VAL:HG22 | 1.92                     | 0.51              |
| 9:I:50:ALA:HB2   | 10:J:128:CYS:HB2 | 1.92                     | 0.51              |
| 4:R:120:GLN:O    | 5:S:134:SER:N    | 2.26                     | 0.51              |
| 6:T:120:THR:HG22 | 6:T:127:PRO:HG3  | 1.92                     | 0.51              |
| 8:V:37:ILE:HG13  | 8:V:83:PHE:HZ    | 1.75                     | 0.51              |
| 3:C:49:ARG:N     | 3:C:210:LYS:O    | 2.41                     | 0.51              |
| 3:C:158:GLY:HA3  | 4:D:55:ASP:HB3   | 1.93                     | 0.51              |
| 8:H:133:SER:HA   | 8:H:136:TYR:HE2  | 1.76                     | 0.51              |
| 6:T:152:ASN:HB2  | 7:U:81:LEU:HD23  | 1.92                     | 0.51              |
| 11:Y:4:LEU:HD22  | 11:Y:45:LEU:HD23 | 1.92                     | 0.51              |
| 6:F:117:GLN:O    | 6:F:120:THR:OG1  | 2.24                     | 0.51              |
| 2:P:183:LEU:HD21 | 2:P:211:ILE:HD12 | 1.93                     | 0.51              |
| 5:S:98:ASN:OD1   | 12:Z:61:ARG:NH2  | 2.44                     | 0.51              |
| 6:F:224:TYR:HD1  | 6:F:228:ASP:HB3  | 1.76                     | 0.50              |
| 2:P:212:CYS:HB2  | 2:P:217:PHE:HD1  | 1.75                     | 0.50              |
| 11:Y:85:ARG:NE   | 11:Y:122:ALA:O   | 2.44                     | 0.50              |
| 1:A:86:ASP:OD1   | 7:G:120:HIS:NE2  | 2.36                     | 0.50              |
| 6:F:120:THR:HG22 | 6:F:127:PRO:HG3  | 1.92                     | 0.50              |
| 4:D:120:GLN:O    | 5:E:134:SER:N    | 2.26                     | 0.50              |
| 8:H:21:THR:HG22  | 8:H:26:ILE:HG12  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:168:GLN:NE2  | 11:K:175:LEU:O    | 2.45                     | 0.50              |
| 8:V:28:ASN:HD21   | 9:W:122:LEU:HD11  | 1.77                     | 0.50              |
| 4:D:116:GLN:NE2   | 5:E:83:ALA:O      | 2.45                     | 0.50              |
| 5:E:98:ASN:OD1    | 12:L:61:ARG:NH2   | 2.44                     | 0.50              |
| 11:K:85:ARG:NE    | 11:K:122:ALA:O    | 2.44                     | 0.50              |
| 9:W:209:THR:OG1   | 10:X:168:GLN:NE2  | 2.38                     | 0.50              |
| 3:Q:158:GLY:HA3   | 4:R:55:ASP:HB3    | 1.93                     | 0.50              |
| 8:H:28:ASN:HD21   | 9:I:122:LEU:HD11  | 1.77                     | 0.50              |
| 4:R:116:GLN:NE2   | 5:S:83:ALA:O      | 2.45                     | 0.50              |
| 11:Y:81:ALA:HA    | 11:Y:104:LEU:HD13 | 1.94                     | 0.50              |
| 14:N:37:ARG:HD2   | 14:N:184:TYR:CE1  | 2.47                     | 0.50              |
| 6:T:189:LYS:HB3   | 6:T:193:ARG:HH12  | 1.77                     | 0.50              |
| 8:V:133:SER:HA    | 8:V:136:TYR:HE2   | 1.76                     | 0.50              |
| 6:F:45:VAL:HG22   | 6:F:214:ILE:HG12  | 1.94                     | 0.50              |
| 11:K:43:LEU:HD12  | 11:K:183:ILE:HD11 | 1.94                     | 0.50              |
| 2:P:83:ARG:HA     | 2:P:86:VAL:HG12   | 1.93                     | 0.50              |
| 10:J:35:THR:HG22  | 11:K:127:ALA:HB2  | 1.92                     | 0.50              |
| 11:K:81:ALA:HA    | 11:K:104:LEU:HD13 | 1.94                     | 0.50              |
| 7:G:71:ARG:NH2    | 7:G:105:ASN:OD1   | 2.45                     | 0.49              |
| 10:J:152:LEU:HB3  | 10:J:165:THR:HG23 | 1.95                     | 0.49              |
| 12:L:8:PHE:CE1    | 12:L:10:HIS:HB2   | 2.47                     | 0.49              |
| 12:L:138:VAL:HG21 | 12:L:162:GLN:HG3  | 1.94                     | 0.49              |
| 13:M:194:ARG:HH11 | 13:M:207:THR:HB   | 1.77                     | 0.49              |
| 12:Z:21:THR:HG22  | 12:Z:26:ILE:HG12  | 1.95                     | 0.49              |
| 12:Z:164:THR:HG22 | 12:Z:170:SER:HB3  | 1.94                     | 0.49              |
| 1:A:49:VAL:HG22   | 1:A:219:VAL:HG12  | 1.94                     | 0.49              |
| 6:T:45:VAL:HG22   | 6:T:214:ILE:HG12  | 1.94                     | 0.49              |
| 9:W:13:VAL:HG22   | 9:W:177:VAL:HG22  | 1.94                     | 0.49              |
| 13:a:4:PRO:O      | 14:b:100:ARG:NH1  | 2.41                     | 0.49              |
| 9:I:13:VAL:HG22   | 9:I:177:VAL:HG22  | 1.94                     | 0.49              |
| 12:L:21:THR:HG22  | 12:L:26:ILE:HG12  | 1.95                     | 0.49              |
| 13:M:36:HIS:HB3   | 14:N:132:TYR:CZ   | 2.48                     | 0.49              |
| 9:I:209:THR:OG1   | 10:J:168:GLN:NE2  | 2.38                     | 0.49              |
| 12:L:45:MET:HG3   | 12:L:52:CYS:HB2   | 1.95                     | 0.49              |
| 10:X:152:LEU:HB3  | 10:X:165:THR:HG23 | 1.95                     | 0.49              |
| 12:Z:45:MET:HG3   | 12:Z:52:CYS:HB2   | 1.95                     | 0.49              |
| 11:Y:168:GLN:NE2  | 11:Y:175:LEU:O    | 2.45                     | 0.49              |
| 12:Z:8:PHE:CE1    | 12:Z:10:HIS:HB2   | 2.48                     | 0.49              |
| 14:b:37:ARG:HD2   | 14:b:184:TYR:CE1  | 2.47                     | 0.49              |
| 6:F:6:TYR:OH      | 7:G:8:ASP:OD2     | 2.27                     | 0.49              |
| 11:K:59:TYR:HE2   | 11:K:87:ASN:HD22  | 1.60                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:53:ALA:HB2   | 14:N:110:MET:HG2  | 1.95                     | 0.49              |
| 1:O:103:TYR:O     | 9:W:81:ARG:HD3    | 2.13                     | 0.49              |
| 13:a:36:HIS:HB3   | 14:b:132:TYR:CZ   | 2.48                     | 0.49              |
| 12:L:164:THR:HG22 | 12:L:170:SER:HB3  | 1.95                     | 0.49              |
| 6:T:192:LEU:HD21  | 6:T:212:ILE:HD11  | 1.95                     | 0.49              |
| 7:U:71:ARG:NH2    | 7:U:105:ASN:OD1   | 2.45                     | 0.49              |
| 13:a:194:ARG:HH11 | 13:a:207:THR:HB   | 1.77                     | 0.49              |
| 1:A:103:TYR:O     | 9:I:81:ARG:HD3    | 2.13                     | 0.49              |
| 14:N:27:LEU:HA    | 14:N:37:ARG:HA    | 1.95                     | 0.49              |
| 6:F:189:LYS:HB3   | 6:F:193:ARG:HH12  | 1.77                     | 0.48              |
| 11:K:45:LEU:HD22  | 11:K:103:LEU:HD23 | 1.95                     | 0.48              |
| 3:Q:3:ARG:NH1     | 5:S:125:GLU:OE2   | 2.46                     | 0.48              |
| 11:Y:43:LEU:HD12  | 11:Y:183:ILE:HD11 | 1.94                     | 0.48              |
| 12:Z:33:LYS:O     | 12:Z:45:MET:N     | 2.41                     | 0.48              |
| 1:A:50:ILE:HD12   | 1:A:79:VAL:HB     | 1.96                     | 0.48              |
| 3:Q:49:ARG:N      | 3:Q:210:LYS:O     | 2.41                     | 0.48              |
| 9:W:59:ILE:HD12   | 9:W:82:MET:HB3    | 1.95                     | 0.48              |
| 14:b:27:LEU:HA    | 14:b:37:ARG:HA    | 1.95                     | 0.48              |
| 11:Y:45:LEU:HD22  | 11:Y:103:LEU:HD23 | 1.95                     | 0.48              |
| 6:F:195:LEU:O     | 6:F:198:THR:OG1   | 2.26                     | 0.48              |
| 9:I:18:THR:HG21   | 9:I:187:ARG:HH12  | 1.77                     | 0.48              |
| 1:O:49:VAL:HG22   | 1:O:219:VAL:HG12  | 1.94                     | 0.48              |
| 12:Z:138:VAL:HG21 | 12:Z:162:GLN:HG3  | 1.94                     | 0.48              |
| 2:B:49:LYS:H      | 2:B:207:ILE:HA    | 1.79                     | 0.48              |
| 3:C:109:GLN:HE21  | 11:K:71:ASN:HD21  | 1.62                     | 0.48              |
| 11:K:45:LEU:O     | 11:K:103:LEU:N    | 2.45                     | 0.48              |
| 4:D:5:ARG:HA      | 5:E:125:GLU:HB2   | 1.96                     | 0.48              |
| 5:E:42:THR:OG1    | 5:E:45:GLY:O      | 2.30                     | 0.48              |
| 6:F:192:LEU:HD21  | 6:F:212:ILE:HD11  | 1.95                     | 0.48              |
| 8:V:176:LEU:HD12  | 8:V:187:GLN:HE21  | 1.78                     | 0.48              |
| 14:b:15:LYS:HE3   | 14:b:135:PRO:HA   | 1.96                     | 0.48              |
| 14:b:53:ALA:HB2   | 14:b:110:MET:HG2  | 1.94                     | 0.48              |
| 14:b:124:TYR:HE1  | 14:b:139:THR:HG22 | 1.79                     | 0.48              |
| 3:C:3:ARG:NH1     | 5:E:125:GLU:OE2   | 2.46                     | 0.48              |
| 7:G:73:VAL:HG22   | 7:G:139:SER:HB3   | 1.95                     | 0.48              |
| 7:G:149:TYR:HD1   | 7:G:159:GLY:HA2   | 1.79                     | 0.48              |
| 8:H:176:LEU:HD12  | 8:H:187:GLN:HE21  | 1.78                     | 0.48              |
| 11:K:19:ARG:NE    | 11:K:177:THR:HB   | 2.28                     | 0.48              |
| 4:R:5:ARG:HA      | 5:S:125:GLU:HB2   | 1.96                     | 0.48              |
| 6:T:26:MET:HA     | 6:T:149:PRO:HG2   | 1.96                     | 0.48              |
| 14:b:25:ASP:HA    | 14:b:187:PHE:HA   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:b:45:VAL:HG11  | 14:b:88:ILE:HD13  | 1.96                     | 0.48              |
| 14:N:15:LYS:HE3   | 14:N:135:PRO:HA   | 1.96                     | 0.48              |
| 13:a:5:TYR:OH     | 13:a:103:PRO:O    | 2.29                     | 0.48              |
| 14:b:25:ASP:OD1   | 14:b:41:ARG:NH2   | 2.47                     | 0.48              |
| 14:b:184:TYR:HE2  | 14:b:186:ARG:HB2  | 1.79                     | 0.48              |
| 9:I:167:LEU:HB3   | 13:a:187:VAL:HB   | 1.95                     | 0.48              |
| 14:N:25:ASP:OD1   | 14:N:41:ARG:NH2   | 2.47                     | 0.48              |
| 2:P:49:LYS:H      | 2:P:207:ILE:HA    | 1.79                     | 0.48              |
| 2:B:38:LYS:HE3    | 2:B:158:LYS:HA    | 1.96                     | 0.48              |
| 7:U:73:VAL:HG22   | 7:U:139:SER:HB3   | 1.95                     | 0.48              |
| 9:W:18:THR:HG21   | 9:W:187:ARG:HH12  | 1.78                     | 0.48              |
| 9:I:12:ILE:HD11   | 9:I:110:LEU:HD12  | 1.96                     | 0.47              |
| 1:O:50:ILE:HD12   | 1:O:79:VAL:HB     | 1.95                     | 0.47              |
| 14:N:144:TYR:HB3  | 9:W:132:LEU:HB3   | 1.96                     | 0.47              |
| 2:P:38:LYS:HE3    | 2:P:158:LYS:HA    | 1.96                     | 0.47              |
| 7:U:149:TYR:HD1   | 7:U:159:GLY:HA2   | 1.79                     | 0.47              |
| 11:Y:19:ARG:NE    | 11:Y:177:THR:HB   | 2.28                     | 0.47              |
| 4:D:87:ALA:HB1    | 4:D:107:ILE:HD11  | 1.96                     | 0.47              |
| 6:F:26:MET:HA     | 6:F:149:PRO:HG2   | 1.96                     | 0.47              |
| 5:E:49:ALA:HB1    | 5:E:202:LEU:HD11  | 1.97                     | 0.47              |
| 9:W:12:ILE:HD11   | 9:W:110:LEU:HD12  | 1.96                     | 0.47              |
| 4:D:83:VAL:HG21   | 4:D:129:ILE:HD11  | 1.97                     | 0.47              |
| 11:K:19:ARG:HE    | 11:K:177:THR:HB   | 1.80                     | 0.47              |
| 5:S:49:ALA:HB1    | 5:S:202:LEU:HD11  | 1.97                     | 0.47              |
| 2:B:88:ARG:HD2    | 2:B:116:VAL:HG11  | 1.96                     | 0.47              |
| 9:I:59:ILE:HD12   | 9:I:82:MET:HB3    | 1.95                     | 0.47              |
| 11:K:29:LYS:HD3   | 11:K:32:HIS:HD2   | 1.80                     | 0.47              |
| 13:M:113:LEU:HD13 | 13:M:198:VAL:HG12 | 1.96                     | 0.47              |
| 14:N:10:SER:OG    | 14:N:142:GLY:N    | 2.48                     | 0.47              |
| 14:N:45:VAL:HG11  | 14:N:88:ILE:HD13  | 1.96                     | 0.47              |
| 2:P:73:LEU:HD13   | 2:P:133:LEU:HD22  | 1.97                     | 0.47              |
| 4:R:83:VAL:HG21   | 4:R:129:ILE:HD11  | 1.97                     | 0.47              |
| 11:Y:59:TYR:HE2   | 11:Y:87:ASN:HD22  | 1.61                     | 0.47              |
| 9:I:97:ALA:HB1    | 9:I:127:MET:HE2   | 1.97                     | 0.47              |
| 2:P:51:GLN:HB3    | 2:P:56:TYR:CD2    | 2.49                     | 0.47              |
| 3:C:161:ALA:HB1   | 3:C:175:LEU:HD13  | 1.97                     | 0.47              |
| 3:Q:161:ALA:HB1   | 3:Q:175:LEU:HD13  | 1.97                     | 0.47              |
| 4:R:87:ALA:HB1    | 4:R:107:ILE:HD11  | 1.96                     | 0.47              |
| 11:Y:19:ARG:HE    | 11:Y:177:THR:HB   | 1.80                     | 0.47              |
| 11:Y:29:LYS:HD3   | 11:Y:32:HIS:HD2   | 1.80                     | 0.47              |
| 4:D:91:CYS:HA     | 4:D:102:VAL:HG11  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:184:TYR:HE2  | 14:N:186:ARG:HB2  | 1.79                     | 0.47              |
| 3:Q:109:GLN:HE21  | 11:Y:71:ASN:HD21  | 1.62                     | 0.47              |
| 6:T:117:GLN:O     | 6:T:120:THR:OG1   | 2.24                     | 0.47              |
| 10:X:55:LEU:HD11  | 11:Y:121:LEU:HD13 | 1.97                     | 0.47              |
| 12:Z:40:TYR:CD2   | 12:Z:73:ARG:HD3   | 2.50                     | 0.47              |
| 10:J:148:MET:HE3  | 10:J:152:LEU:HD11 | 1.97                     | 0.46              |
| 6:T:117:GLN:NE2   | 7:U:83:ASP:HA     | 2.31                     | 0.46              |
| 11:Y:20:VAL:O     | 11:Y:34:LYS:NZ    | 2.48                     | 0.46              |
| 12:L:158:ARG:HD3  | 11:Y:145:ARG:HD3  | 1.97                     | 0.46              |
| 13:M:28:ARG:NH1   | 13:M:187:VAL:O    | 2.49                     | 0.46              |
| 5:S:182:GLN:HA    | 6:T:56:LEU:HD11   | 1.98                     | 0.46              |
| 10:X:58:ASP:OD2   | 10:X:103:TYR:N    | 2.35                     | 0.46              |
| 12:Z:97:MET:CG    | 12:Z:98:GLY:H     | 2.25                     | 0.46              |
| 13:a:113:LEU:HD13 | 13:a:198:VAL:HG12 | 1.96                     | 0.46              |
| 14:b:42:ILE:HD12  | 14:b:188:GLN:HB2  | 1.97                     | 0.46              |
| 5:E:182:GLN:HA    | 6:F:56:LEU:HD11   | 1.98                     | 0.46              |
| 10:J:178:ALA:HB1  | 12:Z:168:ALA:HB1  | 1.97                     | 0.46              |
| 14:N:124:TYR:HE1  | 14:N:139:THR:HG22 | 1.79                     | 0.46              |
| 4:R:168:VAL:HG13  | 4:R:194:ALA:HB1   | 1.98                     | 0.46              |
| 14:N:25:ASP:HA    | 14:N:187:PHE:HA   | 1.96                     | 0.46              |
| 14:b:10:SER:OG    | 14:b:142:GLY:N    | 2.48                     | 0.46              |
| 2:B:73:LEU:HD22   | 2:B:135:ILE:HG12  | 1.98                     | 0.46              |
| 10:J:101:PRO:O    | 11:K:93:ARG:NH2   | 2.49                     | 0.46              |
| 12:L:4:LEU:HB2    | 12:L:160:ILE:HD11 | 1.97                     | 0.46              |
| 12:L:40:TYR:CD2   | 12:L:73:ARG:HD3   | 2.51                     | 0.46              |
| 4:R:92:GLN:HG3    | 11:Y:66:LEU:HB2   | 1.97                     | 0.46              |
| 9:W:97:ALA:HB1    | 9:W:127:MET:HE2   | 1.97                     | 0.46              |
| 2:B:8:SER:HA      | 2:B:124:GLY:HA2   | 1.97                     | 0.46              |
| 10:J:55:LEU:HD11  | 11:K:121:LEU:HD13 | 1.97                     | 0.46              |
| 12:L:97:MET:CG    | 12:L:98:GLY:H     | 2.25                     | 0.46              |
| 12:L:127:SER:O    | 12:L:136:TYR:OH   | 2.23                     | 0.46              |
| 13:M:183:ALA:HA   | 13:M:189:THR:HG23 | 1.97                     | 0.46              |
| 10:X:66:LEU:HD21  | 10:X:86:LEU:HD11  | 1.97                     | 0.46              |
| 13:a:57:PHE:HZ    | 14:b:128:LEU:HB3  | 1.80                     | 0.46              |
| 13:a:68:ILE:HD11  | 13:a:92:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:72:ILE:HA     | 1:A:95:ARG:HG2    | 1.98                     | 0.46              |
| 6:F:70:ILE:HG12   | 6:F:105:VAL:HG22  | 1.98                     | 0.46              |
| 7:G:98:PHE:HE1    | 8:H:66:HIS:HE1    | 1.63                     | 0.46              |
| 10:J:19:VAL:HG23  | 10:J:189:ILE:HD12 | 1.98                     | 0.46              |
| 11:K:12:TYR:OH    | 11:K:151:ILE:HG23 | 2.16                     | 0.46              |
| 1:O:152:TYR:CD1   | 1:O:162:GLY:HA2   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:88:ARG:HD2    | 2:P:116:VAL:HG11  | 1.96                     | 0.46              |
| 11:Y:88:LEU:HG    | 11:Y:122:ALA:HB2  | 1.98                     | 0.46              |
| 1:A:152:TYR:CD1   | 1:A:162:GLY:HA2   | 2.51                     | 0.46              |
| 11:K:20:VAL:O     | 11:K:34:LYS:NZ    | 2.48                     | 0.46              |
| 11:K:174:ASN:N    | 11:Y:172:ILE:O    | 2.41                     | 0.46              |
| 4:R:91:CYS:HA     | 4:R:102:VAL:HG11  | 1.97                     | 0.46              |
| 5:S:42:THR:OG1    | 5:S:45:GLY:O      | 2.30                     | 0.46              |
| 7:U:219:LEU:HD12  | 7:U:220:THR:HG23  | 1.97                     | 0.46              |
| 10:X:101:PRO:O    | 11:Y:93:ARG:NH2   | 2.49                     | 0.46              |
| 10:X:148:MET:HE3  | 10:X:152:LEU:HD11 | 1.97                     | 0.46              |
| 2:B:73:LEU:HD13   | 2:B:133:LEU:HD22  | 1.97                     | 0.46              |
| 7:G:185:THR:O     | 7:G:189:ILE:HG12  | 2.16                     | 0.46              |
| 14:N:42:ILE:HD12  | 14:N:188:GLN:HB2  | 1.97                     | 0.46              |
| 2:P:120:TYR:HD1   | 2:P:126:VAL:HG21  | 1.81                     | 0.46              |
| 6:F:65:HIS:O      | 6:F:89:ARG:NE     | 2.49                     | 0.46              |
| 1:O:14:THR:HG22   | 1:O:24:GLN:HB3    | 1.98                     | 0.46              |
| 2:P:73:LEU:HD22   | 2:P:135:ILE:HG12  | 1.98                     | 0.46              |
| 5:S:22:PHE:HA     | 5:S:25:GLU:HB3    | 1.98                     | 0.46              |
| 12:Z:4:LEU:HB2    | 12:Z:160:ILE:HD11 | 1.96                     | 0.46              |
| 13:a:183:ALA:HA   | 13:a:189:THR:HG23 | 1.97                     | 0.46              |
| 14:b:27:LEU:HD13  | 14:b:184:TYR:HB2  | 1.98                     | 0.46              |
| 2:B:51:GLN:HB3    | 2:B:56:TYR:CD2    | 2.49                     | 0.45              |
| 4:D:92:GLN:HG3    | 11:K:66:LEU:HB2   | 1.97                     | 0.45              |
| 6:F:117:GLN:NE2   | 7:G:83:ASP:HA     | 2.31                     | 0.45              |
| 6:T:6:TYR:OH      | 7:U:8:ASP:OD2     | 2.27                     | 0.45              |
| 11:Y:12:TYR:HB2   | 11:Y:182:ILE:HD11 | 1.98                     | 0.45              |
| 12:Z:179:VAL:HG22 | 12:Z:184:TRP:HB3  | 1.99                     | 0.45              |
| 9:I:202:TYR:HD2   | 10:J:151:SER:HB3  | 1.81                     | 0.45              |
| 13:a:169:ASP:HB3  | 13:a:173:ARG:NH2  | 2.31                     | 0.45              |
| 14:b:25:ASP:O     | 14:b:41:ARG:NH2   | 2.49                     | 0.45              |
| 5:E:22:PHE:HA     | 5:E:25:GLU:HB3    | 1.98                     | 0.45              |
| 13:M:29:LEU:HG    | 13:M:36:HIS:CD2   | 2.51                     | 0.45              |
| 1:A:14:THR:HG22   | 1:A:24:GLN:HB3    | 1.98                     | 0.45              |
| 2:B:133:LEU:HB2   | 2:B:148:SER:HB3   | 1.99                     | 0.45              |
| 7:G:219:LEU:HD12  | 7:G:220:THR:HG23  | 1.97                     | 0.45              |
| 13:M:57:PHE:HZ    | 14:N:128:LEU:HB3  | 1.80                     | 0.45              |
| 2:P:8:SER:HA      | 2:P:124:GLY:HA2   | 1.97                     | 0.45              |
| 5:S:73:HIS:CE1    | 5:S:106:THR:HB    | 2.52                     | 0.45              |
| 1:A:22:LEU:HD13   | 1:A:25:VAL:HG21   | 1.98                     | 0.45              |
| 11:K:88:LEU:HG    | 11:K:122:ALA:HB2  | 1.98                     | 0.45              |
| 2:P:133:LEU:HB2   | 2:P:148:SER:HB3   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:W:202:TYR:HD2  | 10:X:151:SER:HB3  | 1.81                     | 0.45              |
| 11:Y:45:LEU:O    | 11:Y:103:LEU:N    | 2.44                     | 0.45              |
| 11:Y:117:TYR:N   | 11:Y:125:ALA:O    | 2.49                     | 0.45              |
| 13:a:29:LEU:HG   | 13:a:36:HIS:CD2   | 2.51                     | 0.45              |
| 2:B:118:GLN:NE2  | 3:C:82:ASP:HA     | 2.32                     | 0.45              |
| 5:E:73:HIS:CE1   | 5:E:106:THR:HB    | 2.52                     | 0.45              |
| 10:J:66:LEU:HD21 | 10:J:86:LEU:HD11  | 1.97                     | 0.45              |
| 7:U:98:PHE:HE1   | 8:V:66:HIS:HE1    | 1.63                     | 0.45              |
| 14:b:12:LEU:HD21 | 14:b:176:LEU:HD11 | 1.99                     | 0.45              |
| 5:E:41:GLN:HB3   | 5:E:166:ASP:HA    | 1.99                     | 0.45              |
| 10:J:14:LYS:HA   | 10:J:19:VAL:HG12  | 1.98                     | 0.45              |
| 11:K:167:LEU:O   | 11:K:171:PHE:HB3  | 2.16                     | 0.45              |
| 14:N:12:LEU:HD21 | 14:N:176:LEU:HD11 | 1.99                     | 0.45              |
| 1:O:22:LEU:HD13  | 1:O:25:VAL:HG21   | 1.98                     | 0.45              |
| 4:R:31:THR:OG1   | 4:R:163:ARG:O     | 2.31                     | 0.45              |
| 6:T:69:HIS:CD2   | 6:T:70:ILE:HG13   | 2.52                     | 0.45              |
| 10:X:14:LYS:HA   | 10:X:19:VAL:HG12  | 1.98                     | 0.45              |
| 10:X:19:VAL:HG23 | 10:X:189:ILE:HD12 | 1.98                     | 0.45              |
| 11:Y:9:GLY:HA3   | 11:Y:12:TYR:CZ    | 2.52                     | 0.45              |
| 5:E:160:GLY:HA3  | 6:F:79:ALA:HB2    | 1.99                     | 0.45              |
| 11:K:9:GLY:HA3   | 11:K:12:TYR:CZ    | 2.52                     | 0.45              |
| 12:L:33:LYS:O    | 12:L:45:MET:N     | 2.41                     | 0.45              |
| 2:P:118:GLN:NE2  | 3:Q:82:ASP:HA     | 2.32                     | 0.45              |
| 6:T:47:VAL:HG22  | 6:T:212:ILE:HG12  | 1.99                     | 0.45              |
| 6:T:65:HIS:O     | 6:T:89:ARG:NE     | 2.49                     | 0.45              |
| 7:U:185:THR:O    | 7:U:189:ILE:HG12  | 2.16                     | 0.45              |
| 11:Y:167:LEU:O   | 11:Y:171:PHE:HB3  | 2.16                     | 0.45              |
| 2:B:120:TYR:HD1  | 2:B:126:VAL:HG21  | 1.81                     | 0.45              |
| 4:D:168:VAL:HG13 | 4:D:194:ALA:HB1   | 1.98                     | 0.45              |
| 13:M:68:ILE:HD11 | 13:M:92:LEU:HD13  | 1.97                     | 0.45              |
| 1:O:72:ILE:HA    | 1:O:95:ARG:HG2    | 1.98                     | 0.45              |
| 1:O:86:ASP:OD1   | 7:U:120:HIS:NE2   | 2.36                     | 0.45              |
| 11:K:117:TYR:N   | 11:K:125:ALA:O    | 2.49                     | 0.45              |
| 8:V:1:THR:HG21   | 8:V:46:SER:HA     | 1.99                     | 0.45              |
| 11:Y:77:PRO:HD2  | 11:Y:108:ASP:HB2  | 1.99                     | 0.45              |
| 13:a:28:ARG:NH1  | 13:a:187:VAL:O    | 2.49                     | 0.45              |
| 4:D:140:GLY:O    | 4:D:213:ARG:CZ    | 2.64                     | 0.44              |
| 10:J:57:THR:O    | 11:K:85:ARG:NH2   | 2.51                     | 0.44              |
| 14:N:27:LEU:HD13 | 14:N:184:TYR:HB2  | 1.98                     | 0.44              |
| 14:N:96:MET:HE1  | 14:N:106:LEU:HB2  | 1.99                     | 0.44              |
| 4:R:88:ARG:HH11  | 11:Y:70:ARG:HA    | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:S:160:GLY:HA3   | 6:T:79:ALA:HB2    | 1.99                     | 0.44              |
| 6:T:70:ILE:HG12   | 6:T:105:VAL:HG22  | 1.98                     | 0.44              |
| 9:W:83:LEU:HB2    | 9:W:113:ILE:HD13  | 1.99                     | 0.44              |
| 4:D:88:ARG:HH11   | 11:K:70:ARG:HA    | 1.82                     | 0.44              |
| 6:F:69:HIS:CD2    | 6:F:70:ILE:HG13   | 2.52                     | 0.44              |
| 10:J:24:ASP:OD1   | 10:J:40:LYS:NZ    | 2.34                     | 0.44              |
| 2:P:124:GLY:H     | 3:Q:127:LYS:HE3   | 1.82                     | 0.44              |
| 6:T:10:VAL:HB     | 6:T:21:GLN:HG2    | 1.99                     | 0.44              |
| 14:b:96:MET:HE1   | 14:b:106:LEU:HB2  | 1.99                     | 0.44              |
| 6:F:192:LEU:HD13  | 6:F:233:LEU:HD23  | 2.00                     | 0.44              |
| 5:S:41:GLN:HA     | 5:S:46:VAL:HG12   | 1.99                     | 0.44              |
| 11:K:12:TYR:HB2   | 11:K:182:ILE:HD11 | 1.98                     | 0.44              |
| 5:S:41:GLN:HB3    | 5:S:166:ASP:HA    | 1.99                     | 0.44              |
| 6:T:192:LEU:HD13  | 6:T:233:LEU:HD23  | 2.00                     | 0.44              |
| 12:Z:33:LYS:HA    | 12:Z:45:MET:HE2   | 1.99                     | 0.44              |
| 3:C:172:VAL:O     | 3:C:176:LYS:HG3   | 2.18                     | 0.44              |
| 5:E:195:ILE:HG22  | 5:E:237:VAL:HG11  | 2.00                     | 0.44              |
| 12:L:179:VAL:HG22 | 12:L:184:TRP:HB3  | 1.99                     | 0.44              |
| 3:Q:172:VAL:O     | 3:Q:176:LYS:HG3   | 2.18                     | 0.44              |
| 10:X:55:LEU:HG    | 10:X:57:THR:HG22  | 2.00                     | 0.44              |
| 10:X:57:THR:O     | 11:Y:85:ARG:NH2   | 2.51                     | 0.44              |
| 11:Y:12:TYR:OH    | 11:Y:151:ILE:HG23 | 2.16                     | 0.44              |
| 13:a:29:LEU:HG    | 13:a:36:HIS:HD2   | 1.83                     | 0.44              |
| 1:A:158:GLY:O     | 2:B:83:ARG:NH2    | 2.51                     | 0.44              |
| 12:L:5:ALA:HA     | 12:L:13:ILE:O     | 2.18                     | 0.44              |
| 5:S:195:ILE:HG22  | 5:S:237:VAL:HG11  | 2.00                     | 0.44              |
| 6:F:47:VAL:HG22   | 6:F:212:ILE:HG12  | 1.99                     | 0.44              |
| 10:J:58:ASP:OD2   | 10:J:103:TYR:N    | 2.35                     | 0.44              |
| 13:M:11:THR:HG21  | 13:M:141:ALA:HB3  | 2.00                     | 0.44              |
| 2:P:70:HIS:CD2    | 2:P:71:ILE:HG13   | 2.53                     | 0.44              |
| 5:S:59:MET:SD     | 5:S:64:ILE:HD11   | 2.58                     | 0.44              |
| 7:U:215:TRP:HE1   | 7:U:219:LEU:HD11  | 1.83                     | 0.44              |
| 11:Y:156:ALA:O    | 11:Y:160:LEU:N    | 2.42                     | 0.44              |
| 14:b:72:ILE:O     | 14:b:76:LEU:HG    | 2.18                     | 0.44              |
| 5:E:41:GLN:HA     | 5:E:46:VAL:HG12   | 1.99                     | 0.44              |
| 9:I:8:TYR:CE2     | 9:I:13:VAL:HG23   | 2.53                     | 0.44              |
| 12:L:33:LYS:HA    | 12:L:45:MET:HE2   | 1.99                     | 0.44              |
| 3:Q:60:PHE:O      | 3:Q:62:SER:N      | 2.50                     | 0.44              |
| 3:C:60:PHE:O      | 3:C:62:SER:N      | 2.50                     | 0.44              |
| 5:E:59:MET:SD     | 5:E:64:ILE:HD11   | 2.58                     | 0.44              |
| 6:F:45:VAL:HG11   | 6:F:188:VAL:HG22  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:S:27:ALA:HB1   | 5:S:138:GLY:HA2   | 2.00                     | 0.44              |
| 10:X:67:LYS:HE3  | 10:X:71:ASN:HD21  | 1.83                     | 0.44              |
| 7:G:119:VAL:HG13 | 7:G:131:PHE:HD2   | 1.82                     | 0.43              |
| 10:J:25:ARG:HB3  | 10:J:36:THR:O     | 2.18                     | 0.43              |
| 7:U:119:VAL:HG13 | 7:U:131:PHE:HD2   | 1.82                     | 0.43              |
| 9:W:8:TYR:CE2    | 9:W:13:VAL:HG23   | 2.53                     | 0.43              |
| 7:G:215:TRP:HE1  | 7:G:219:LEU:HD11  | 1.83                     | 0.43              |
| 10:J:11:MET:HE3  | 10:J:166:ILE:HG13 | 2.00                     | 0.43              |
| 14:N:25:ASP:O    | 14:N:41:ARG:NH2   | 2.50                     | 0.43              |
| 8:V:142:THR:HG23 | 8:V:155:PHE:HE1   | 1.84                     | 0.43              |
| 9:W:174:ASP:OD1  | 9:W:187:ARG:NH1   | 2.51                     | 0.43              |
| 12:Z:103:GLY:HA2 | 12:Z:179:VAL:HG11 | 2.00                     | 0.43              |
| 13:M:5:TYR:OH    | 13:M:103:PRO:O    | 2.29                     | 0.43              |
| 1:O:158:GLY:O    | 2:P:83:ARG:NH2    | 2.51                     | 0.43              |
| 5:S:141:LEU:HB2  | 5:S:156:MET:HE2   | 2.00                     | 0.43              |
| 6:T:45:VAL:HG11  | 6:T:188:VAL:HG22  | 2.00                     | 0.43              |
| 12:Z:5:ALA:HA    | 12:Z:13:ILE:O     | 2.18                     | 0.43              |
| 12:Z:8:PHE:HE1   | 12:Z:10:HIS:HB2   | 1.83                     | 0.43              |
| 2:B:124:GLY:H    | 3:C:127:LYS:HE3   | 1.82                     | 0.43              |
| 8:H:142:THR:HG23 | 8:H:155:PHE:HE1   | 1.84                     | 0.43              |
| 9:I:163:ILE:HD13 | 9:I:192:PRO:HG2   | 2.00                     | 0.43              |
| 8:H:1:THR:HG21   | 8:H:46:SER:HA     | 1.99                     | 0.43              |
| 12:L:8:PHE:HE1   | 12:L:10:HIS:HB2   | 1.83                     | 0.43              |
| 13:M:57:PHE:CZ   | 14:N:128:LEU:HB3  | 2.53                     | 0.43              |
| 14:N:72:ILE:O    | 14:N:76:LEU:HG    | 2.18                     | 0.43              |
| 9:W:43:CYS:SG    | 9:W:98:LEU:HB3    | 2.58                     | 0.43              |
| 9:W:163:ILE:HD13 | 9:W:192:PRO:HG2   | 2.01                     | 0.43              |
| 4:D:31:THR:OG1   | 4:D:163:ARG:O     | 2.31                     | 0.43              |
| 5:E:41:GLN:NE2   | 5:E:152:GLN:HA    | 2.33                     | 0.43              |
| 12:L:58:LEU:HD12 | 12:L:61:ARG:HD3   | 2.01                     | 0.43              |
| 4:R:140:GLY:O    | 4:R:213:ARG:CZ    | 2.65                     | 0.43              |
| 10:X:25:ARG:HB3  | 10:X:36:THR:O     | 2.18                     | 0.43              |
| 10:X:117:LYS:HD2 | 10:X:118:PRO:HD2  | 2.01                     | 0.43              |
| 12:Z:167:ASP:HB3 | 12:Z:170:SER:HB2  | 2.01                     | 0.43              |
| 13:a:57:PHE:CZ   | 14:b:128:LEU:HB3  | 2.53                     | 0.43              |
| 9:I:43:CYS:SG    | 9:I:98:LEU:HB3    | 2.58                     | 0.43              |
| 13:M:29:LEU:HG   | 13:M:36:HIS:HD2   | 1.83                     | 0.43              |
| 13:M:169:ASP:HB3 | 13:M:173:ARG:NH2  | 2.31                     | 0.43              |
| 4:R:45:VAL:HG11  | 4:R:61:LYS:HB2    | 2.01                     | 0.43              |
| 13:a:8:ASN:OD1   | 13:a:58:HIS:N     | 2.41                     | 0.43              |
| 2:B:70:HIS:CD2   | 2:B:71:ILE:HG13   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:83:LEU:HB2   | 9:I:113:ILE:HD13  | 1.99                     | 0.43              |
| 10:J:55:LEU:HG   | 10:J:57:THR:HG22  | 2.00                     | 0.43              |
| 11:K:29:LYS:HE3  | 11:K:32:HIS:HA    | 2.01                     | 0.43              |
| 12:L:100:MET:HB3 | 12:L:111:LEU:HD11 | 2.00                     | 0.43              |
| 7:U:215:TRP:HZ3  | 7:U:227:VAL:HG13  | 1.84                     | 0.43              |
| 9:W:112:SER:HB3  | 9:W:125:VAL:HG21  | 2.00                     | 0.43              |
| 7:G:68:ASN:OD1   | 7:G:224:HIS:ND1   | 2.52                     | 0.43              |
| 11:K:77:PRO:HD2  | 11:K:108:ASP:HB2  | 1.99                     | 0.43              |
| 10:X:6:ASN:ND2   | 10:X:28:GLY:O     | 2.44                     | 0.43              |
| 13:a:11:THR:HG21 | 13:a:141:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:132:ARG:HD3  | 7:G:12:SER:HA     | 2.01                     | 0.43              |
| 7:G:215:TRP:HZ3  | 7:G:227:VAL:HG13  | 1.84                     | 0.43              |
| 9:I:112:SER:HB3  | 9:I:125:VAL:HG21  | 2.00                     | 0.43              |
| 9:I:122:LEU:HD22 | 9:I:125:VAL:HG12  | 2.00                     | 0.43              |
| 6:T:39:LYS:HB2   | 6:T:142:PRO:HB2   | 2.01                     | 0.43              |
| 8:V:19:ARG:NH1   | 8:V:168:GLY:O     | 2.46                     | 0.43              |
| 9:W:126:THR:OG1  | 9:W:135:MET:SD    | 2.72                     | 0.43              |
| 12:Z:58:LEU:HD12 | 12:Z:61:ARG:HD3   | 2.01                     | 0.43              |
| 3:C:171:ALA:HB2  | 3:C:200:THR:HG21  | 2.01                     | 0.42              |
| 9:I:19:ARG:NH1   | 9:I:167:LEU:O     | 2.51                     | 0.42              |
| 10:J:117:LYS:HD2 | 10:J:118:PRO:HD2  | 2.01                     | 0.42              |
| 12:L:3:THR:OG1   | 12:L:128:VAL:HB   | 2.19                     | 0.42              |
| 14:N:1:THR:N     | 14:N:105:PRO:O    | 2.36                     | 0.42              |
| 10:X:51:GLY:C    | 10:X:52:LEU:HD12  | 2.44                     | 0.42              |
| 3:C:214:ALA:HB2  | 3:C:227:VAL:HG22  | 2.00                     | 0.42              |
| 3:Q:214:ALA:HB2  | 3:Q:227:VAL:HG22  | 2.00                     | 0.42              |
| 5:S:69:GLU:HG2   | 5:S:226:PHE:CD2   | 2.55                     | 0.42              |
| 10:X:11:MET:HE3  | 10:X:166:ILE:HG13 | 2.00                     | 0.42              |
| 2:B:38:LYS:HG3   | 2:B:43:VAL:HG22   | 2.01                     | 0.42              |
| 5:E:27:ALA:HB1   | 5:E:138:GLY:HA2   | 2.00                     | 0.42              |
| 6:F:10:VAL:HB    | 6:F:21:GLN:HG2    | 1.99                     | 0.42              |
| 6:F:47:VAL:HG11  | 6:F:192:LEU:HD23  | 2.01                     | 0.42              |
| 10:J:67:LYS:HE3  | 10:J:71:ASN:HD21  | 1.83                     | 0.42              |
| 14:N:166:ARG:NH2 | 14:N:200:GLU:OE1  | 2.43                     | 0.42              |
| 2:P:38:LYS:HG3   | 2:P:43:VAL:HG22   | 2.01                     | 0.42              |
| 12:Z:100:MET:HB3 | 12:Z:111:LEU:HD11 | 2.00                     | 0.42              |
| 13:a:27:THR:O    | 13:a:40:SER:N     | 2.53                     | 0.42              |
| 2:B:108:GLN:HE22 | 10:J:76:LYS:HG2   | 1.85                     | 0.42              |
| 4:D:64:ALA:O     | 4:D:88:ARG:NE     | 2.53                     | 0.42              |
| 11:K:42:ILE:HG22 | 11:K:106:GLY:HA3  | 2.02                     | 0.42              |
| 11:K:47:VAL:O    | 11:K:101:ASN:N    | 2.41                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:185:ARG:HA   | 9:W:26:VAL:HB     | 2.02                     | 0.42              |
| 1:O:159:TYR:CZ    | 1:O:161:CYS:HB3   | 2.55                     | 0.42              |
| 3:Q:119:GLN:HE22  | 4:R:79:ASP:HA     | 1.84                     | 0.42              |
| 5:S:41:GLN:NE2    | 5:S:152:GLN:HA    | 2.33                     | 0.42              |
| 9:W:19:ARG:NH1    | 9:W:167:LEU:O     | 2.51                     | 0.42              |
| 2:B:121:THR:HG22  | 2:B:128:PRO:HB3   | 2.02                     | 0.42              |
| 3:C:86:LEU:HD22   | 3:C:114:LEU:HD11  | 2.01                     | 0.42              |
| 9:I:174:ASP:OD1   | 9:I:187:ARG:NH1   | 2.51                     | 0.42              |
| 12:L:103:GLY:HA2  | 12:L:179:VAL:HG11 | 2.00                     | 0.42              |
| 14:N:187:PHE:HE1  | 14:N:189:ILE:HD11 | 1.85                     | 0.42              |
| 1:O:132:ARG:HD3   | 7:U:12:SER:HA     | 2.01                     | 0.42              |
| 9:W:122:LEU:HD22  | 9:W:125:VAL:HG12  | 2.00                     | 0.42              |
| 10:J:121:CYS:SG   | 10:J:122:SER:N    | 2.92                     | 0.42              |
| 13:M:27:THR:O     | 13:M:40:SER:N     | 2.53                     | 0.42              |
| 6:T:95:SER:O      | 6:T:99:PHE:N      | 2.47                     | 0.42              |
| 10:X:121:CYS:SG   | 10:X:122:SER:N    | 2.92                     | 0.42              |
| 12:Z:3:THR:OG1    | 12:Z:128:VAL:HB   | 2.19                     | 0.42              |
| 5:E:141:LEU:HB2   | 5:E:156:MET:HE2   | 2.00                     | 0.42              |
| 6:F:39:LYS:HB2    | 6:F:142:PRO:HB2   | 2.01                     | 0.42              |
| 10:J:12:ALA:HA    | 10:J:21:ILE:HA    | 2.01                     | 0.42              |
| 10:J:51:GLY:C     | 10:J:52:LEU:HD12  | 2.44                     | 0.42              |
| 13:M:4:PRO:O      | 14:N:100:ARG:NH1  | 2.41                     | 0.42              |
| 7:U:21:PHE:HB3    | 7:U:25:TYR:CE2    | 2.55                     | 0.42              |
| 11:Y:13:VAL:HG11  | 11:Y:106:GLY:N    | 2.35                     | 0.42              |
| 13:a:108:ASN:HB2  | 13:a:124:PHE:HB2  | 2.01                     | 0.42              |
| 5:E:69:GLU:HG2    | 5:E:226:PHE:CD2   | 2.55                     | 0.42              |
| 5:E:110:GLU:HA    | 5:E:154:PHE:HE2   | 1.85                     | 0.42              |
| 10:J:142:ALA:HB1  | 10:J:146:TYR:HE2  | 1.85                     | 0.42              |
| 14:N:56:ASP:N     | 14:N:107:TRP:HD1  | 2.17                     | 0.42              |
| 10:X:44:MET:HE3   | 10:X:66:LEU:HD23  | 2.02                     | 0.42              |
| 11:Y:14:LEU:HD12  | 11:Y:182:ILE:HD13 | 2.01                     | 0.42              |
| 13:a:166:LEU:HD11 | 13:a:171:ALA:HB2  | 2.02                     | 0.42              |
| 2:P:121:THR:HG22  | 2:P:128:PRO:HB3   | 2.01                     | 0.42              |
| 3:Q:86:LEU:HD22   | 3:Q:114:LEU:HD11  | 2.01                     | 0.42              |
| 9:W:187:ARG:CB    | 9:W:188:PRO:CD    | 2.86                     | 0.42              |
| 11:Y:29:LYS:HE3   | 11:Y:32:HIS:HA    | 2.01                     | 0.42              |
| 1:A:191:PHE:H     | 1:A:194:THR:HG23  | 1.85                     | 0.42              |
| 14:N:92:LEU:HD21  | 14:N:110:MET:SD   | 2.60                     | 0.42              |
| 11:Y:29:LYS:HD3   | 11:Y:32:HIS:CD2   | 2.55                     | 0.42              |
| 12:Z:40:TYR:OH    | 12:Z:74:ILE:HG22  | 2.20                     | 0.42              |
| 14:b:187:PHE:HE1  | 14:b:189:ILE:HD11 | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:29:LYS:HD3   | 11:K:32:HIS:CD2   | 2.55                     | 0.41              |
| 2:P:108:GLN:HE22  | 10:X:76:LYS:HG2   | 1.85                     | 0.41              |
| 3:Q:122:THR:HG22  | 3:Q:129:PRO:HB3   | 2.02                     | 0.41              |
| 5:S:68:VAL:HB     | 5:S:93:ARG:HH21   | 1.85                     | 0.41              |
| 5:S:73:HIS:CD2    | 5:S:74:ILE:HG13   | 2.55                     | 0.41              |
| 10:X:142:ALA:HB1  | 10:X:146:TYR:HE2  | 1.85                     | 0.41              |
| 11:Y:42:ILE:HG22  | 11:Y:106:GLY:HA3  | 2.02                     | 0.41              |
| 1:A:159:TYR:CZ    | 1:A:161:CYS:HB3   | 2.55                     | 0.41              |
| 12:L:167:ASP:HB3  | 12:L:170:SER:HB2  | 2.01                     | 0.41              |
| 2:P:72:GLY:HA3    | 2:P:217:PHE:CE2   | 2.55                     | 0.41              |
| 3:Q:171:ALA:HB2   | 3:Q:200:THR:HG21  | 2.01                     | 0.41              |
| 6:T:47:VAL:HG11   | 6:T:192:LEU:HD23  | 2.01                     | 0.41              |
| 10:X:110:GLY:HA2  | 10:X:189:ILE:HD13 | 2.02                     | 0.41              |
| 11:Y:29:LYS:HZ3   | 12:Z:122:SER:C    | 2.27                     | 0.41              |
| 5:E:73:HIS:CD2    | 5:E:74:ILE:HG13   | 2.55                     | 0.41              |
| 8:H:99:ILE:HA     | 8:H:113:SER:HA    | 2.02                     | 0.41              |
| 10:J:44:MET:HE3   | 10:J:66:LEU:HD23  | 2.02                     | 0.41              |
| 11:K:6:GLY:HA3    | 11:K:15:VAL:HG12  | 2.02                     | 0.41              |
| 7:U:68:ASN:OD1    | 7:U:224:HIS:ND1   | 2.52                     | 0.41              |
| 9:W:18:THR:OG1    | 9:W:172:ASN:HB2   | 2.20                     | 0.41              |
| 11:Y:6:GLY:HA3    | 11:Y:15:VAL:HG12  | 2.02                     | 0.41              |
| 11:Y:9:GLY:HA3    | 11:Y:12:TYR:CE2   | 2.56                     | 0.41              |
| 4:D:45:VAL:HG11   | 4:D:61:LYS:HB2    | 2.01                     | 0.41              |
| 4:D:65:LEU:HD22   | 4:D:87:ALA:HB3    | 2.02                     | 0.41              |
| 8:H:133:SER:HA    | 8:H:136:TYR:CE2   | 2.55                     | 0.41              |
| 9:I:8:TYR:HE2     | 9:I:13:VAL:HG23   | 1.86                     | 0.41              |
| 9:I:18:THR:OG1    | 9:I:172:ASN:HB2   | 2.20                     | 0.41              |
| 11:K:9:GLY:HA3    | 11:K:12:TYR:CE2   | 2.55                     | 0.41              |
| 12:L:179:VAL:HA   | 12:L:184:TRP:HA   | 2.03                     | 0.41              |
| 13:M:36:HIS:HB3   | 14:N:132:TYR:CE2  | 2.55                     | 0.41              |
| 13:M:166:LEU:HD11 | 13:M:171:ALA:HB2  | 2.02                     | 0.41              |
| 14:b:56:ASP:N     | 14:b:107:TRP:HD1  | 2.17                     | 0.41              |
| 1:A:122:SER:HA    | 1:A:125:TYR:HD2   | 1.86                     | 0.41              |
| 3:C:119:GLN:HE22  | 4:D:79:ASP:HA     | 1.84                     | 0.41              |
| 9:I:1:THR:HG21    | 9:I:46:ALA:HA     | 2.03                     | 0.41              |
| 11:K:14:LEU:HD12  | 11:K:182:ILE:HD13 | 2.01                     | 0.41              |
| 11:K:29:LYS:HE3   | 11:K:31:ASP:O     | 2.21                     | 0.41              |
| 4:R:64:ALA:O      | 4:R:88:ARG:NE     | 2.53                     | 0.41              |
| 2:B:72:GLY:HA3    | 2:B:217:PHE:CE2   | 2.55                     | 0.41              |
| 5:E:68:VAL:HB     | 5:E:93:ARG:HH21   | 1.85                     | 0.41              |
| 6:F:144:ILE:O     | 6:F:144:ILE:HG22  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:21:PHE:HB3    | 7:G:25:TYR:CE2    | 2.55                     | 0.41              |
| 7:G:45:VAL:HG13   | 7:G:148:LEU:HD12  | 2.02                     | 0.41              |
| 7:G:150:MET:HE2   | 7:G:160:TYR:CZ    | 2.56                     | 0.41              |
| 12:L:40:TYR:OH    | 12:L:74:ILE:HG22  | 2.20                     | 0.41              |
| 12:L:91:LYS:NZ    | 12:L:117:GLU:O    | 2.52                     | 0.41              |
| 7:U:47:PHE:HZ     | 7:U:138:GLY:HA3   | 1.86                     | 0.41              |
| 11:Y:47:VAL:O     | 11:Y:101:ASN:N    | 2.41                     | 0.41              |
| 14:b:166:ARG:NH2  | 14:b:200:GLU:OE1  | 2.43                     | 0.41              |
| 7:G:131:PHE:O     | 7:G:153:PRO:HB3   | 2.21                     | 0.41              |
| 11:K:173:LEU:HD23 | 11:Y:173:LEU:HD23 | 2.02                     | 0.41              |
| 2:P:10:THR:HG22   | 2:P:18:LEU:HD22   | 2.02                     | 0.41              |
| 6:T:103:LEU:HD23  | 6:T:104:PRO:O     | 2.21                     | 0.41              |
| 8:V:133:SER:HA    | 8:V:136:TYR:CE2   | 2.55                     | 0.41              |
| 13:a:49:LYS:HD2   | 13:a:113:LEU:HB2  | 2.02                     | 0.41              |
| 11:K:13:VAL:HG11  | 11:K:106:GLY:N    | 2.35                     | 0.41              |
| 13:M:108:ASN:HB2  | 13:M:124:PHE:HB2  | 2.01                     | 0.41              |
| 11:Y:129:PHE:HB2  | 11:Y:143:LEU:HD13 | 2.03                     | 0.41              |
| 13:a:36:HIS:HB3   | 14:b:132:TYR:CE2  | 2.55                     | 0.41              |
| 14:b:92:LEU:HD21  | 14:b:110:MET:SD   | 2.60                     | 0.41              |
| 1:A:69:LEU:HD13   | 1:A:216:GLU:HG3   | 2.03                     | 0.41              |
| 1:A:152:TYR:HD1   | 1:A:162:GLY:HA2   | 1.86                     | 0.41              |
| 4:D:66:ASP:OD1    | 4:D:67:ASP:N      | 2.50                     | 0.41              |
| 5:E:68:VAL:HB     | 5:E:93:ARG:NH2    | 2.36                     | 0.41              |
| 7:G:69:VAL:HA     | 7:G:92:ARG:HG2    | 2.03                     | 0.41              |
| 8:H:19:ARG:NH1    | 8:H:168:GLY:O     | 2.46                     | 0.41              |
| 11:K:38:MET:HB2   | 11:K:42:ILE:HG13  | 2.03                     | 0.41              |
| 12:L:41:LEU:HD21  | 12:L:101:ILE:HG23 | 2.03                     | 0.41              |
| 13:M:49:LYS:HD2   | 13:M:113:LEU:HB2  | 2.02                     | 0.41              |
| 14:N:67:LEU:HD11  | 14:N:88:ILE:HG23  | 2.02                     | 0.41              |
| 1:O:191:PHE:H     | 1:O:194:THR:HG23  | 1.85                     | 0.41              |
| 4:R:65:LEU:HD22   | 4:R:87:ALA:HB3    | 2.02                     | 0.41              |
| 5:S:110:GLU:HA    | 5:S:154:PHE:HE2   | 1.85                     | 0.41              |
| 7:U:88:ALA:O      | 7:U:92:ARG:HG3    | 2.21                     | 0.41              |
| 10:X:12:ALA:HA    | 10:X:21:ILE:HA    | 2.01                     | 0.41              |
| 12:Z:41:LEU:HD21  | 12:Z:101:ILE:HG23 | 2.03                     | 0.41              |
| 10:J:110:GLY:HA2  | 10:J:189:ILE:HD13 | 2.02                     | 0.41              |
| 11:K:129:PHE:HB2  | 11:K:143:LEU:HD13 | 2.03                     | 0.41              |
| 12:L:180:ARG:HH21 | 12:L:185:ILE:HG21 | 1.86                     | 0.41              |
| 13:M:85:THR:HG21  | 13:M:120:ALA:HB3  | 2.02                     | 0.41              |
| 2:P:32:ALA:HA     | 2:P:33:PRO:HD3    | 1.98                     | 0.41              |
| 6:T:106:SER:OG    | 14:b:79:ASP:OD2   | 2.39                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:53:HIS:HB3   | 3:C:56:LEU:HG    | 2.04                     | 0.40              |
| 7:G:88:ALA:O     | 7:G:92:ARG:HG3   | 2.21                     | 0.40              |
| 3:Q:123:GLN:HG3  | 4:R:125:ARG:HG2  | 2.02                     | 0.40              |
| 6:T:144:ILE:HG22 | 6:T:144:ILE:O    | 2.20                     | 0.40              |
| 9:W:8:TYR:HE2    | 9:W:13:VAL:HG23  | 1.86                     | 0.40              |
| 11:Y:108:ASP:HB3 | 11:Y:111:GLU:HB3 | 2.03                     | 0.40              |
| 12:Z:179:VAL:HA  | 12:Z:184:TRP:HA  | 2.03                     | 0.40              |
| 3:C:122:THR:HG22 | 3:C:129:PRO:HB3  | 2.02                     | 0.40              |
| 5:E:166:ASP:HB3  | 5:E:185:TYR:CZ   | 2.56                     | 0.40              |
| 13:M:185:ARG:HG2 | 9:W:29:LYS:NZ    | 2.36                     | 0.40              |
| 9:W:112:SER:HB3  | 9:W:125:VAL:HG11 | 2.03                     | 0.40              |
| 11:Y:29:LYS:HE3  | 11:Y:31:ASP:O    | 2.21                     | 0.40              |
| 7:G:47:PHE:HZ    | 7:G:138:GLY:HA3  | 1.86                     | 0.40              |
| 7:G:215:TRP:CE3  | 7:G:227:VAL:HG22 | 2.56                     | 0.40              |
| 1:O:152:TYR:HD1  | 1:O:162:GLY:HA2  | 1.86                     | 0.40              |
| 11:Y:38:MET:HB2  | 11:Y:42:ILE:HG13 | 2.03                     | 0.40              |
| 11:Y:92:LEU:HD12 | 11:Y:93:ARG:HG3  | 2.03                     | 0.40              |
| 1:A:72:ILE:HG21  | 1:A:114:LEU:HD21 | 2.03                     | 0.40              |
| 2:B:10:THR:HG22  | 2:B:18:LEU:HD22  | 2.02                     | 0.40              |
| 7:G:39:ILE:HD12  | 7:G:193:VAL:HG22 | 2.04                     | 0.40              |
| 9:I:114:TYR:HD1  | 9:I:127:MET:HE3  | 1.87                     | 0.40              |
| 4:R:115:LYS:NZ   | 4:R:147:THR:OG1  | 2.42                     | 0.40              |
| 9:W:1:THR:HG21   | 9:W:46:ALA:HA    | 2.03                     | 0.40              |
| 3:C:123:GLN:HG3  | 4:D:125:ARG:HG2  | 2.02                     | 0.40              |
| 6:F:95:SER:O     | 6:F:99:PHE:N     | 2.47                     | 0.40              |
| 10:J:29:ILE:HG22 | 10:J:30:GLN:N    | 2.32                     | 0.40              |
| 11:K:108:ASP:HB3 | 11:K:111:GLU:HB3 | 2.03                     | 0.40              |
| 13:M:55:SER:OG   | 13:M:107:TYR:HB2 | 2.22                     | 0.40              |
| 3:Q:53:HIS:HB3   | 3:Q:56:LEU:HG    | 2.04                     | 0.40              |
| 5:S:166:ASP:HB3  | 5:S:185:TYR:CZ   | 2.56                     | 0.40              |
| 6:T:35:THR:HG22  | 6:T:48:ALA:HB1   | 2.04                     | 0.40              |
| 7:U:69:VAL:HA    | 7:U:92:ARG:HG2   | 2.03                     | 0.40              |
| 7:U:87:LEU:HD13  | 7:U:135:PHE:CE2  | 2.57                     | 0.40              |
| 7:U:131:PHE:O    | 7:U:153:PRO:HB3  | 2.21                     | 0.40              |
| 8:V:7:GLN:HB2    | 8:V:111:VAL:HG23 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 238/246 (97%) | 229 (96%) | 8 (3%)  | 1 (0%)   | 30          | 64  |
| 1   | O     | 238/246 (97%) | 227 (95%) | 11 (5%) | 0        | 100         | 100 |
| 2   | B     | 227/234 (97%) | 222 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 2   | P     | 227/234 (97%) | 222 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 3   | C     | 245/261 (94%) | 231 (94%) | 14 (6%) | 0        | 100         | 100 |
| 3   | Q     | 245/261 (94%) | 231 (94%) | 14 (6%) | 0        | 100         | 100 |
| 4   | D     | 230/248 (93%) | 223 (97%) | 6 (3%)  | 1 (0%)   | 30          | 64  |
| 4   | R     | 230/248 (93%) | 223 (97%) | 6 (3%)  | 1 (0%)   | 30          | 64  |
| 5   | E     | 231/241 (96%) | 225 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 5   | S     | 231/241 (96%) | 225 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 6   | F     | 231/263 (88%) | 227 (98%) | 3 (1%)  | 1 (0%)   | 30          | 64  |
| 6   | T     | 231/263 (88%) | 227 (98%) | 3 (1%)  | 1 (0%)   | 30          | 64  |
| 7   | G     | 237/255 (93%) | 232 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 7   | U     | 237/255 (93%) | 232 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 8   | H     | 200/205 (98%) | 197 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 8   | V     | 200/205 (98%) | 197 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 9   | I     | 218/234 (93%) | 205 (94%) | 13 (6%) | 0        | 100         | 100 |
| 9   | W     | 218/234 (93%) | 205 (94%) | 13 (6%) | 0        | 100         | 100 |
| 10  | J     | 202/205 (98%) | 194 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 10  | X     | 202/205 (98%) | 194 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 11  | K     | 194/201 (96%) | 189 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 11  | Y     | 194/201 (96%) | 189 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 12  | L     | 198/204 (97%) | 195 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 12  | Z     | 198/204 (97%) | 195 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 13  | M     | 210/213 (99%) | 203 (97%) | 7 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 13  | a     | 210/213 (99%)   | 203 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 14  | N     | 210/219 (96%)   | 206 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 14  | b     | 210/219 (96%)   | 206 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| All | All   | 6142/6458 (95%) | 5954 (97%) | 183 (3%) | 5 (0%)   | 49          | 80  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 184 | LYS  |
| 4   | D     | 216 | SER  |
| 4   | R     | 216 | SER  |
| 6   | F     | 59  | HIS  |
| 6   | T     | 59  | HIS  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 163/210 (78%) | 163 (100%) | 0        | 100         | 100 |
| 1   | O     | 163/210 (78%) | 163 (100%) | 0        | 100         | 100 |
| 2   | B     | 150/191 (78%) | 150 (100%) | 0        | 100         | 100 |
| 2   | P     | 150/191 (78%) | 150 (100%) | 0        | 100         | 100 |
| 3   | C     | 160/221 (72%) | 160 (100%) | 0        | 100         | 100 |
| 3   | Q     | 160/221 (72%) | 160 (100%) | 0        | 100         | 100 |
| 4   | D     | 136/211 (64%) | 136 (100%) | 0        | 100         | 100 |
| 4   | R     | 136/211 (64%) | 136 (100%) | 0        | 100         | 100 |
| 5   | E     | 158/203 (78%) | 158 (100%) | 0        | 100         | 100 |
| 5   | S     | 158/203 (78%) | 158 (100%) | 0        | 100         | 100 |
| 6   | F     | 160/224 (71%) | 160 (100%) | 0        | 100         | 100 |
| 6   | T     | 160/224 (71%) | 160 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 7   | G     | 162/212 (76%)   | 162 (100%)  | 0        | 100         | 100 |
| 7   | U     | 162/212 (76%)   | 162 (100%)  | 0        | 100         | 100 |
| 8   | H     | 140/159 (88%)   | 140 (100%)  | 0        | 100         | 100 |
| 8   | V     | 140/159 (88%)   | 140 (100%)  | 0        | 100         | 100 |
| 9   | I     | 157/195 (80%)   | 157 (100%)  | 0        | 100         | 100 |
| 9   | W     | 157/195 (80%)   | 157 (100%)  | 0        | 100         | 100 |
| 10  | J     | 155/174 (89%)   | 155 (100%)  | 0        | 100         | 100 |
| 10  | X     | 155/174 (89%)   | 155 (100%)  | 0        | 100         | 100 |
| 11  | K     | 148/171 (86%)   | 148 (100%)  | 0        | 100         | 100 |
| 11  | Y     | 148/171 (86%)   | 148 (100%)  | 0        | 100         | 100 |
| 12  | L     | 138/159 (87%)   | 138 (100%)  | 0        | 100         | 100 |
| 12  | Z     | 138/159 (87%)   | 138 (100%)  | 0        | 100         | 100 |
| 13  | M     | 158/178 (89%)   | 158 (100%)  | 0        | 100         | 100 |
| 13  | a     | 158/178 (89%)   | 158 (100%)  | 0        | 100         | 100 |
| 14  | N     | 149/181 (82%)   | 149 (100%)  | 0        | 100         | 100 |
| 14  | b     | 149/181 (82%)   | 149 (100%)  | 0        | 100         | 100 |
| All | All   | 4268/5378 (79%) | 4268 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | GLN  |
| 1   | A     | 128 | ASN  |
| 1   | A     | 193 | GLN  |
| 2   | B     | 51  | GLN  |
| 2   | B     | 87  | HIS  |
| 2   | B     | 108 | GLN  |
| 3   | C     | 88  | ASN  |
| 3   | C     | 102 | GLN  |
| 3   | C     | 109 | GLN  |
| 3   | C     | 167 | ASN  |
| 4   | D     | 54  | GLN  |
| 4   | D     | 92  | GLN  |
| 4   | D     | 154 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 175 | ASN  |
| 5   | E     | 97  | GLN  |
| 5   | E     | 225 | ASN  |
| 6   | F     | 43  | HIS  |
| 6   | F     | 69  | HIS  |
| 6   | F     | 175 | HIS  |
| 8   | H     | 7   | GLN  |
| 8   | H     | 38  | HIS  |
| 8   | H     | 123 | GLN  |
| 8   | H     | 187 | GLN  |
| 9   | I     | 66  | HIS  |
| 10  | J     | 92  | ASN  |
| 10  | J     | 168 | GLN  |
| 10  | J     | 187 | HIS  |
| 11  | K     | 32  | HIS  |
| 11  | K     | 55  | GLN  |
| 11  | K     | 61  | GLN  |
| 11  | K     | 63  | ASN  |
| 11  | K     | 87  | ASN  |
| 11  | K     | 101 | ASN  |
| 13  | M     | 108 | ASN  |
| 13  | M     | 146 | GLN  |
| 13  | M     | 157 | ASN  |
| 14  | N     | 69  | GLN  |
| 14  | N     | 81  | HIS  |
| 14  | N     | 188 | GLN  |
| 1   | O     | 24  | GLN  |
| 1   | O     | 128 | ASN  |
| 1   | O     | 193 | GLN  |
| 2   | P     | 51  | GLN  |
| 2   | P     | 87  | HIS  |
| 2   | P     | 108 | GLN  |
| 3   | Q     | 88  | ASN  |
| 3   | Q     | 102 | GLN  |
| 3   | Q     | 109 | GLN  |
| 4   | R     | 54  | GLN  |
| 4   | R     | 92  | GLN  |
| 4   | R     | 146 | GLN  |
| 4   | R     | 154 | HIS  |
| 4   | R     | 175 | ASN  |
| 5   | S     | 97  | GLN  |
| 5   | S     | 225 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | T     | 43  | HIS  |
| 6   | T     | 175 | HIS  |
| 8   | V     | 7   | GLN  |
| 8   | V     | 38  | HIS  |
| 8   | V     | 123 | GLN  |
| 8   | V     | 187 | GLN  |
| 10  | X     | 92  | ASN  |
| 10  | X     | 168 | GLN  |
| 11  | Y     | 32  | HIS  |
| 11  | Y     | 55  | GLN  |
| 11  | Y     | 61  | GLN  |
| 11  | Y     | 63  | ASN  |
| 11  | Y     | 87  | ASN  |
| 11  | Y     | 101 | ASN  |
| 13  | a     | 108 | ASN  |
| 13  | a     | 146 | GLN  |
| 13  | a     | 157 | ASN  |
| 14  | b     | 69  | GLN  |
| 14  | b     | 81  | HIS  |
| 14  | b     | 188 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

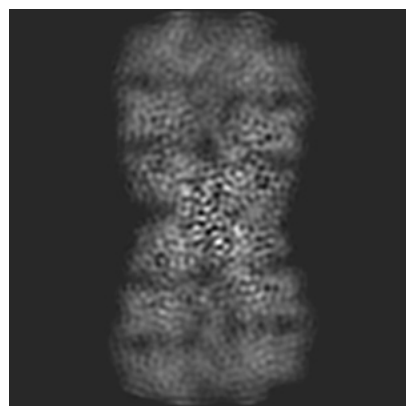
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31727. These allow visual inspection of the internal detail of the map and identification of artifacts.

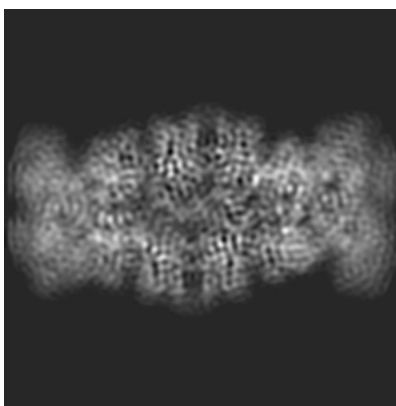
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

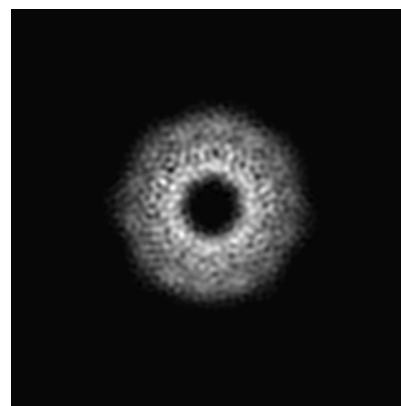
#### 6.1.1 Primary map



X

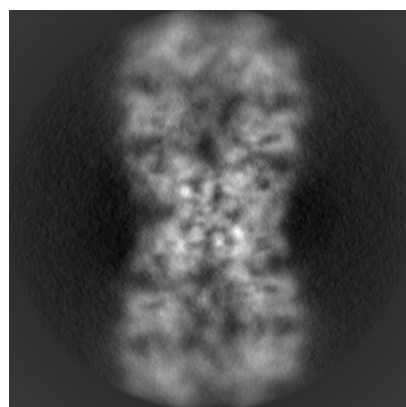


Y

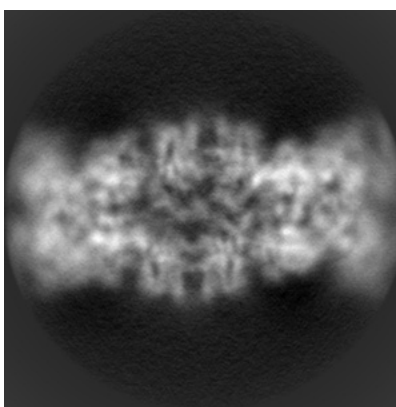


Z

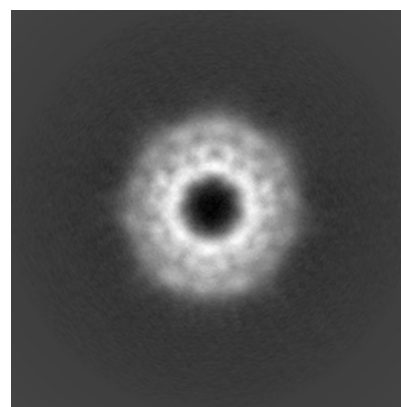
#### 6.1.2 Raw map



X



Y

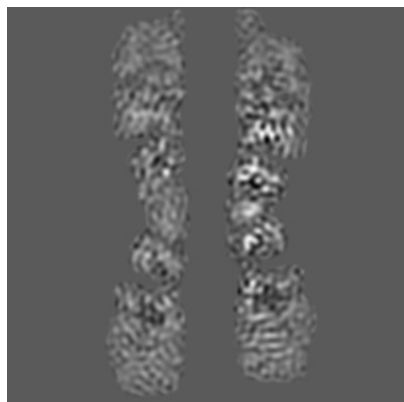


Z

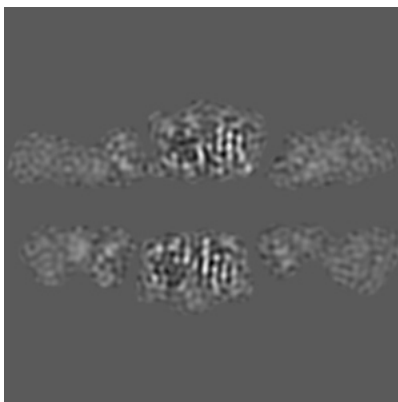
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

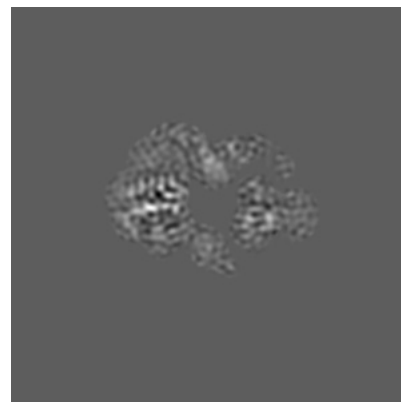
### 6.2.1 Primary map



X Index: 128

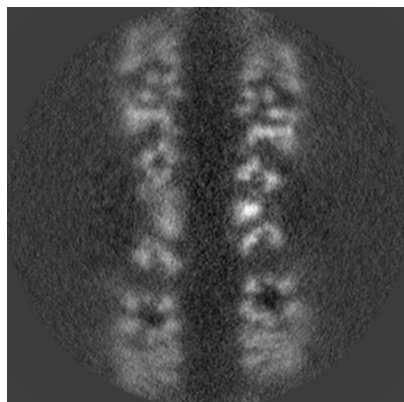


Y Index: 128

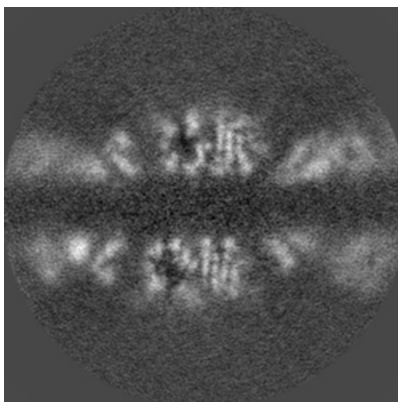


Z Index: 128

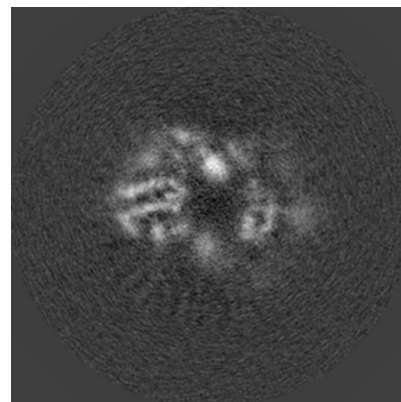
### 6.2.2 Raw map



X Index: 128



Y Index: 128

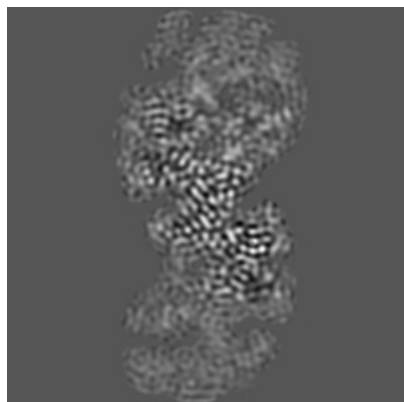


Z Index: 128

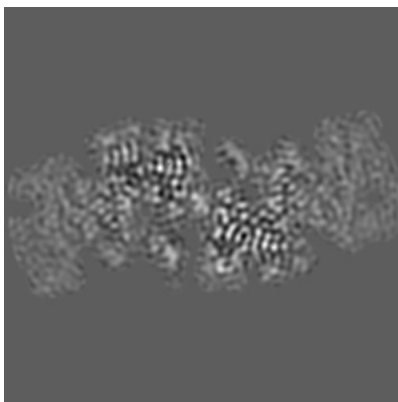
The images above show central slices of the map in three orthogonal directions.

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

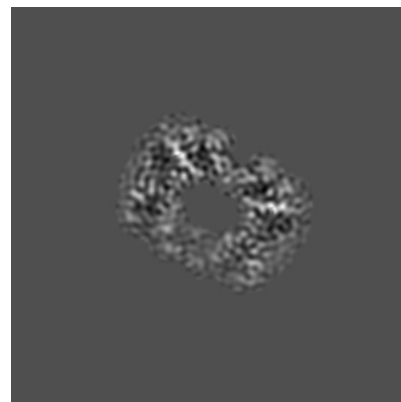
### 6.3.1 Primary map



X Index: 154

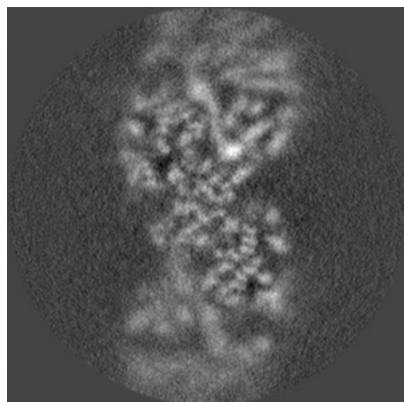


Y Index: 156

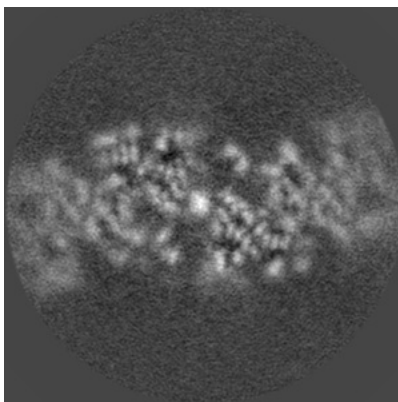


Z Index: 144

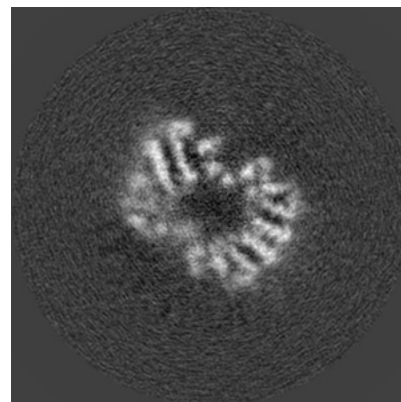
### 6.3.2 Raw map



X Index: 151



Y Index: 154

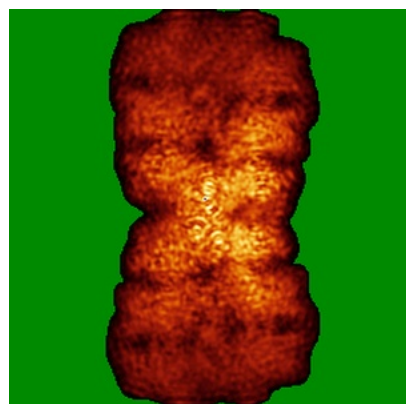


Z Index: 149

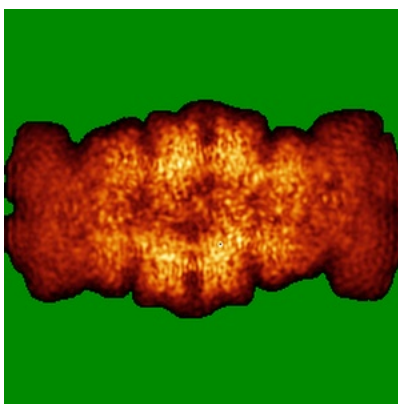
The images above show the largest variance slices of the map in three orthogonal directions.

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

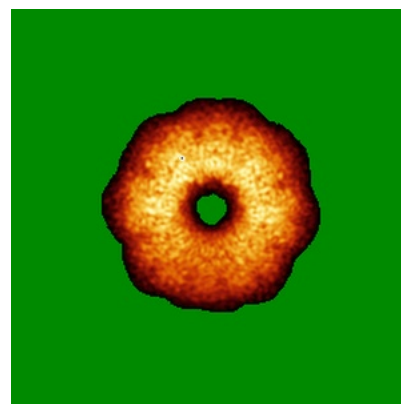
### 6.4.1 Primary map



X

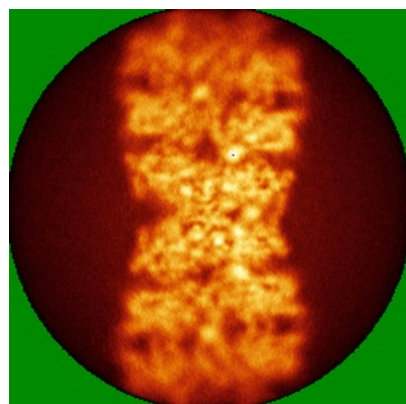


Y

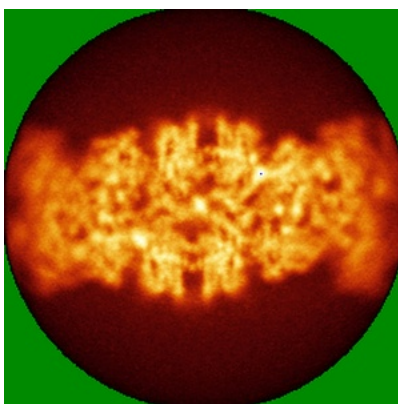


Z

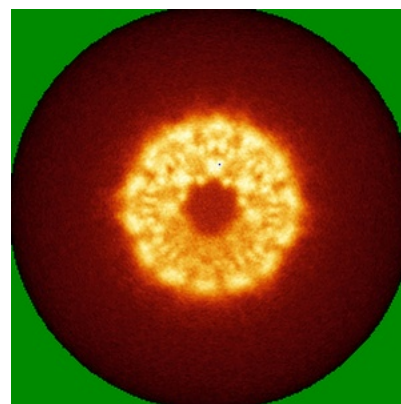
### 6.4.2 Raw map



X



Y



Z

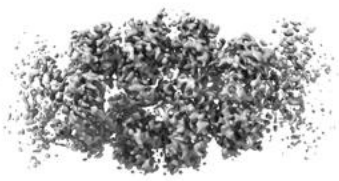
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



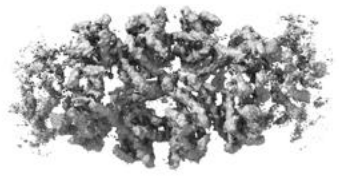
Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

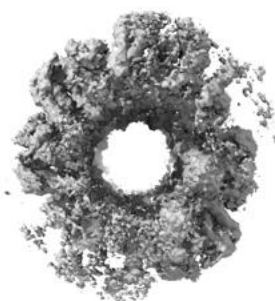
### 6.5.2 Raw map



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.

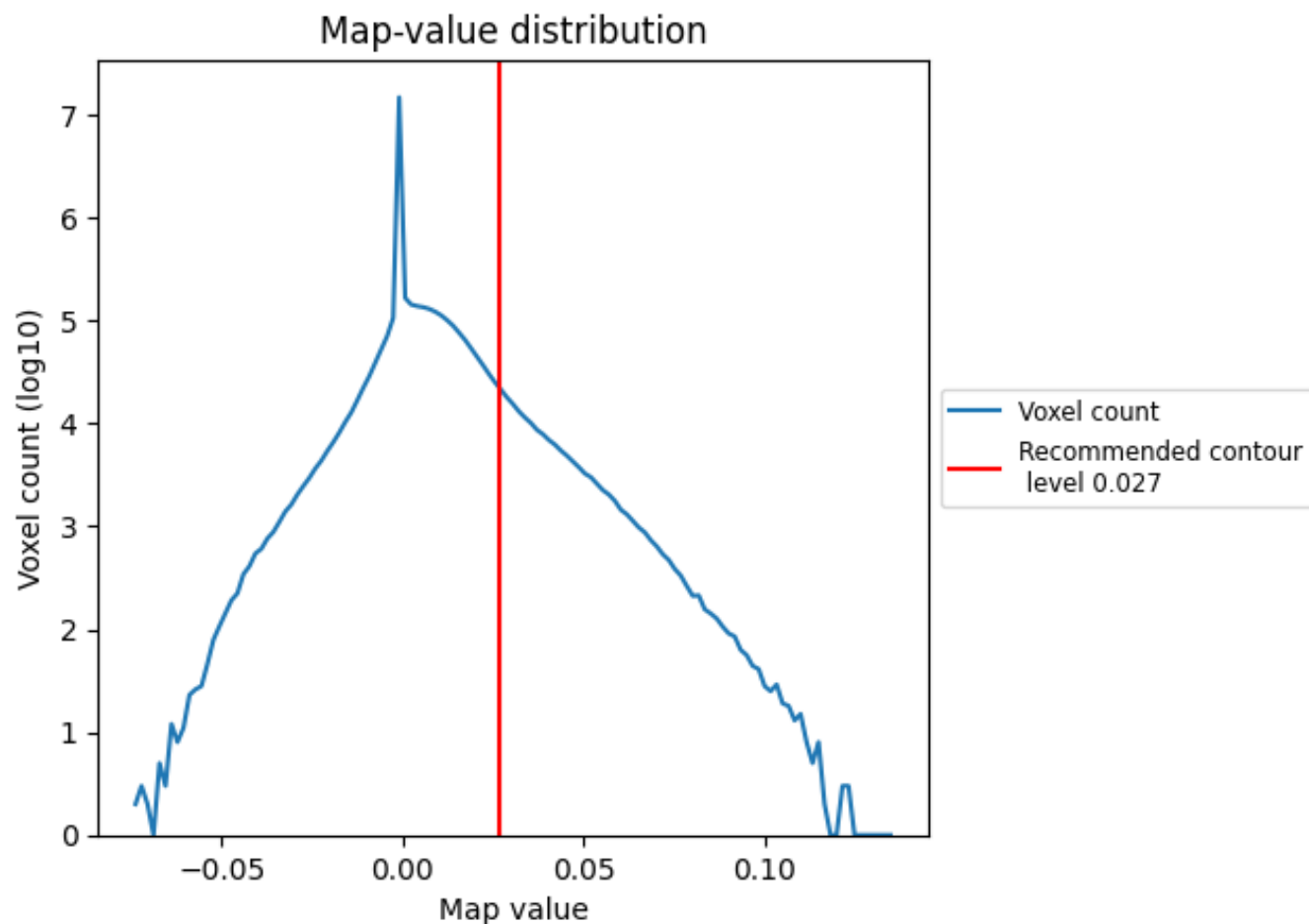
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

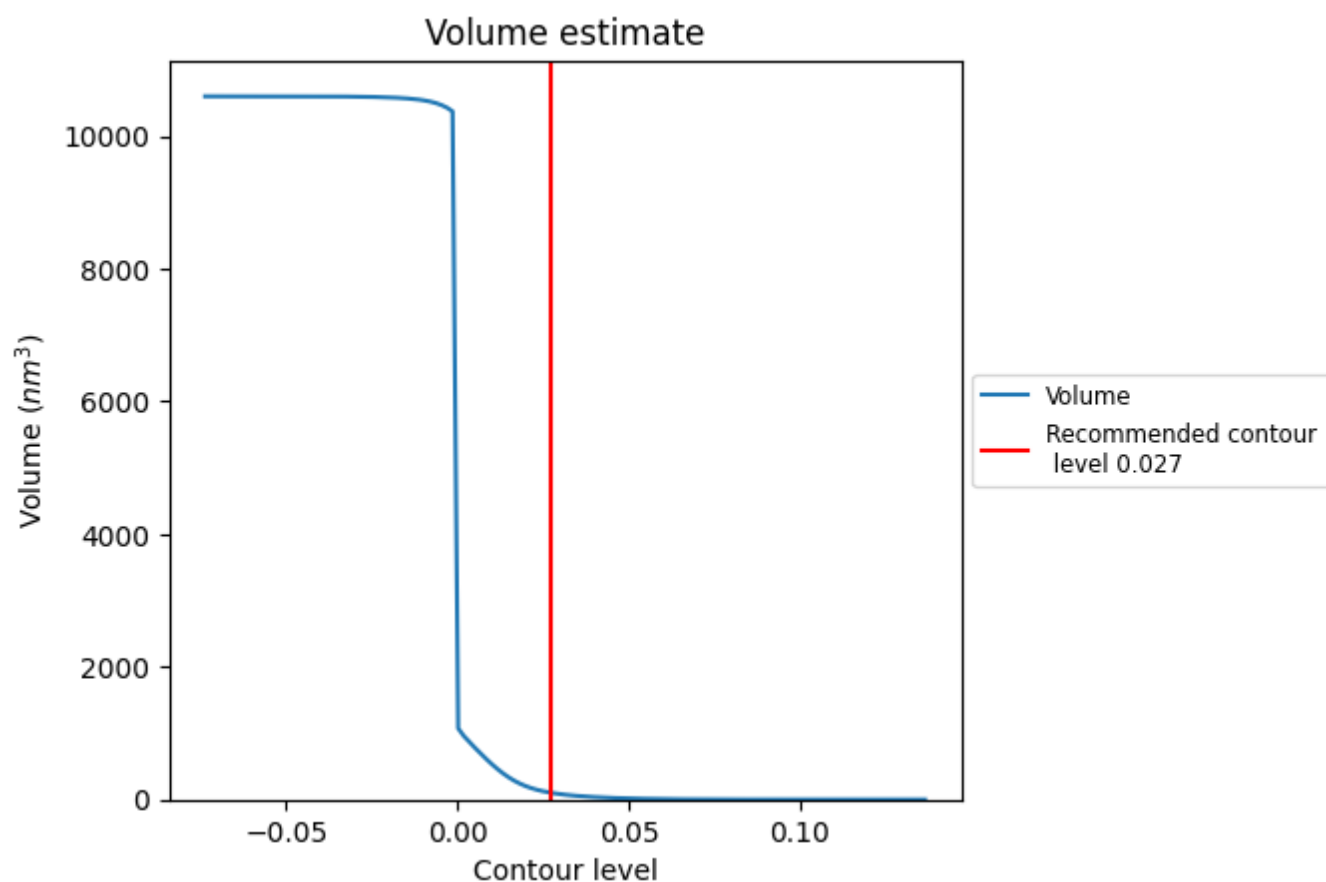
This section contains the results of statistical analysis of the map.

### 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.

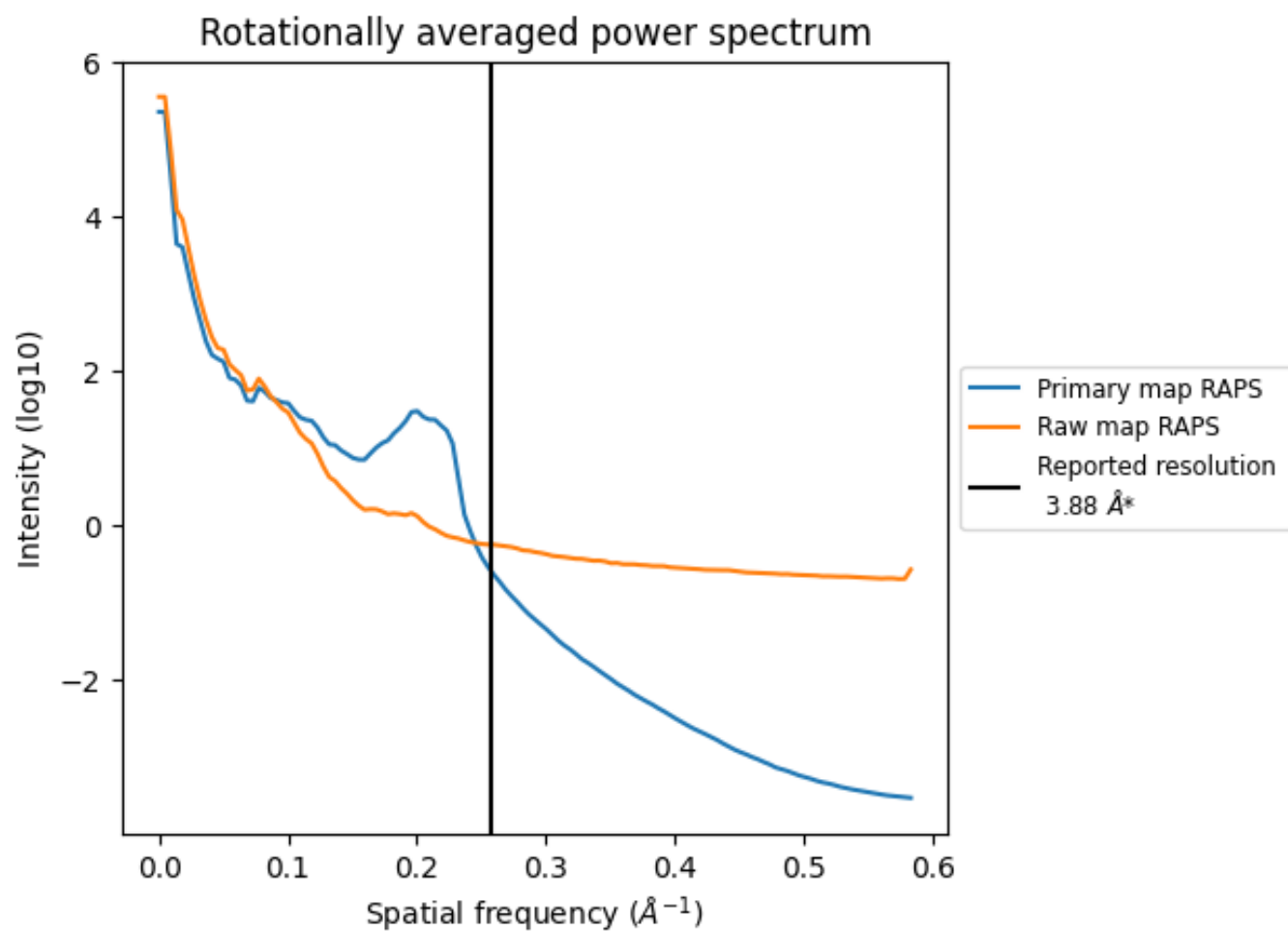
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105  $\text{nm}^3$ ; this corresponds to an approximate mass of 95 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 ⓘ

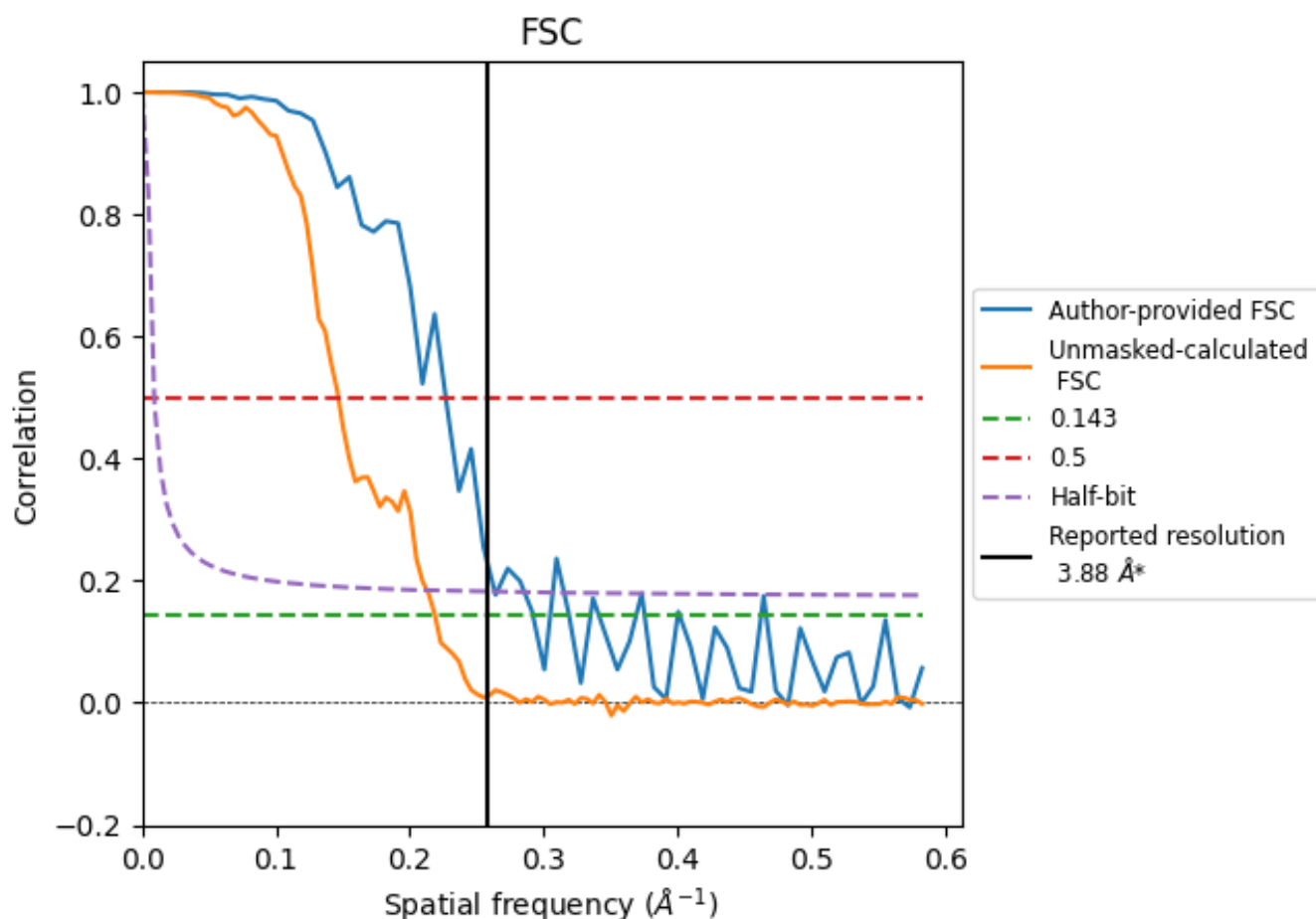


\*Reported resolution corresponds to spatial frequency of 0.258 Å<sup>-1</sup>

## 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 0.258 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        | 3.88                               | -    | -        |
| Author-provided FSC curve | 3.42                               | 4.41 | 3.81     |
| Unmasked-calculated*      | 4.57                               | 6.83 | 4.70     |

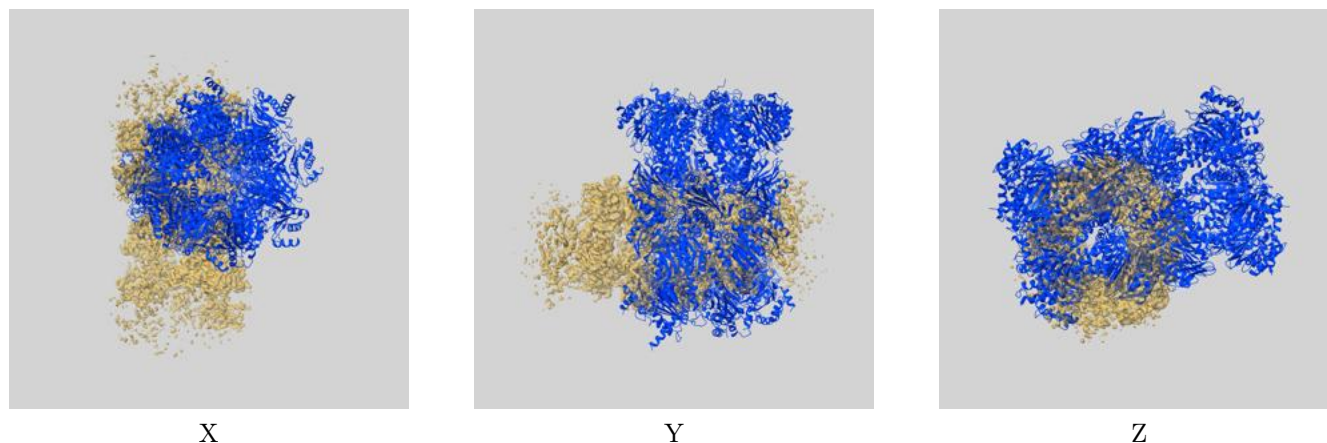
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.88 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.88 by more than 10 %

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

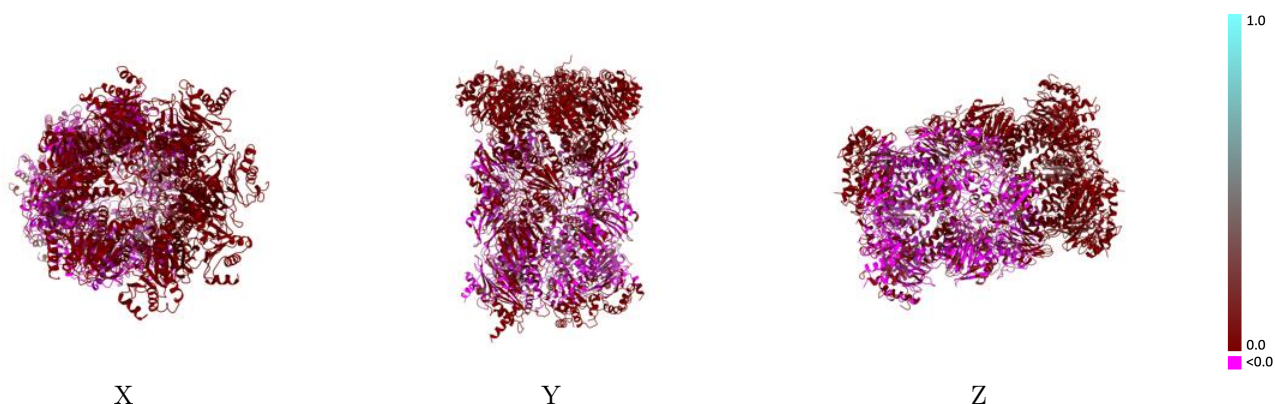
This section contains information regarding the fit between EMDB map EMD-31727 and PDB model 7V5M. Per-residue inclusion information can be found in section 3 on page 7.

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



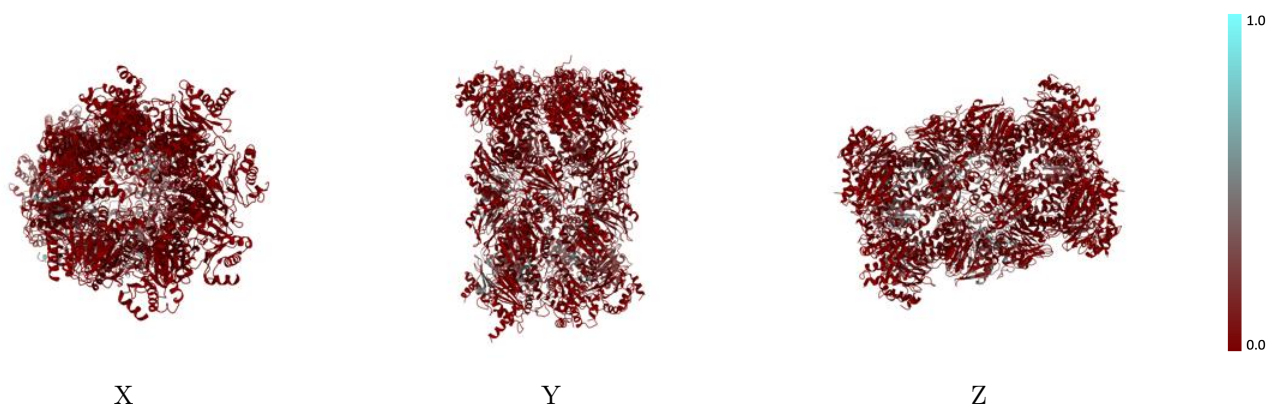
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



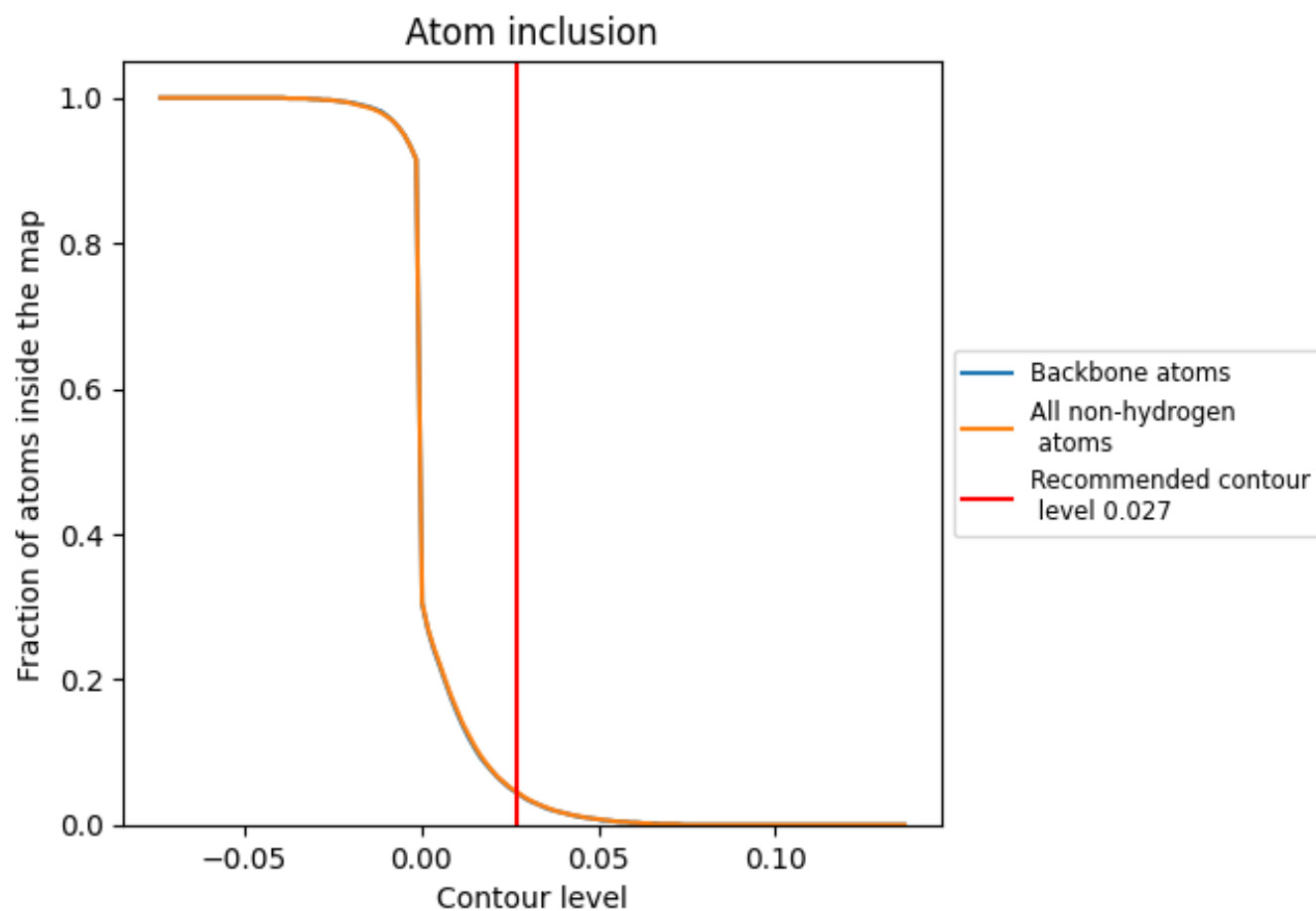
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 4% of all backbone atoms, 4% 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 (0.027) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.0450         | -0.0060 |
| A     | 0.0000         | 0.0000  |
| B     | 0.0000         | 0.0000  |
| C     | 0.0000         | -0.0010 |
| D     | 0.0000         | 0.0000  |
| E     | 0.0000         | 0.0000  |
| F     | 0.0000         | 0.0000  |
| G     | 0.0000         | 0.0000  |
| H     | 0.0080         | -0.0180 |
| I     | 0.0260         | 0.0010  |
| J     | 0.0980         | -0.0040 |
| K     | 0.0920         | -0.0070 |
| L     | 0.0180         | -0.0030 |
| M     | 0.0010         | 0.0010  |
| N     | 0.0120         | -0.0020 |
| O     | 0.0360         | -0.0030 |
| P     | 0.0120         | -0.0070 |
| Q     | 0.0470         | -0.0030 |
| R     | 0.1570         | -0.0510 |
| S     | 0.1170         | -0.0110 |
| T     | 0.0110         | -0.0200 |
| U     | 0.0310         | -0.0250 |
| V     | 0.0900         | -0.0020 |
| W     | 0.0720         | -0.0030 |
| X     | 0.0440         | -0.0010 |
| Y     | 0.1430         | 0.0110  |
| Z     | 0.0770         | -0.0170 |
| a     | 0.1120         | -0.0100 |
| b     | 0.0840         | 0.0090  |

