



## Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 07:18 AM UTC

PDB ID : 6WXG / pdb\_00006wxg  
EMDB ID : EMD-21957  
Title : Cryo-EM reconstruction of VP5\*/VP8\* assembly from rhesus rotavirus particles - Reversed conformation  
Authors : Herrmann, T.; Harrison, S.C.; Jenni, S.  
Deposited on : 2020-05-10  
Resolution : 3.30 Å (reported)  
Based on initial models : 4V7Q, 1SLQ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

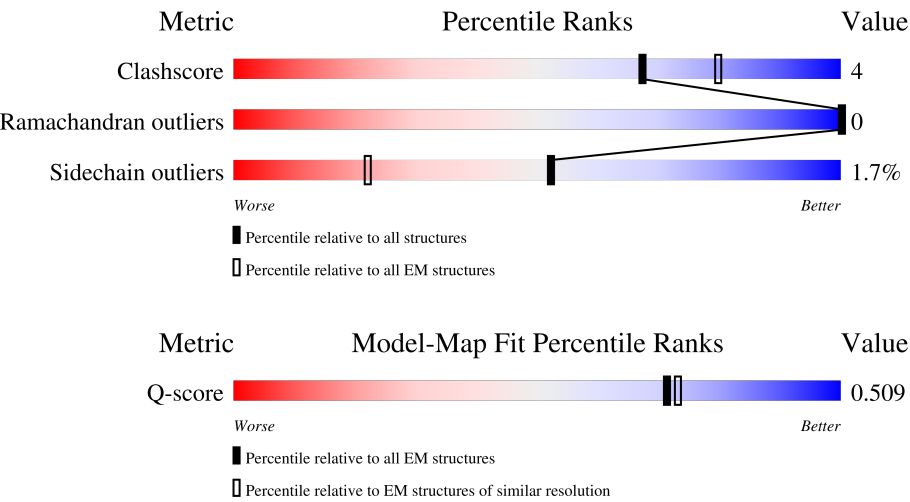
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 15087 ( 2.80 - 3.80 )                                    |

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 >=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 <=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   | 1     | 776    | <div><div>34%</div><div><div></div><div></div><div></div><div></div></div><div>31%</div><div>65%</div></div> |
| 1   | 2     | 776    | <div><div>33%</div><div><div></div><div></div><div></div><div></div></div><div>32%</div><div>65%</div></div> |
| 1   | 3     | 776    | <div><div>33%</div><div><div></div><div></div><div></div><div></div></div><div>31%</div><div>65%</div></div> |
| 2   | A     | 397    | <div><div>28%</div><div><div></div><div></div><div></div><div></div></div><div>88%</div><div>12%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 2   | B     | 397    | <div> <div>32%</div> <div>90%</div> <div>10%</div> </div>                |
| 2   | C     | 397    | <div> <div>31%</div> <div>89%</div> <div>11%</div> </div>                |
| 2   | D     | 397    | <div> <div>29%</div> <div>88%</div> <div>12%</div> </div>                |
| 2   | E     | 397    | <div> <div>31%</div> <div>87%</div> <div>12%</div> </div>                |
| 2   | F     | 397    | <div> <div>29%</div> <div>88%</div> <div>11%</div> </div>                |
| 2   | G     | 397    | <div> <div>29%</div> <div>88%</div> <div>12%</div> </div>                |
| 2   | H     | 397    | <div> <div>32%</div> <div>90%</div> <div>10%</div> </div>                |
| 2   | I     | 397    | <div> <div>31%</div> <div>89%</div> <div>10%</div> </div>                |
| 2   | J     | 397    | <div> <div>36%</div> <div>90%</div> <div>10%</div> </div>                |
| 2   | K     | 397    | <div> <div>35%</div> <div>88%</div> <div>12%</div> </div>                |
| 2   | L     | 397    | <div> <div>37%</div> <div>88%</div> <div>12%</div> </div>                |
| 2   | M     | 397    | <div> <div>34%</div> <div>89%</div> <div>11%</div> </div>                |
| 2   | N     | 397    | <div> <div>37%</div> <div>91%</div> <div>9%</div> </div>                 |
| 2   | O     | 397    | <div> <div>39%</div> <div>90%</div> <div>9%</div> </div>                 |
| 2   | P     | 397    | <div> <div>34%</div> <div>87%</div> <div>13%</div> </div>                |
| 2   | Q     | 397    | <div> <div>32%</div> <div>90%</div> <div>10%</div> </div>                |
| 2   | R     | 397    | <div> <div>38%</div> <div>90%</div> <div>10%</div> </div>                |
| 3   | a     | 326    | <div> <div>51%</div> <div>69%</div> <div>11%</div> <div>21%</div> </div> |
| 3   | b     | 326    | <div> <div>48%</div> <div>71%</div> <div>13%</div> <div>17%</div> </div> |
| 3   | c     | 326    | <div> <div>44%</div> <div>71%</div> <div>9%</div> <div>20%</div> </div>  |
| 3   | d     | 326    | <div> <div>43%</div> <div>72%</div> <div>10%</div> <div>19%</div> </div> |
| 3   | e     | 326    | <div> <div>40%</div> <div>67%</div> <div>12%</div> <div>20%</div> </div> |
| 3   | f     | 326    | <div> <div>44%</div> <div>71%</div> <div>10%</div> <div>19%</div> </div> |
| 3   | g     | 326    | <div> <div>54%</div> <div>74%</div> <div>9%</div> <div>17%</div> </div>  |
| 3   | h     | 326    | <div> <div>50%</div> <div>71%</div> <div>8%</div> <div>21%</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 3   | i     | 326    | <div> <div>48%</div> <div>74%</div> <div>10%</div> <div>17%</div> </div> |
| 3   | j     | 326    | <div> <div>52%</div> <div>73%</div> <div>10%</div> <div>17%</div> </div> |
| 3   | k     | 326    | <div> <div>51%</div> <div>73%</div> <div>8%</div> <div>19%</div> </div>  |
| 3   | l     | 326    | <div> <div>47%</div> <div>71%</div> <div>10%</div> <div>19%</div> </div> |
| 3   | m     | 326    | <div> <div>51%</div> <div>73%</div> <div>10%</div> <div>17%</div> </div> |
| 3   | n     | 326    | <div> <div>52%</div> <div>73%</div> <div>9%</div> <div>19%</div> </div>  |
| 3   | o     | 326    | <div> <div>50%</div> <div>73%</div> <div>8%</div> <div>19%</div> </div>  |
| 3   | p     | 326    | <div> <div>56%</div> <div>75%</div> <div>8%</div> <div>17%</div> </div>  |
| 3   | q     | 326    | <div> <div>52%</div> <div>73%</div> <div>6%</div> <div>21%</div> </div>  |
| 3   | r     | 326    | <div> <div>53%</div> <div>74%</div> <div>9%</div> <div>17%</div> </div>  |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 201212 atoms, of which 99503 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 Outer capsid protein VP4.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 1   | 1     | 275      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4291  | 1382 | 2107 | 368 | 427 | 7 |         |       |
| 1   | 2     | 275      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4291  | 1382 | 2107 | 368 | 427 | 7 |         |       |
| 1   | 3     | 275      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4291  | 1382 | 2107 | 368 | 427 | 7 |         |       |

- Molecule 2 is a protein called Intermediate capsid protein VP6.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | A     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | B     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | C     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | D     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | E     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |
| 2   | F     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |
| 2   | G     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |
| 2   | H     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |
| 2   | I     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | J     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | K     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | L     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | M     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |
| 2   | N     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | O     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |
| 2   | P     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |
| 2   | Q     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6276  | 2004 | 3113 | 551 | 593 | 15 |         |       |
| 2   | R     | 397      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6275  | 2004 | 3112 | 551 | 593 | 15 |         |       |

- Molecule 3 is a protein called Outer capsid glycoprotein VP7.

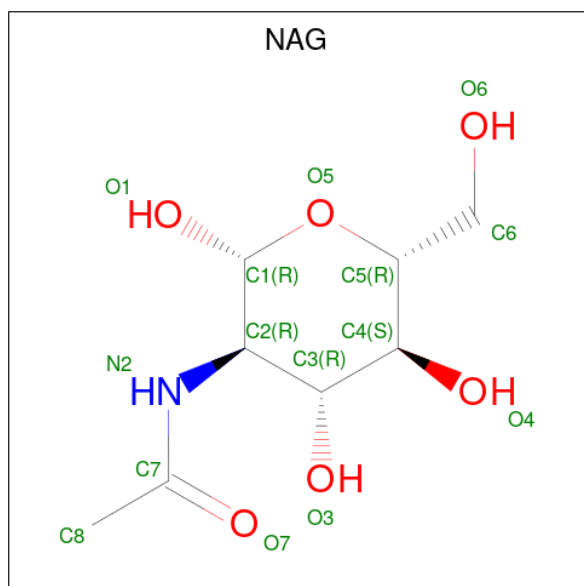
| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 3   | a     | 259      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4041  | 1298 | 1994 | 324 | 409 | 16 |         |       |
| 3   | b     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4254  | 1369 | 2099 | 342 | 428 | 16 |         |       |
| 3   | c     | 261      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4074  | 1308 | 2011 | 327 | 412 | 16 |         |       |
| 3   | d     | 265      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4133  | 1328 | 2037 | 333 | 419 | 16 |         |       |
| 3   | e     | 260      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4050  | 1302 | 1998 | 323 | 411 | 16 |         |       |
| 3   | f     | 265      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4133  | 1328 | 2037 | 333 | 419 | 16 |         |       |
| 3   | g     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4254  | 1369 | 2099 | 342 | 428 | 16 |         |       |
| 3   | h     | 259      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4041  | 1298 | 1994 | 324 | 409 | 16 |         |       |
| 3   | i     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4254  | 1369 | 2099 | 342 | 428 | 16 |         |       |
| 3   | j     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4254  | 1369 | 2099 | 342 | 428 | 16 |         |       |
| 3   | k     | 265      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4133  | 1328 | 2037 | 333 | 419 | 16 |         |       |
| 3   | l     | 265      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4133  | 1328 | 2037 | 333 | 419 | 16 |         |       |
| 3   | m     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4254  | 1369 | 2099 | 342 | 428 | 16 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 3   | n     | 265      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4133  | 1328 | 2037 | 333 | 419 | 16 |         |       |
| 3   | o     | 265      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4133  | 1328 | 2037 | 333 | 419 | 16 |         |       |
| 3   | p     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4254  | 1369 | 2099 | 342 | 428 | 16 |         |       |
| 3   | q     | 259      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4041  | 1298 | 1994 | 324 | 409 | 16 |         |       |
| 3   | r     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4254  | 1369 | 2099 | 342 | 428 | 16 |         |       |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |    |   |   | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 4   | a     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | b     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | c     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | d     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | e     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | f     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |

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| Mol | Chain | Residues | Atoms |   |    |   |   | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 4   | g     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | h     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | i     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | j     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | k     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | l     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | m     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | n     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | o     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | p     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | q     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |
| 4   | r     | 1        | Total | C | H  | N | O | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 5   | a     | 5        | Total | Ca | 0       |
|     |       |          | 5     | 5  |         |
| 5   | b     | 3        | Total | Ca | 0       |
|     |       |          | 3     | 3  |         |
| 5   | c     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 5   | d     | 5        | Total | Ca | 0       |
|     |       |          | 5     | 5  |         |
| 5   | e     | 3        | Total | Ca | 0       |
|     |       |          | 3     | 3  |         |
| 5   | f     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 5   | g     | 5        | Total | Ca | 0       |
|     |       |          | 5     | 5  |         |

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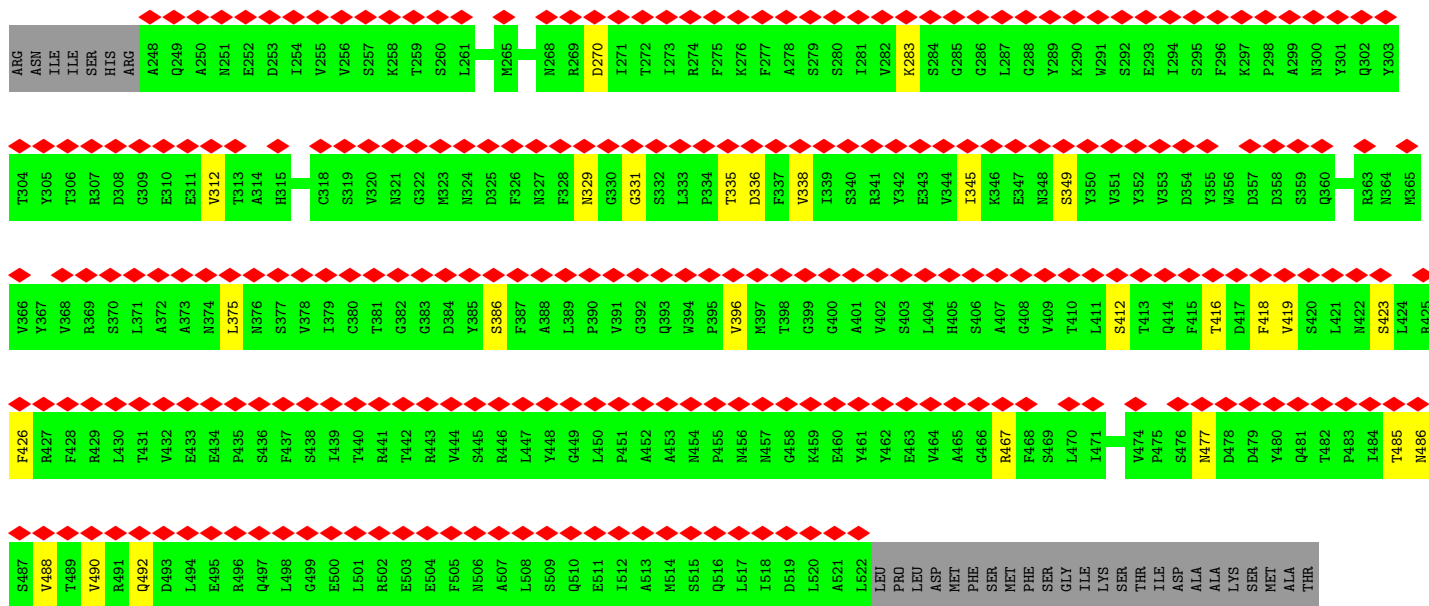
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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 5   | h     | 3        | Total<br>3 | Ca<br>3 | 0       |
| 5   | i     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 5   | j     | 5        | Total<br>5 | Ca<br>5 | 0       |
| 5   | k     | 3        | Total<br>3 | Ca<br>3 | 0       |
| 5   | l     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 5   | m     | 5        | Total<br>5 | Ca<br>5 | 0       |
| 5   | n     | 3        | Total<br>3 | Ca<br>3 | 0       |
| 5   | o     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 5   | p     | 5        | Total<br>5 | Ca<br>5 | 0       |
| 5   | q     | 3        | Total<br>3 | Ca<br>3 | 0       |
| 5   | r     | 1        | Total<br>1 | Ca<br>1 | 0       |



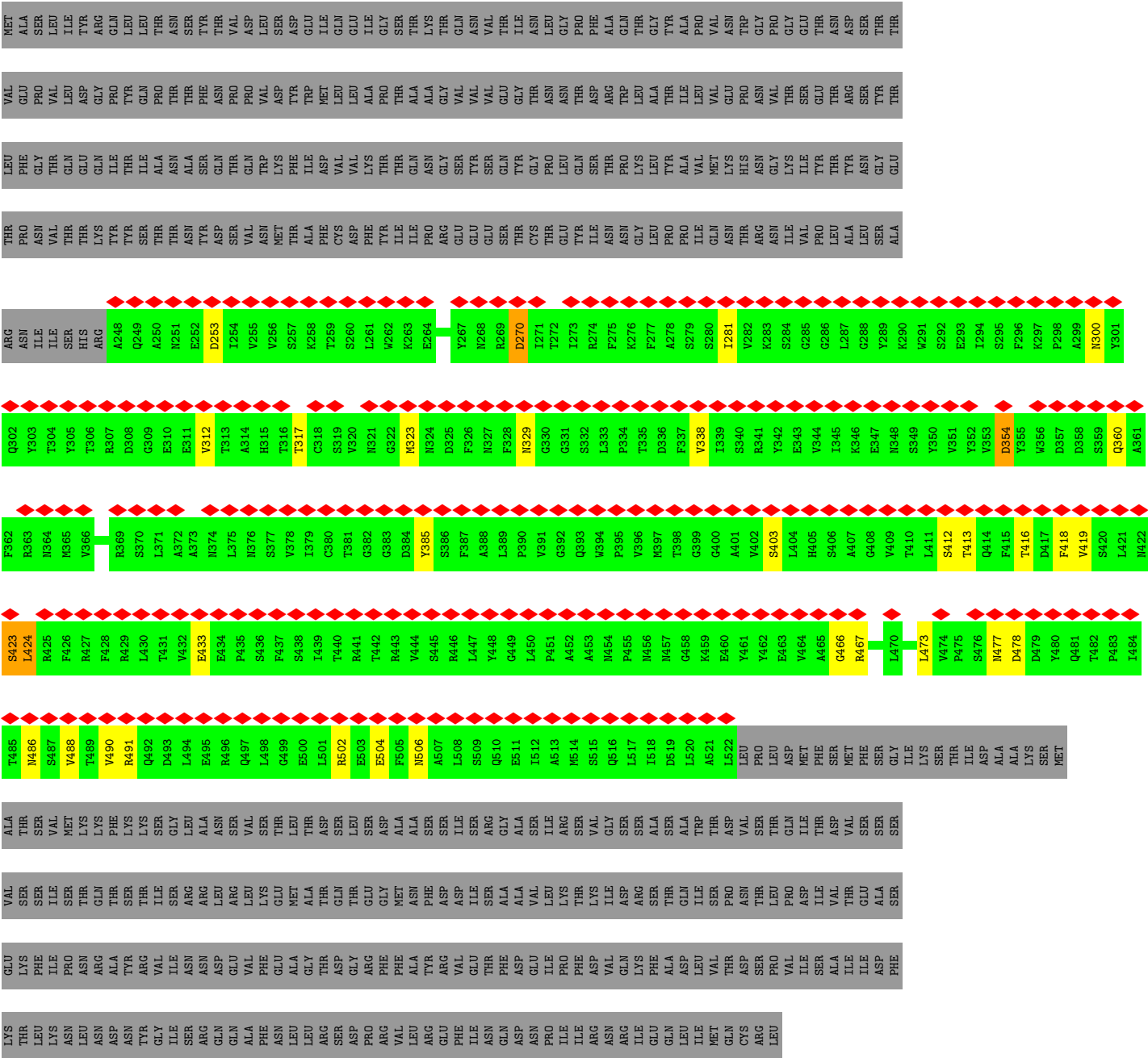
[illegible]

- Molecule 1: Outer capsid protein VP4

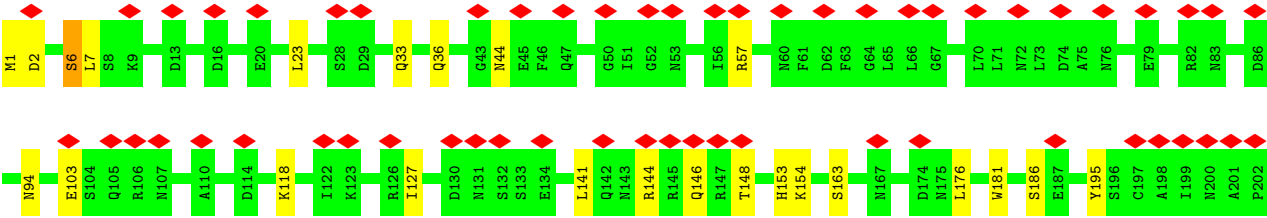
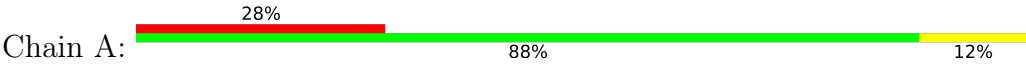
[illegible][illegible]

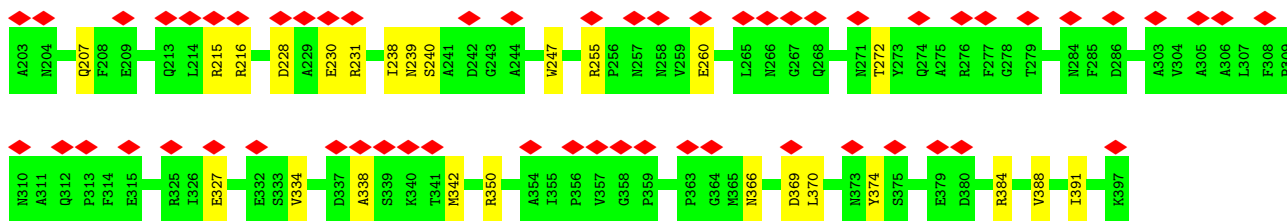
- Molecule 1: Outer capsid protein VP4



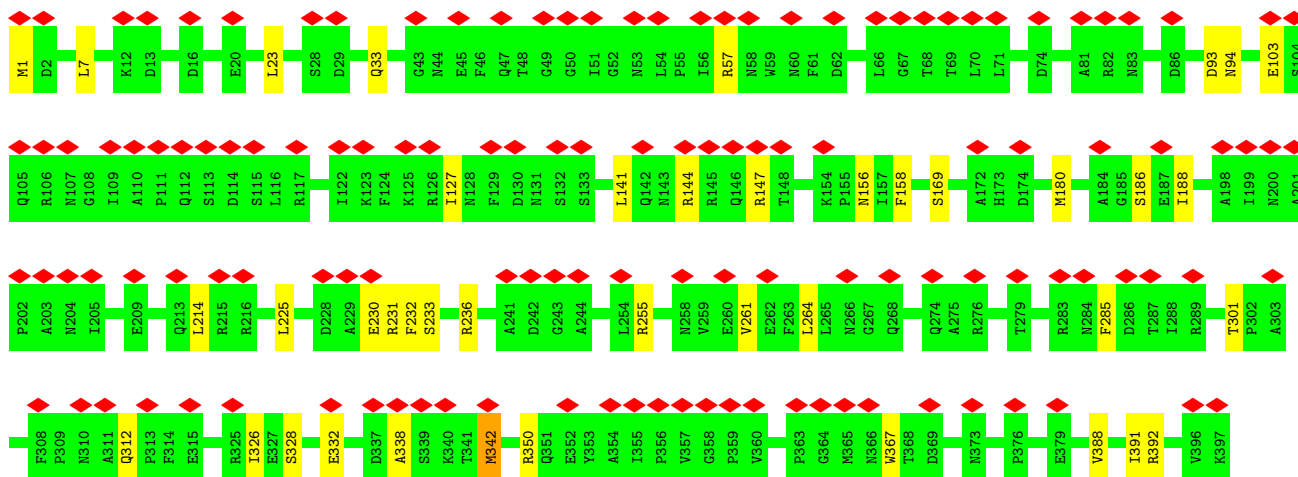
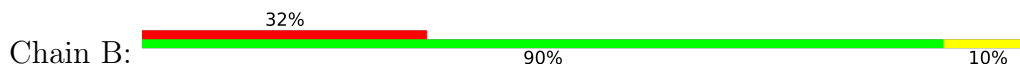


● Molecule 2: Intermediate capsid protein VP6

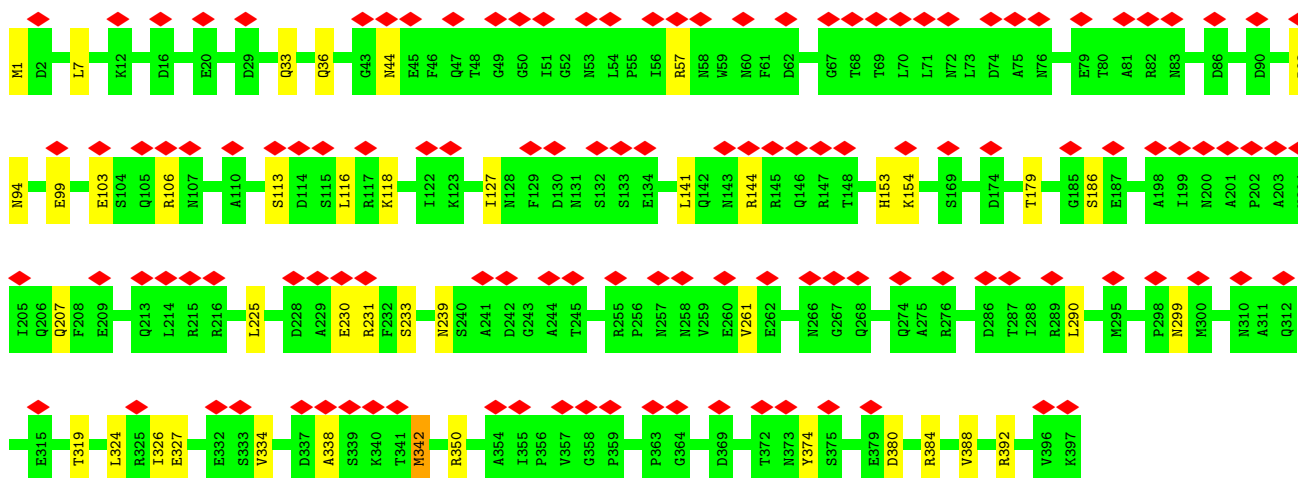
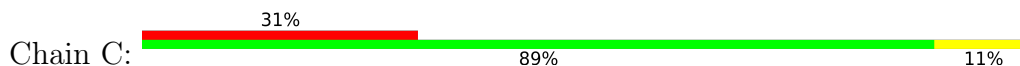




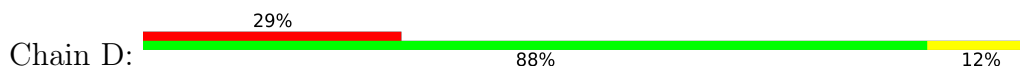
• Molecule 2: Intermediate capsid protein VP6

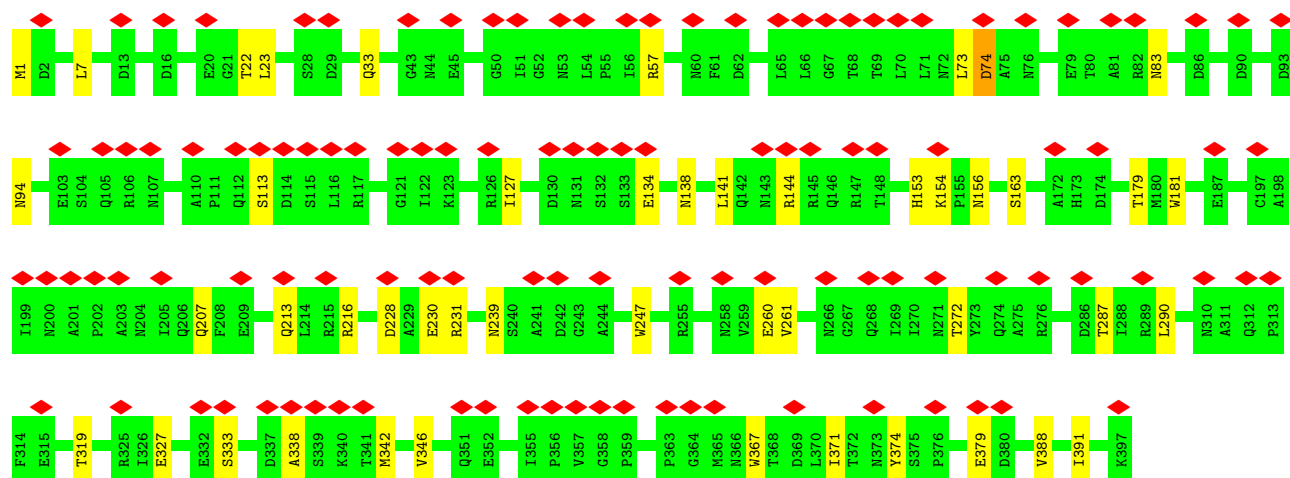


• Molecule 2: Intermediate capsid protein VP6

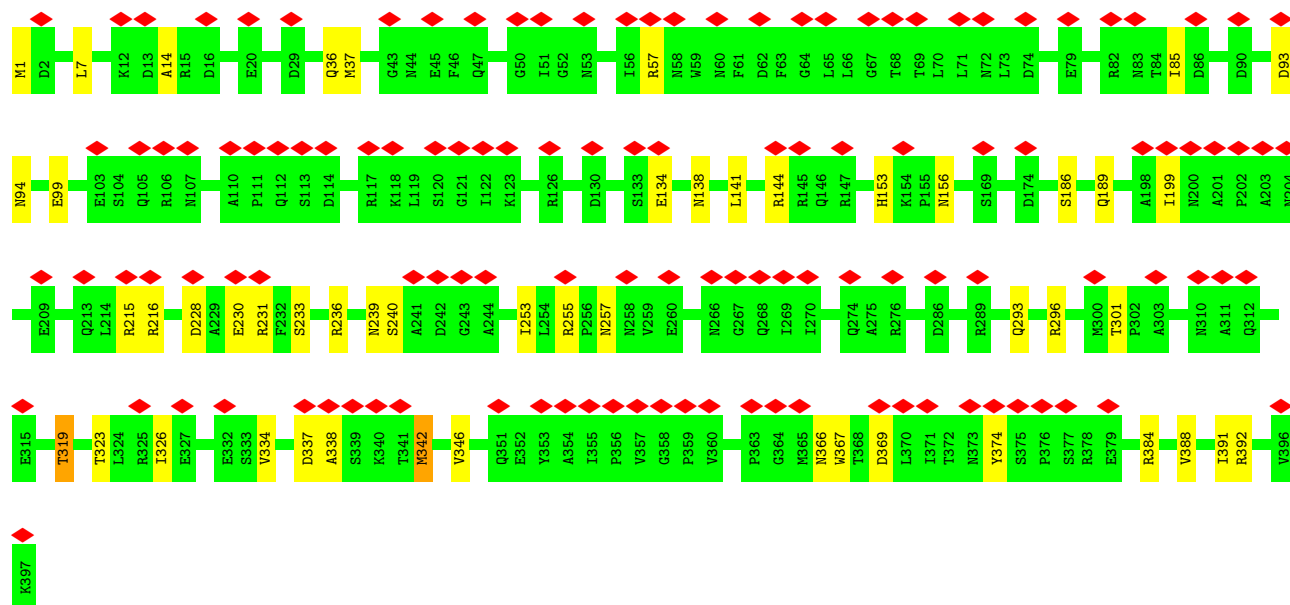
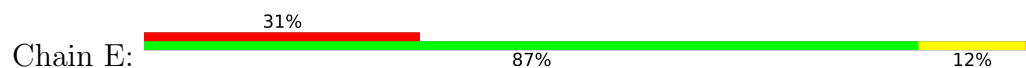


• Molecule 2: Intermediate capsid protein VP6

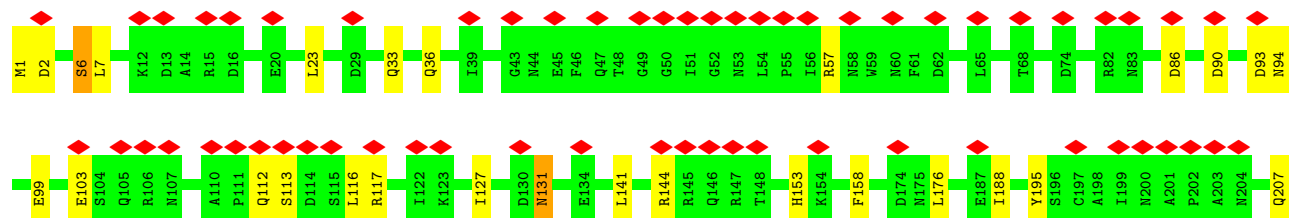
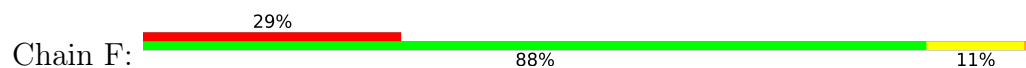


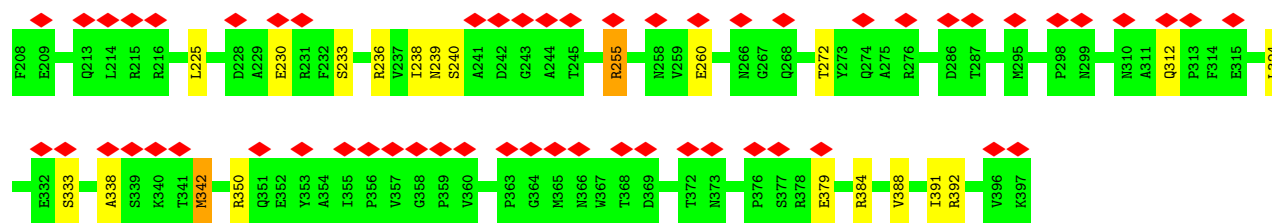


• Molecule 2: Intermediate capsid protein VP6

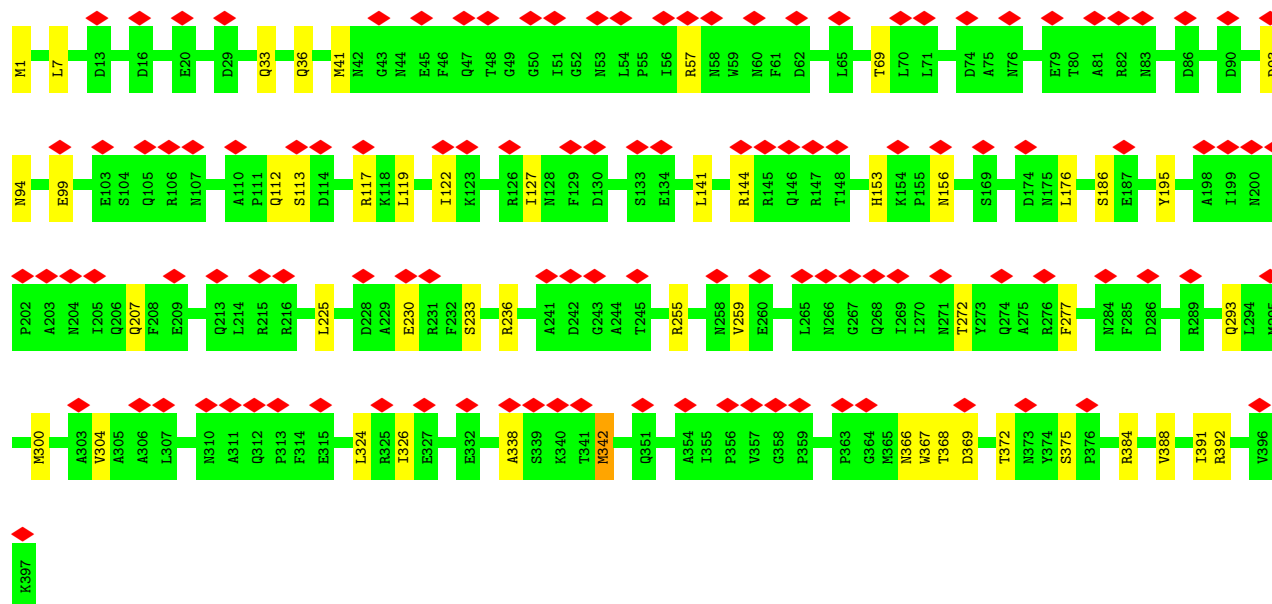
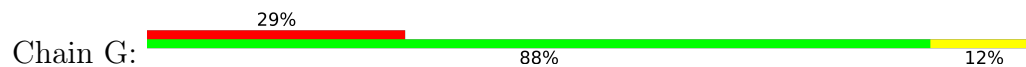


• Molecule 2: Intermediate capsid protein VP6

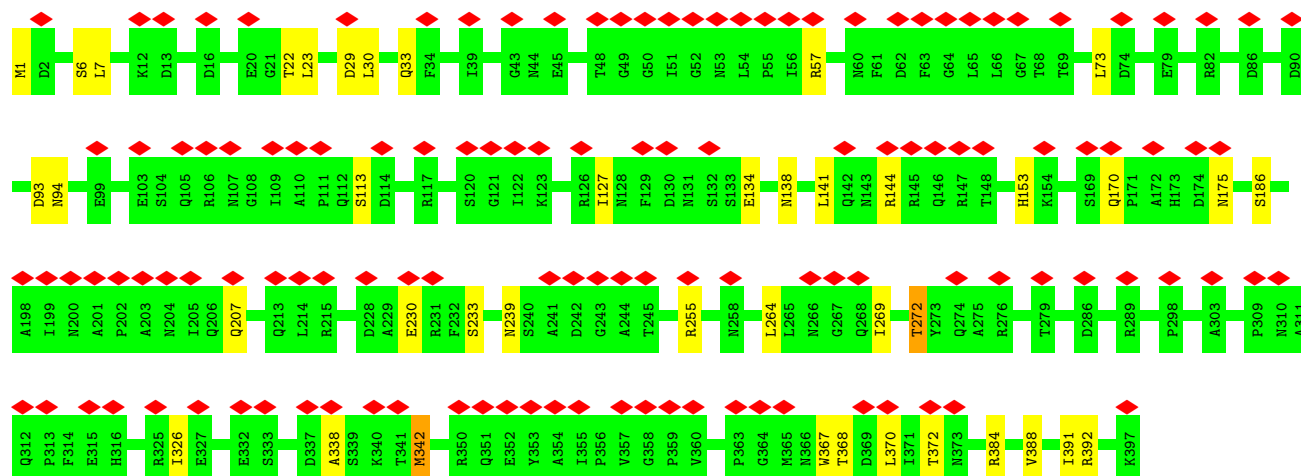
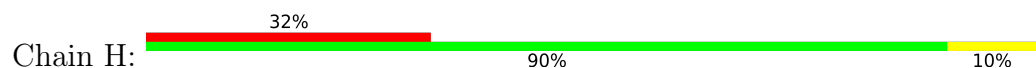




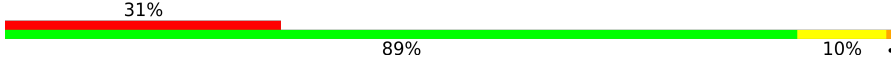
• Molecule 2: Intermediate capsid protein VP6

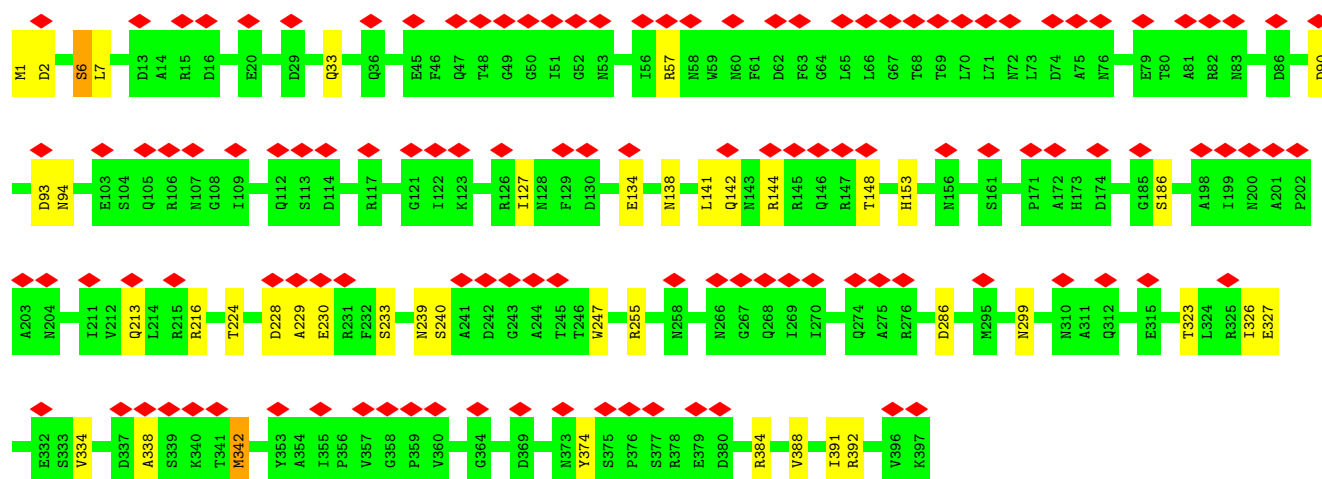


• Molecule 2: Intermediate capsid protein VP6

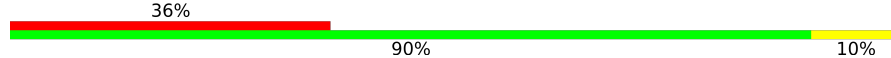


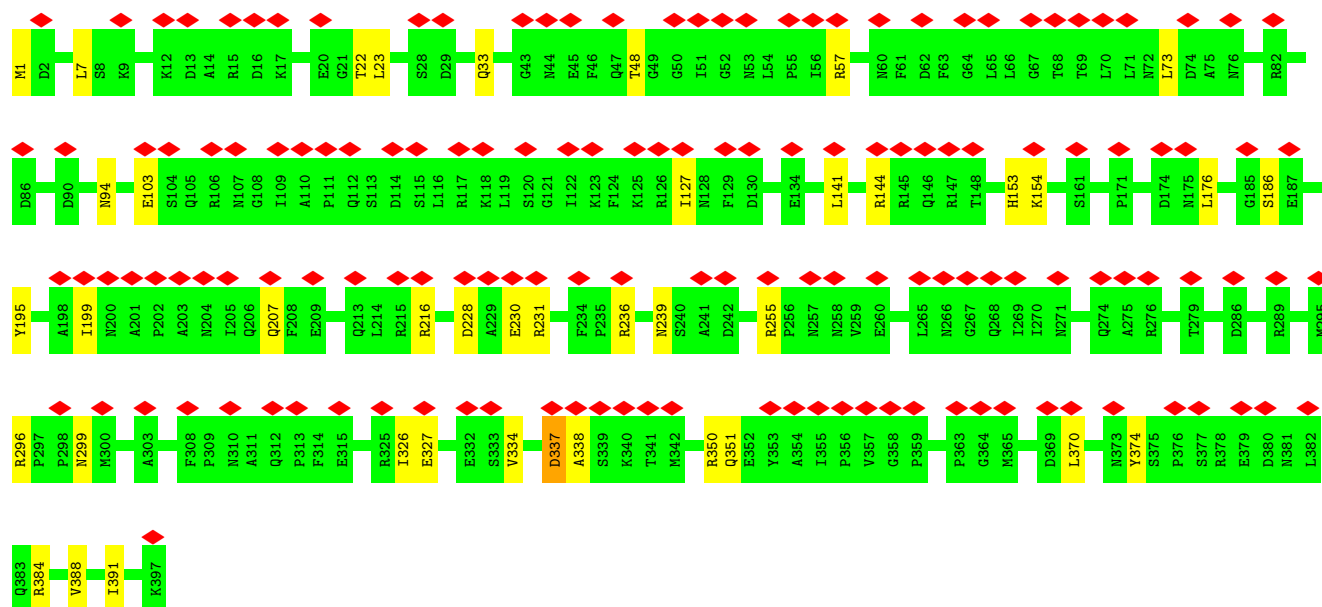
• Molecule 2: Intermediate capsid protein VP6

Chain I: 

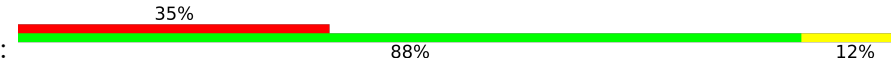


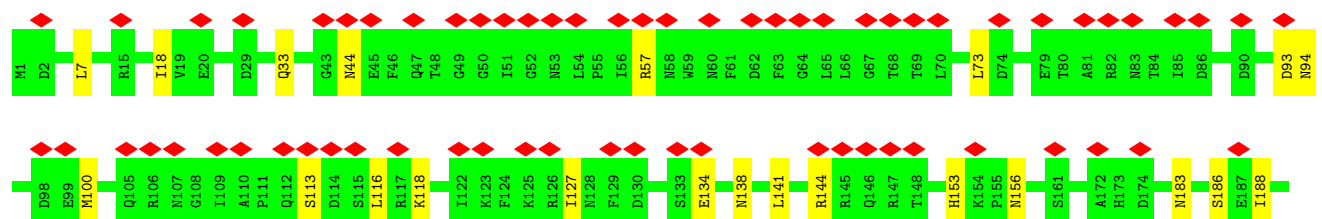
• Molecule 2: Intermediate capsid protein VP6

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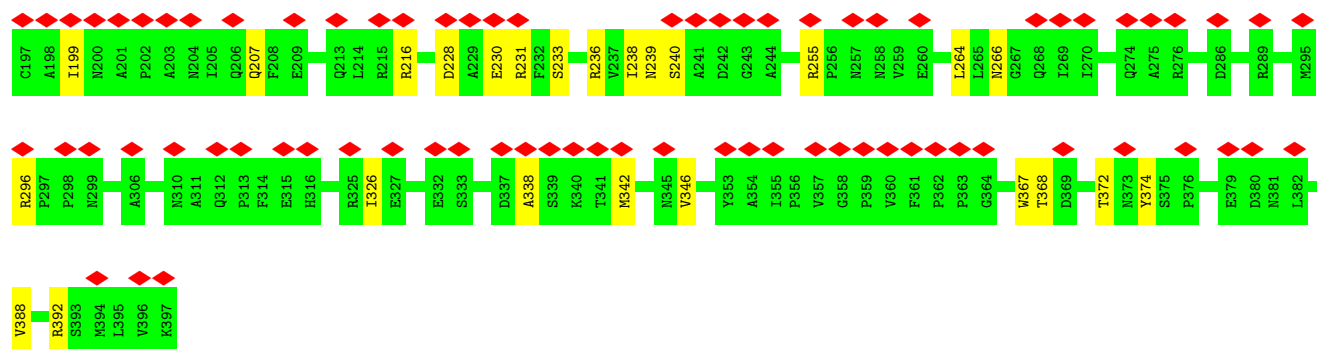


• Molecule 2: Intermediate capsid protein VP6

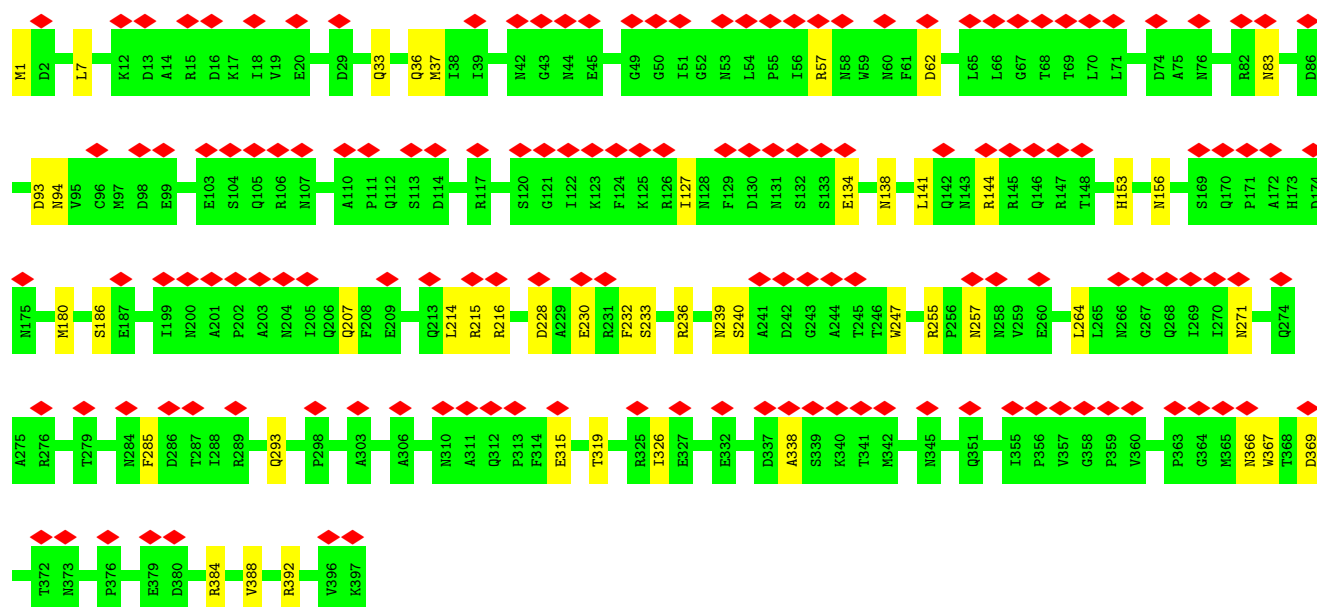
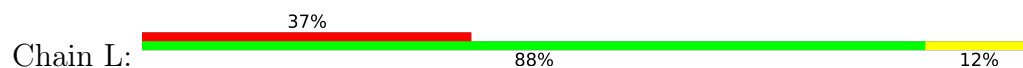
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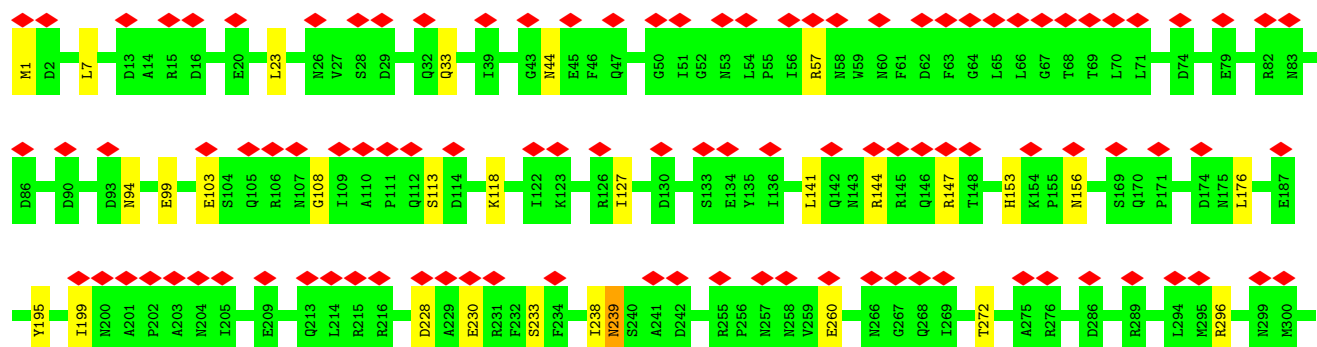
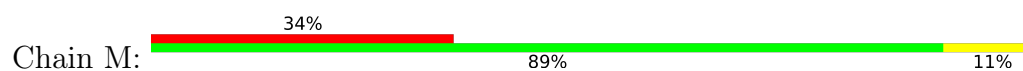


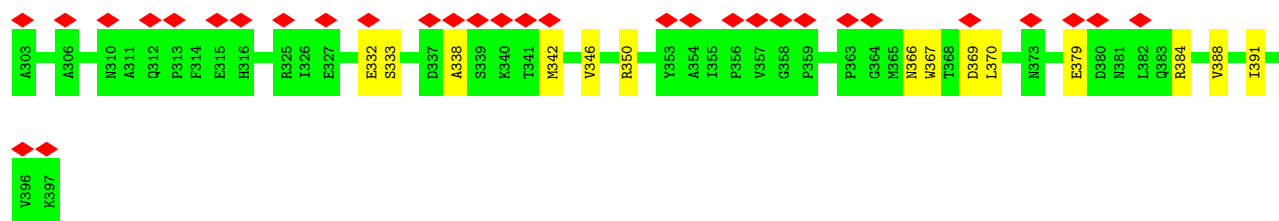


• Molecule 2: Intermediate capsid protein VP6

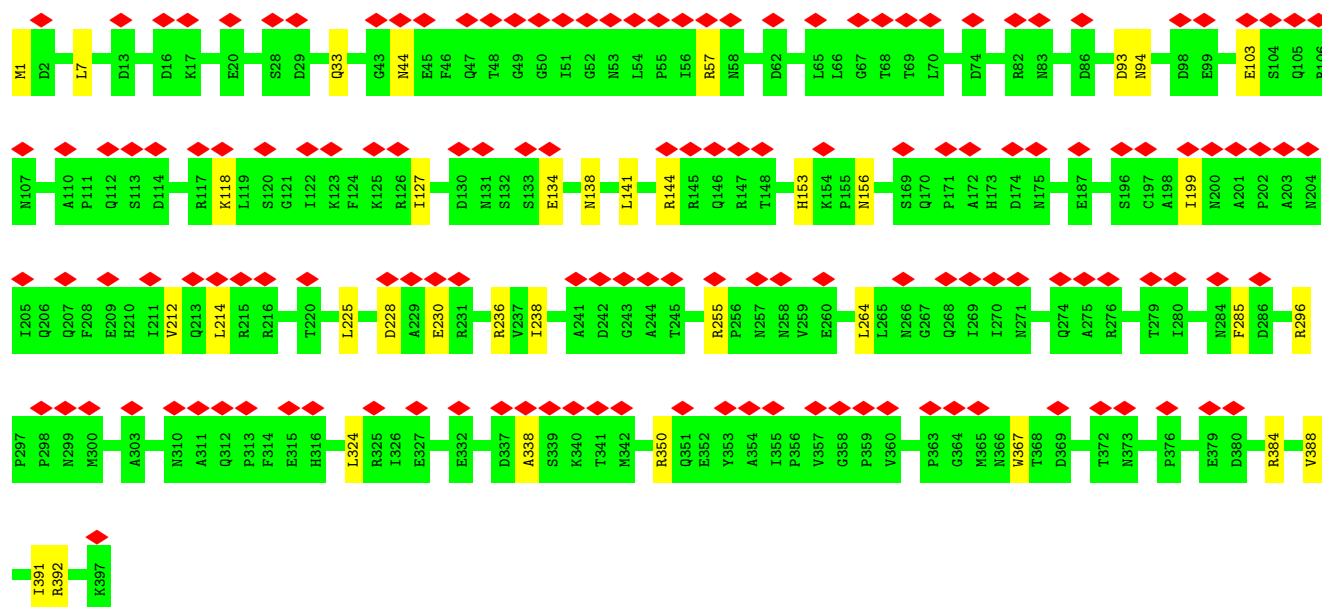
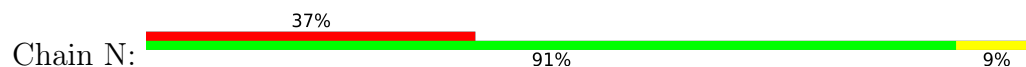


• Molecule 2: Intermediate capsid protein VP6

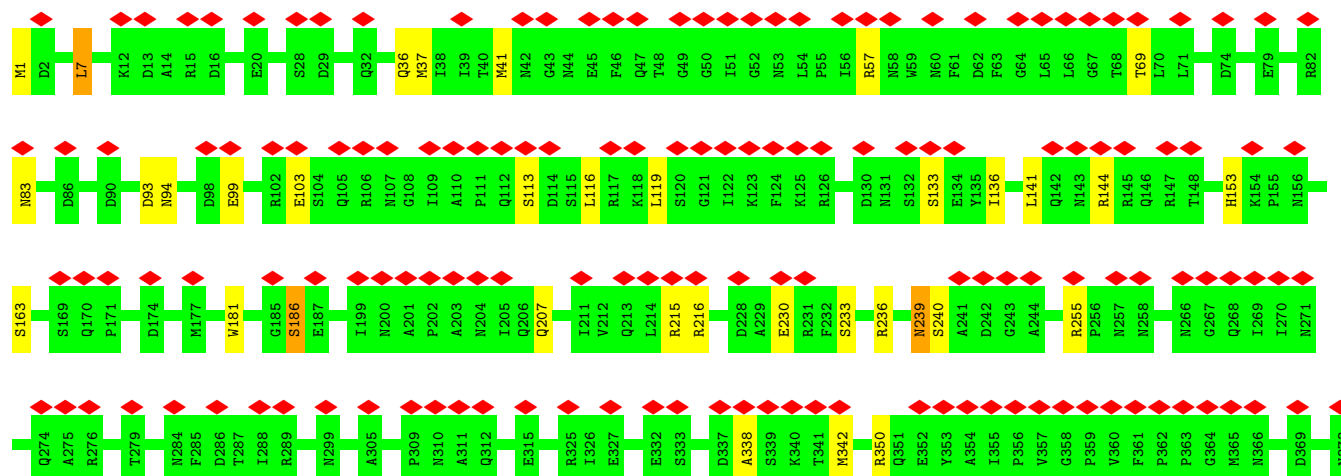
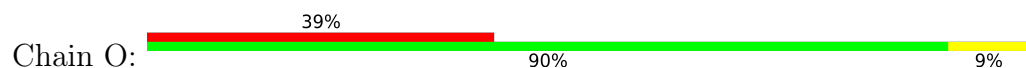


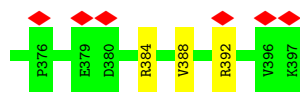


• Molecule 2: Intermediate capsid protein VP6

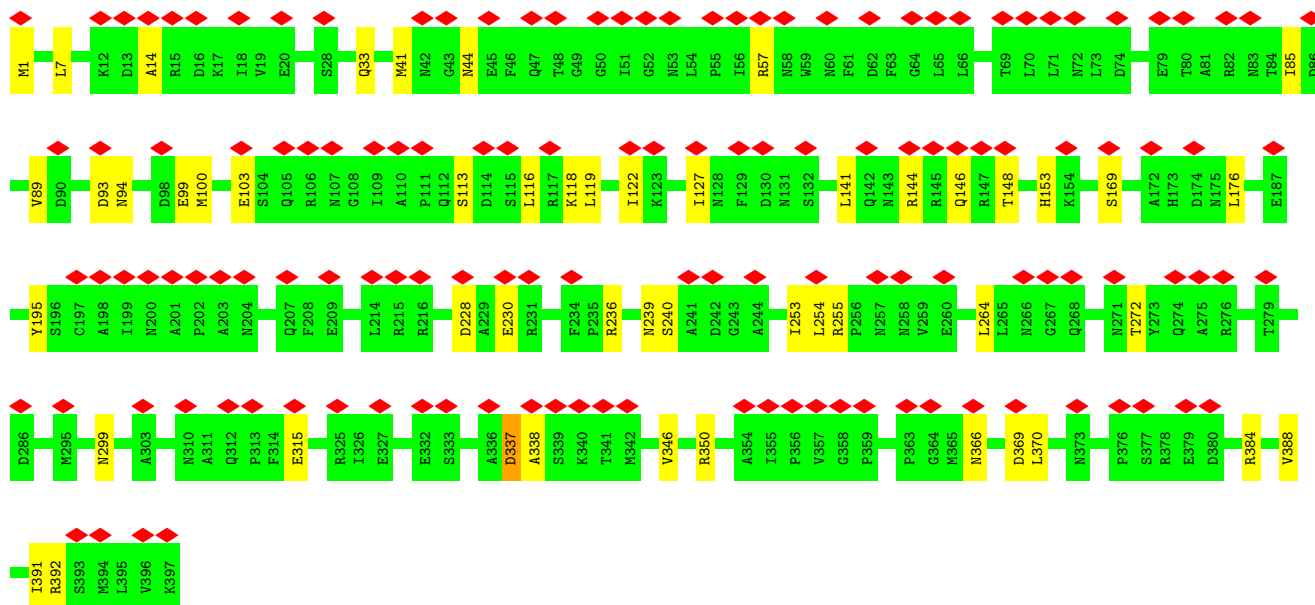
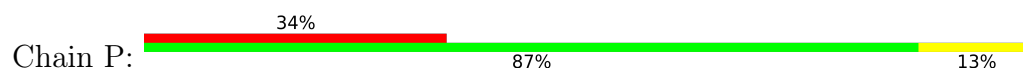


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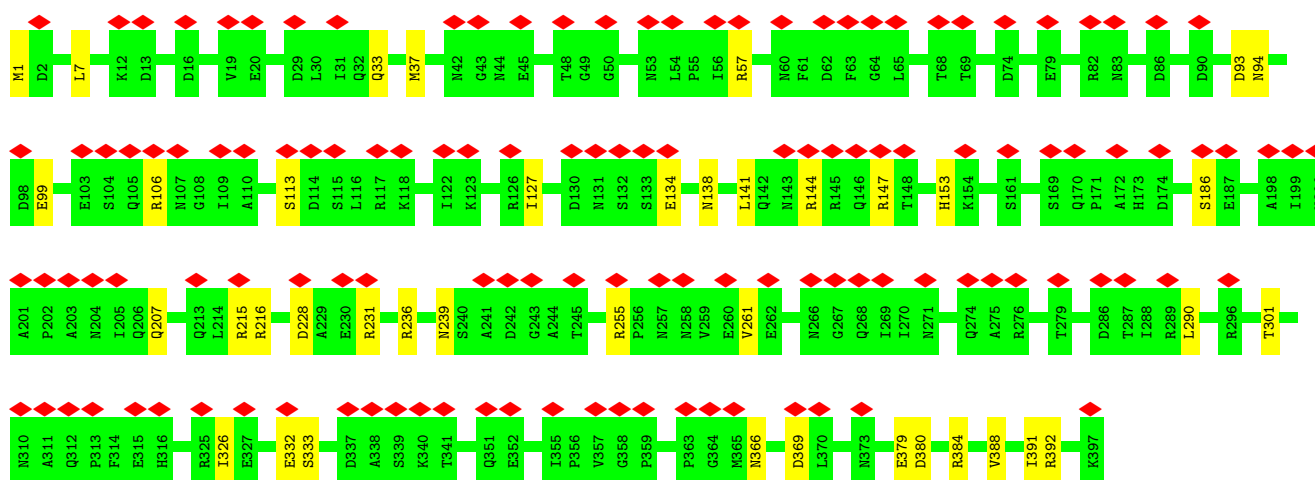
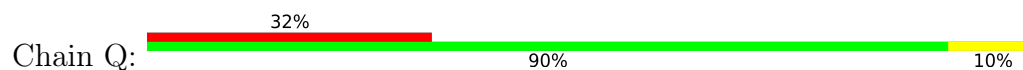




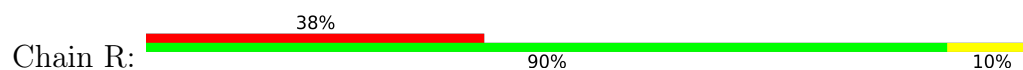
• Molecule 2: Intermediate capsid protein VP6

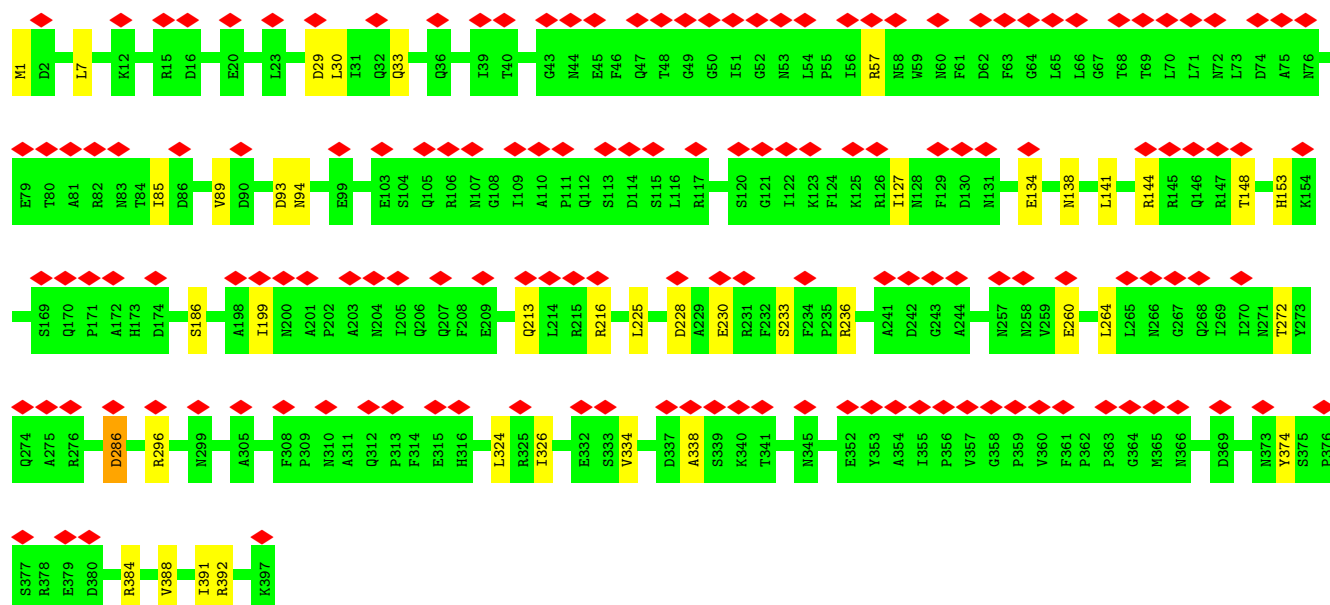


• Molecule 2: Intermediate capsid protein VP6

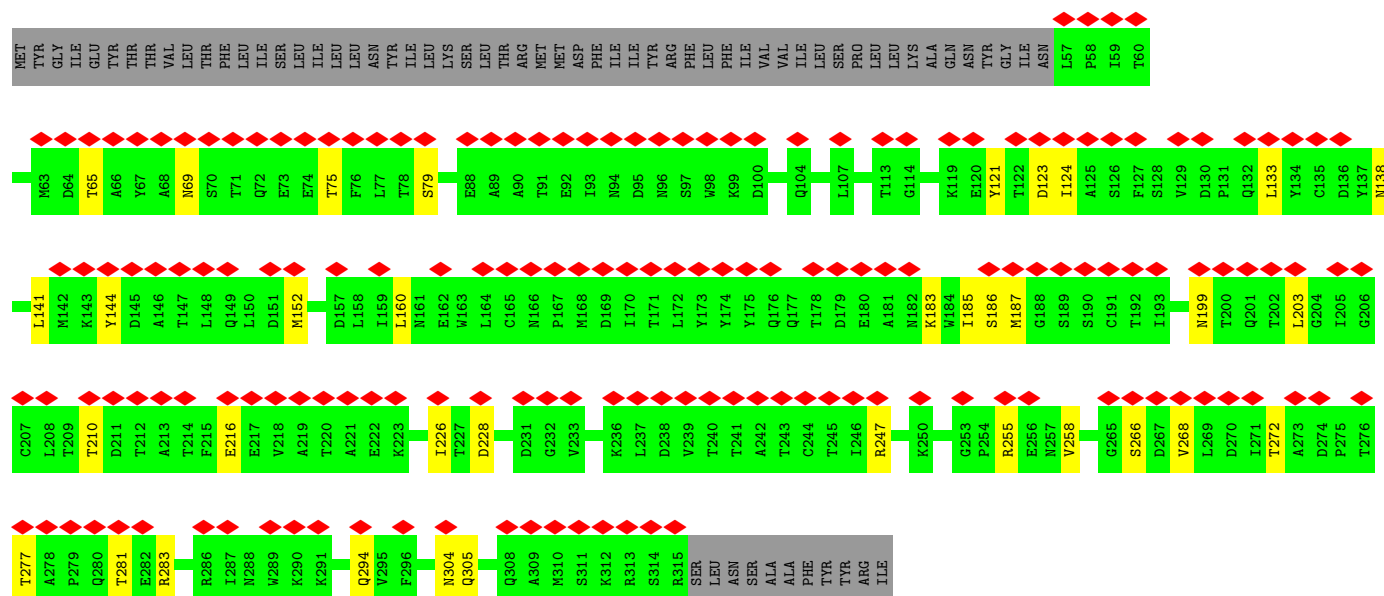


• Molecule 2: Intermediate capsid protein VP6

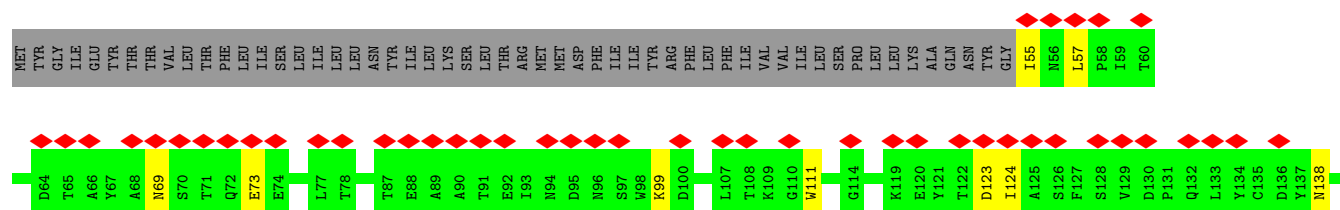


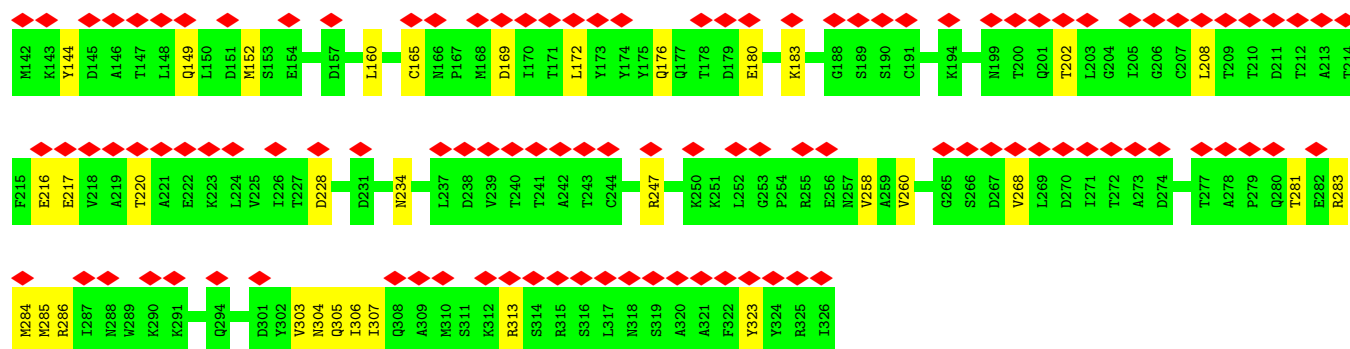


• Molecule 3: Outer capsid glycoprotein VP7

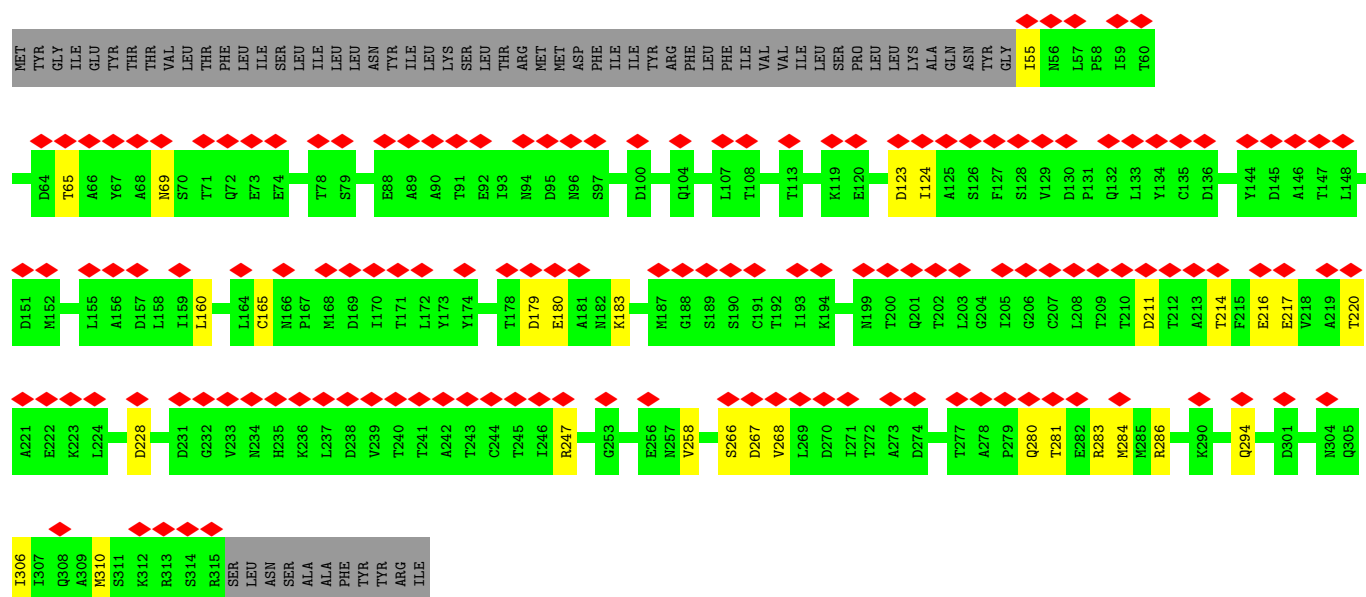


• Molecule 3: Outer capsid glycoprotein VP7

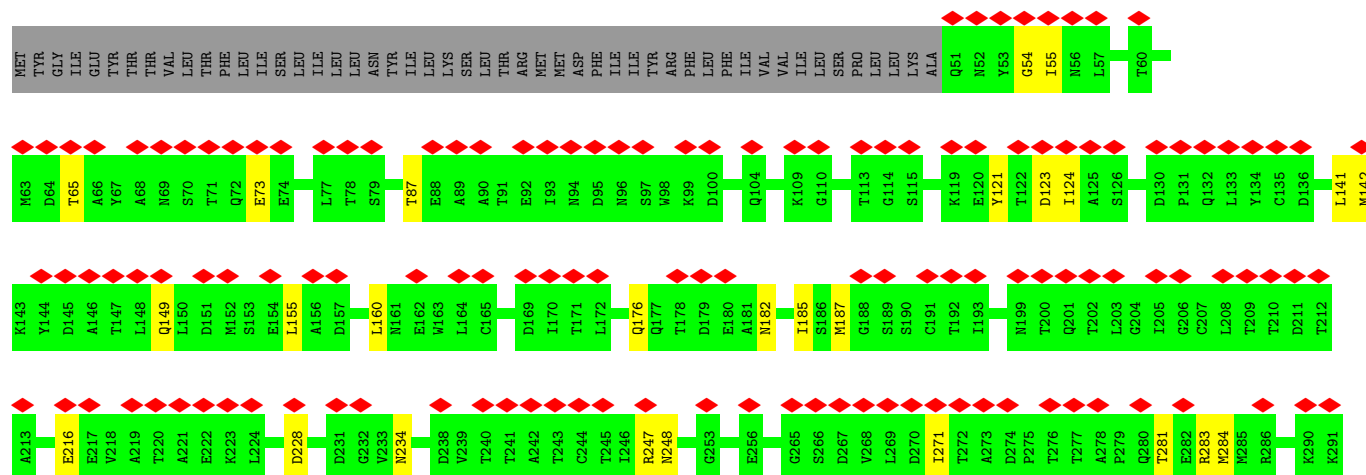
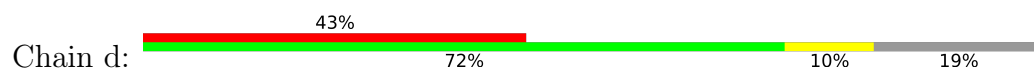


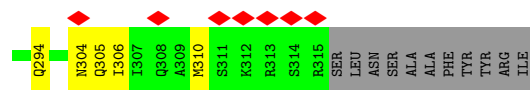


• Molecule 3: Outer capsid glycoprotein VP7

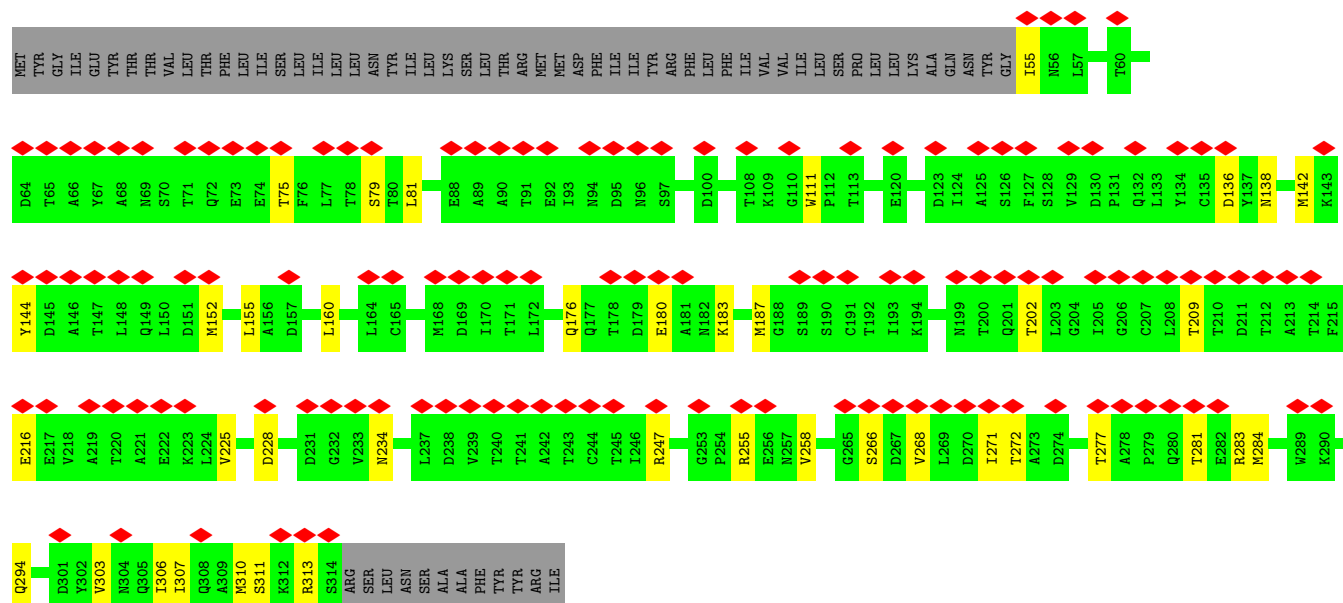
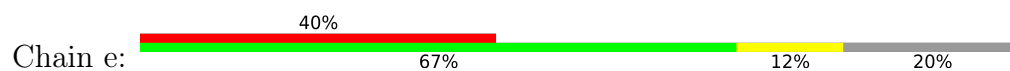


• Molecule 3: Outer capsid glycoprotein VP7

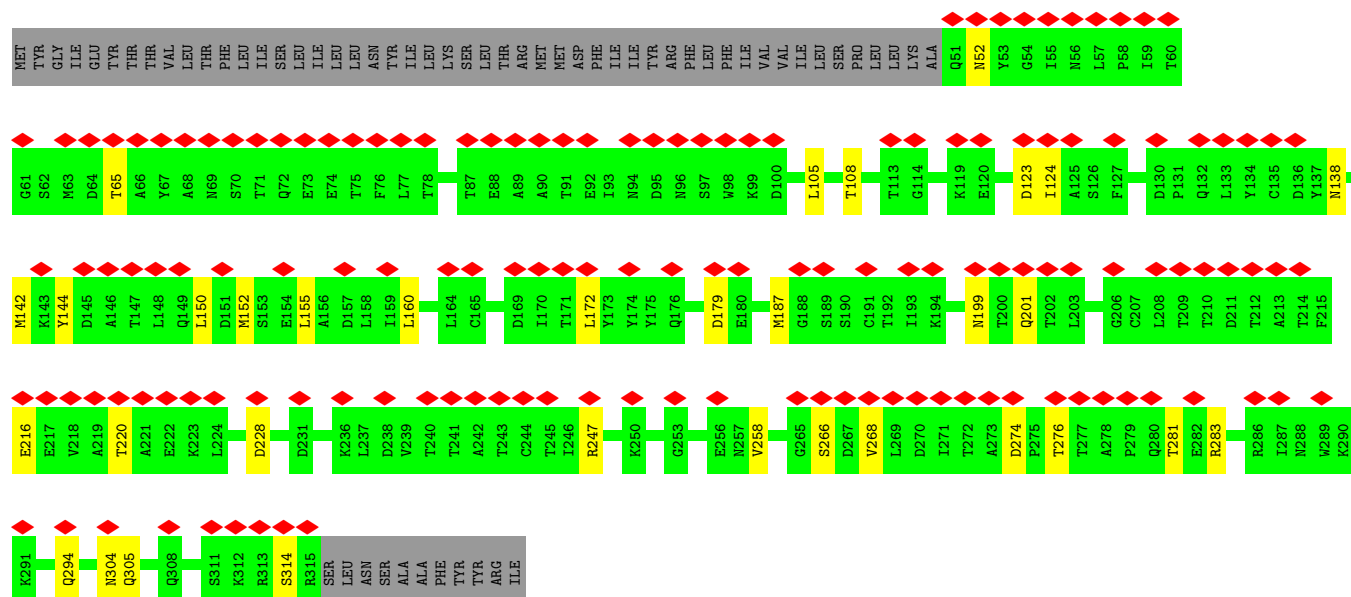
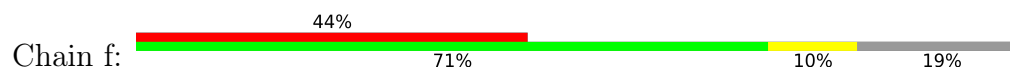




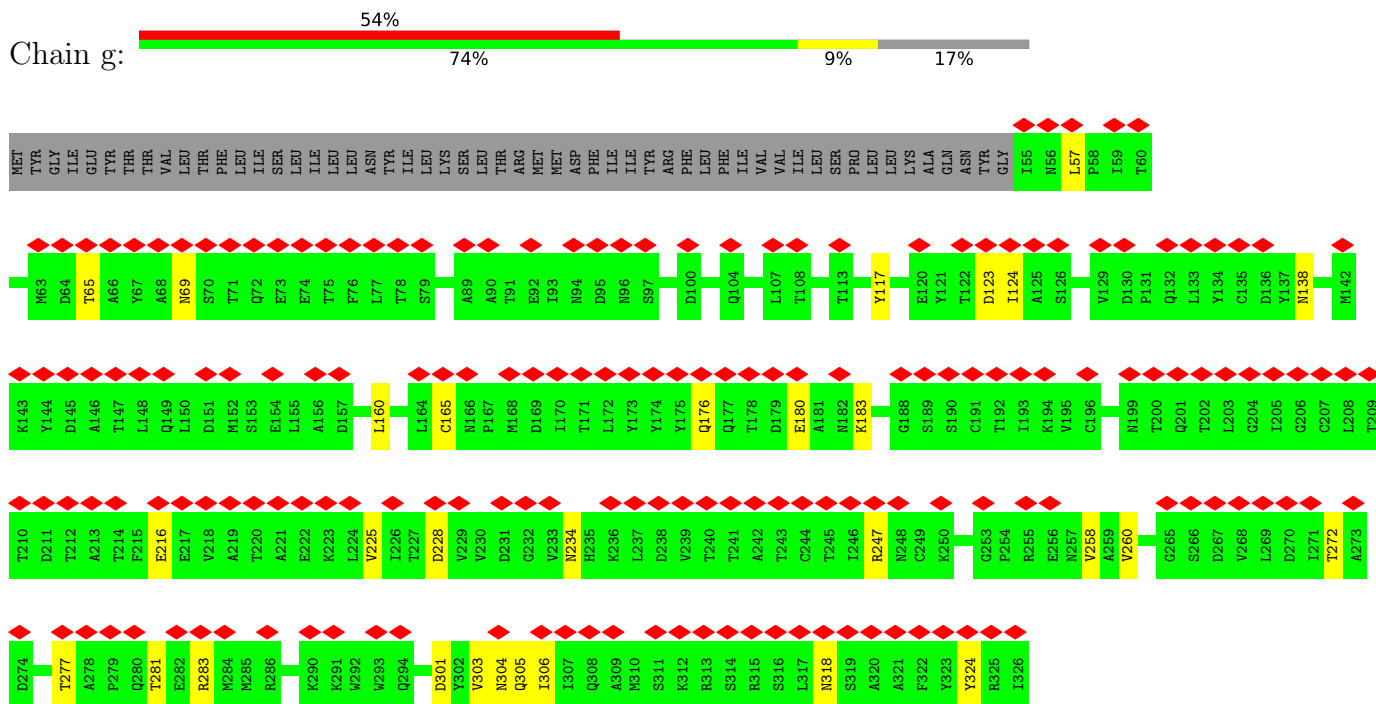
• Molecule 3: Outer capsid glycoprotein VP7



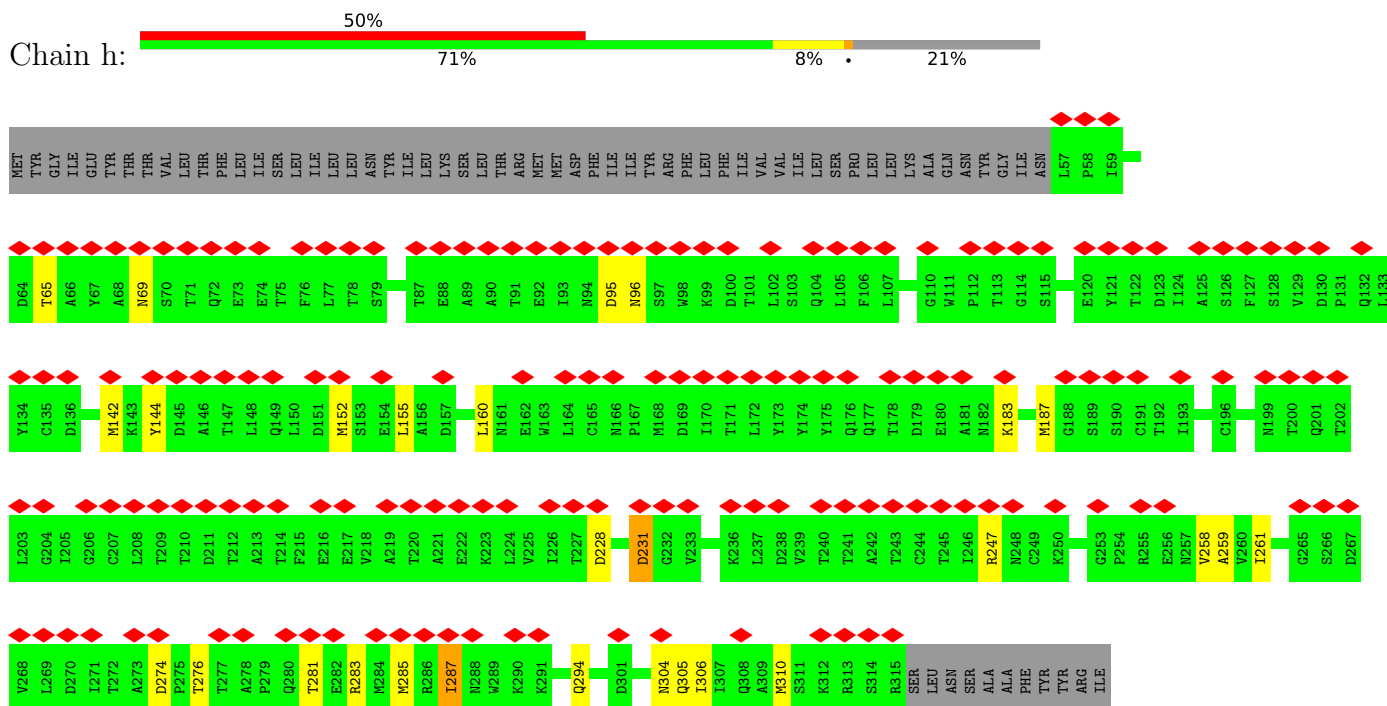
• Molecule 3: Outer capsid glycoprotein VP7



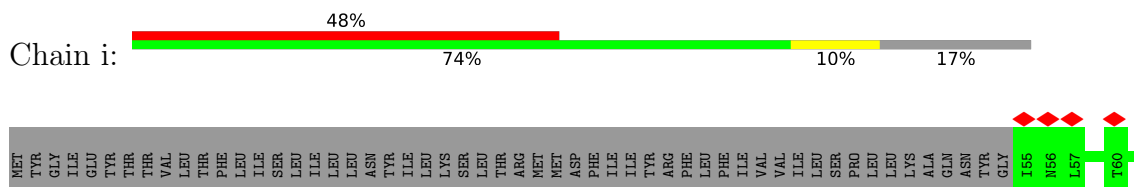
• Molecule 3: Outer capsid glycoprotein VP7

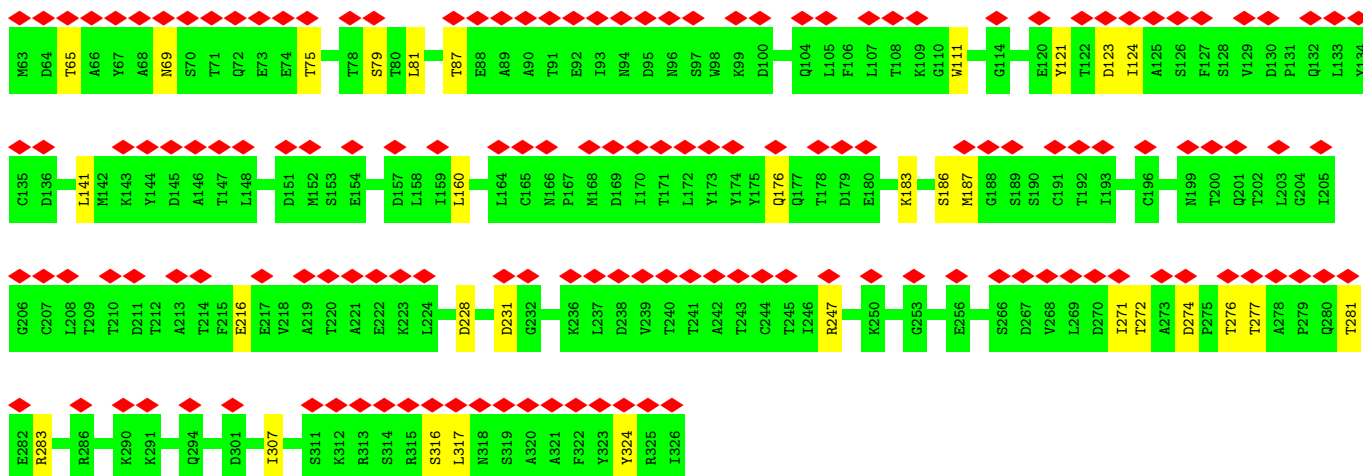


- Molecule 3: Outer capsid glycoprotein VP7

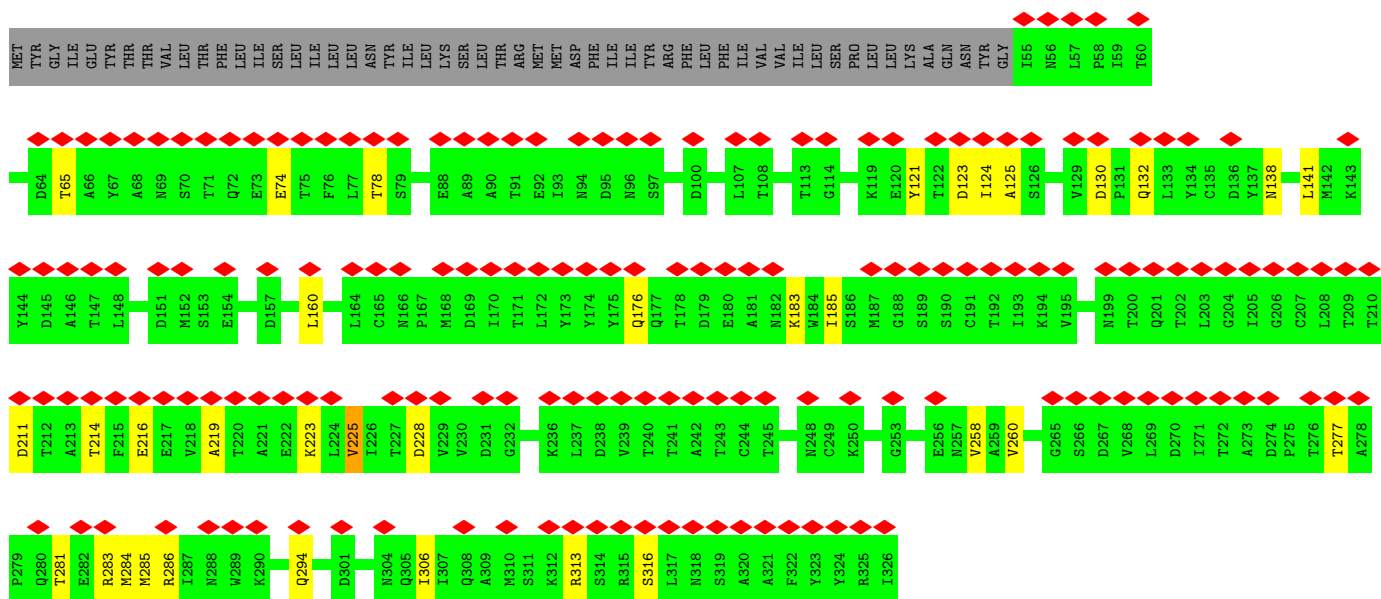
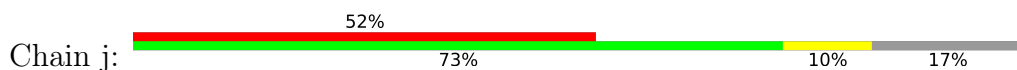


- Molecule 3: Outer capsid glycoprotein VP7

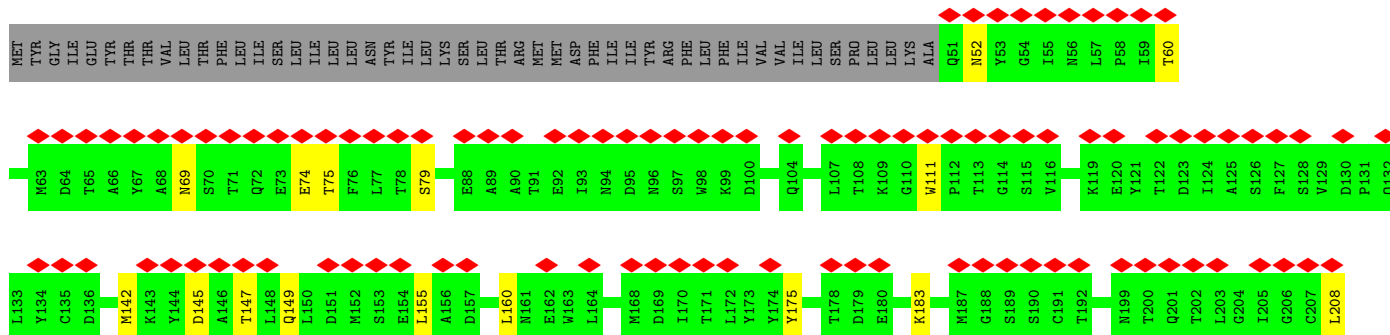
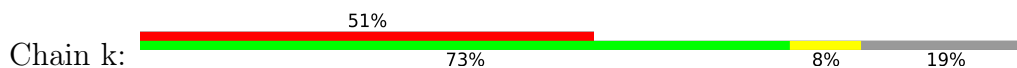




• Molecule 3: Outer capsid glycoprotein VP7

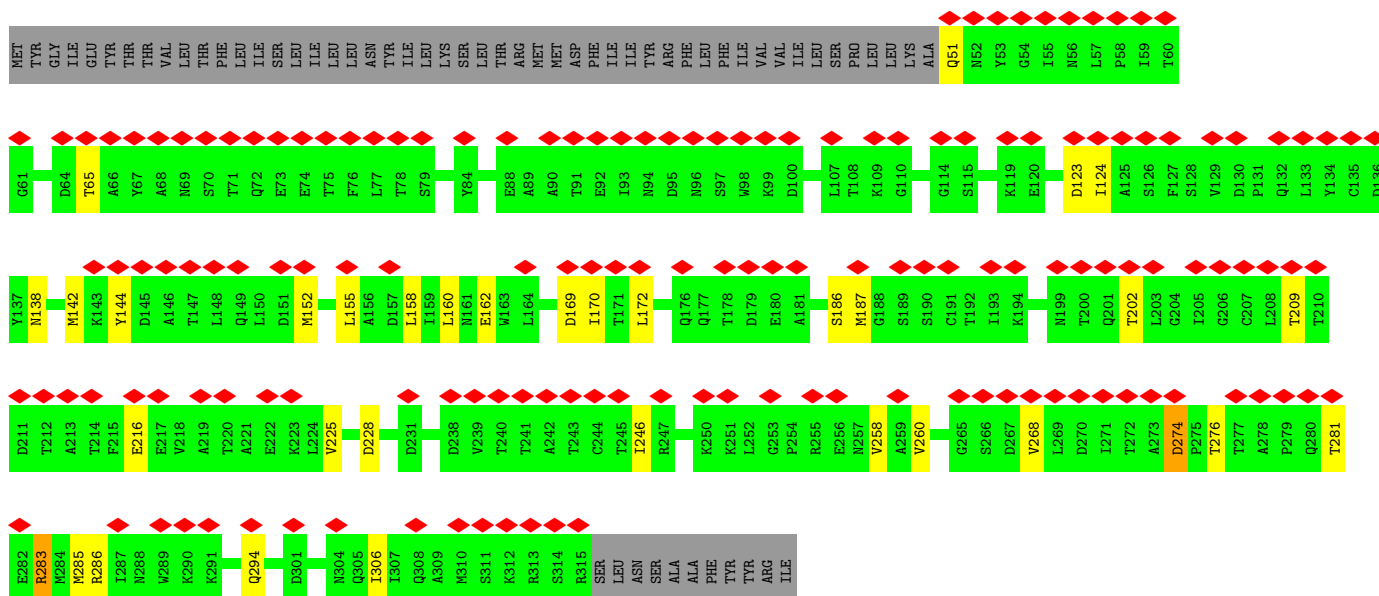


• Molecule 3: Outer capsid glycoprotein VP7

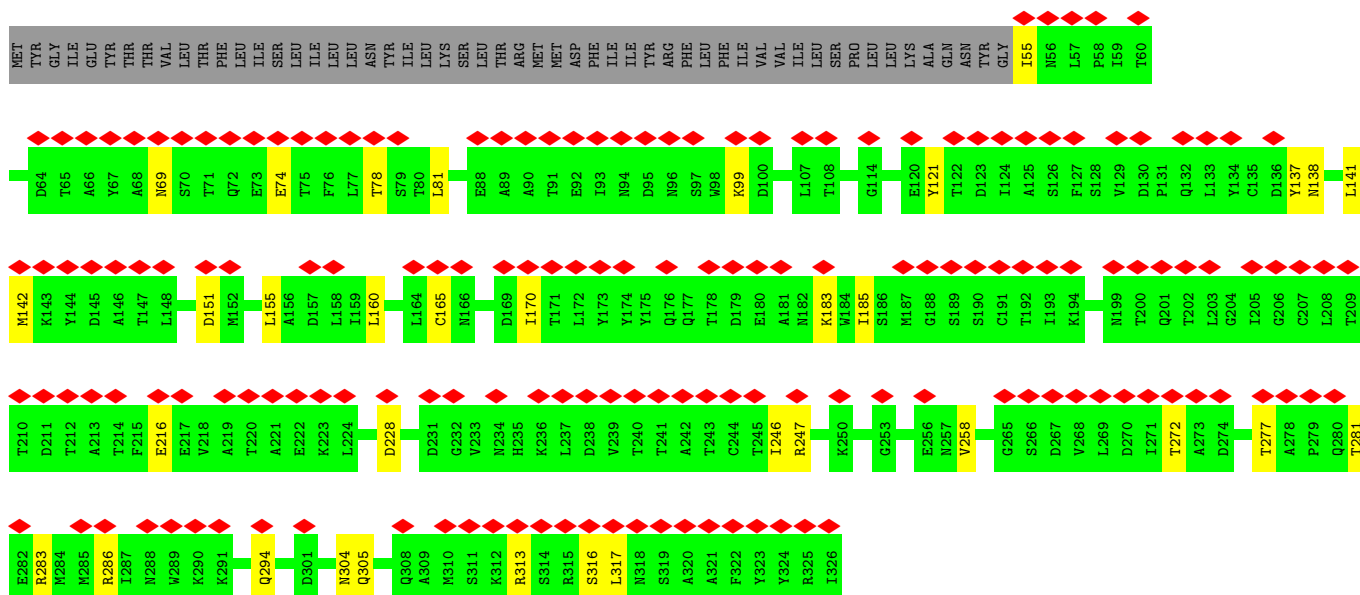
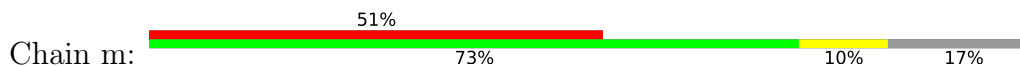




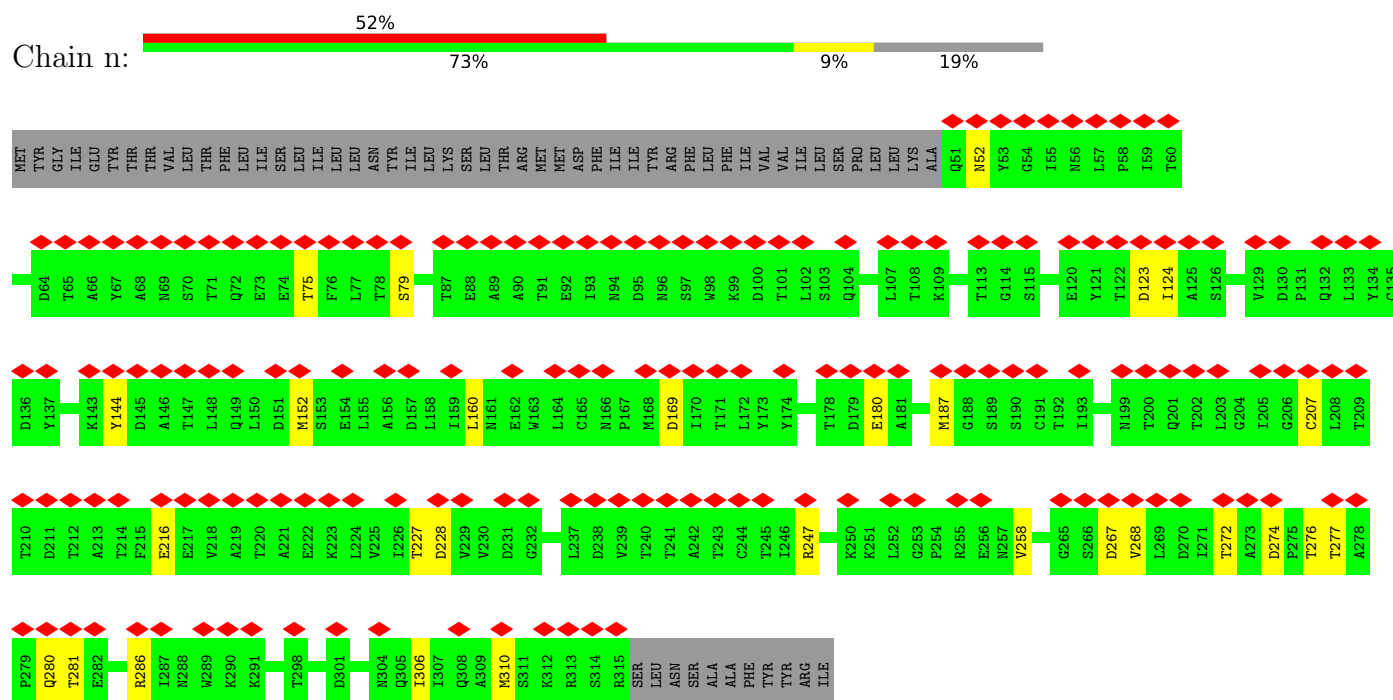
- Molecule 3: Outer capsid glycoprotein VP7



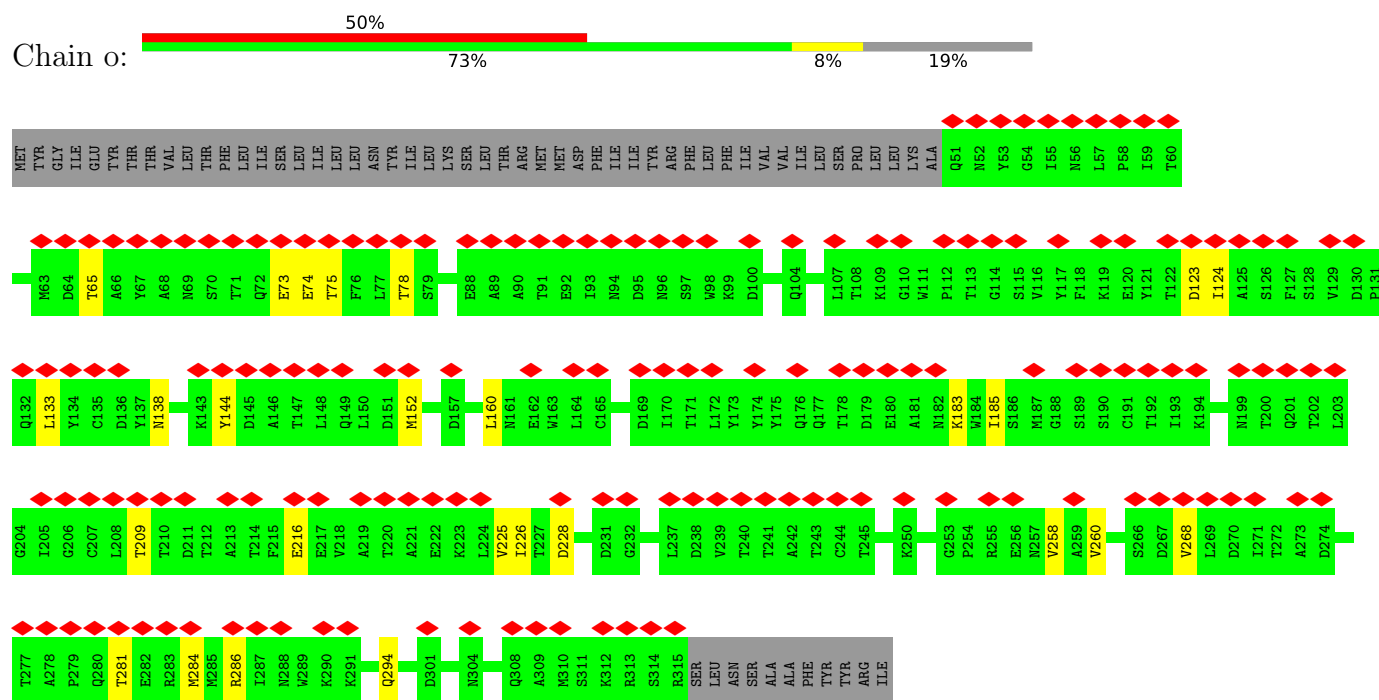
- Molecule 3: Outer capsid glycoprotein VP7



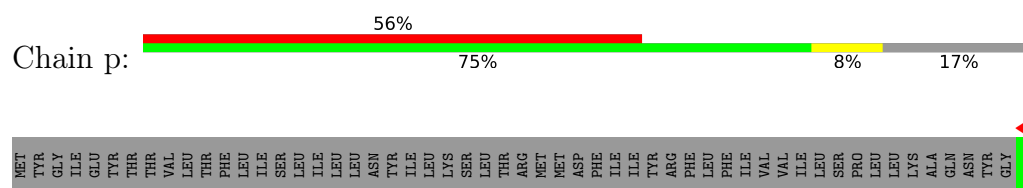
- Molecule 3: Outer capsid glycoprotein VP7



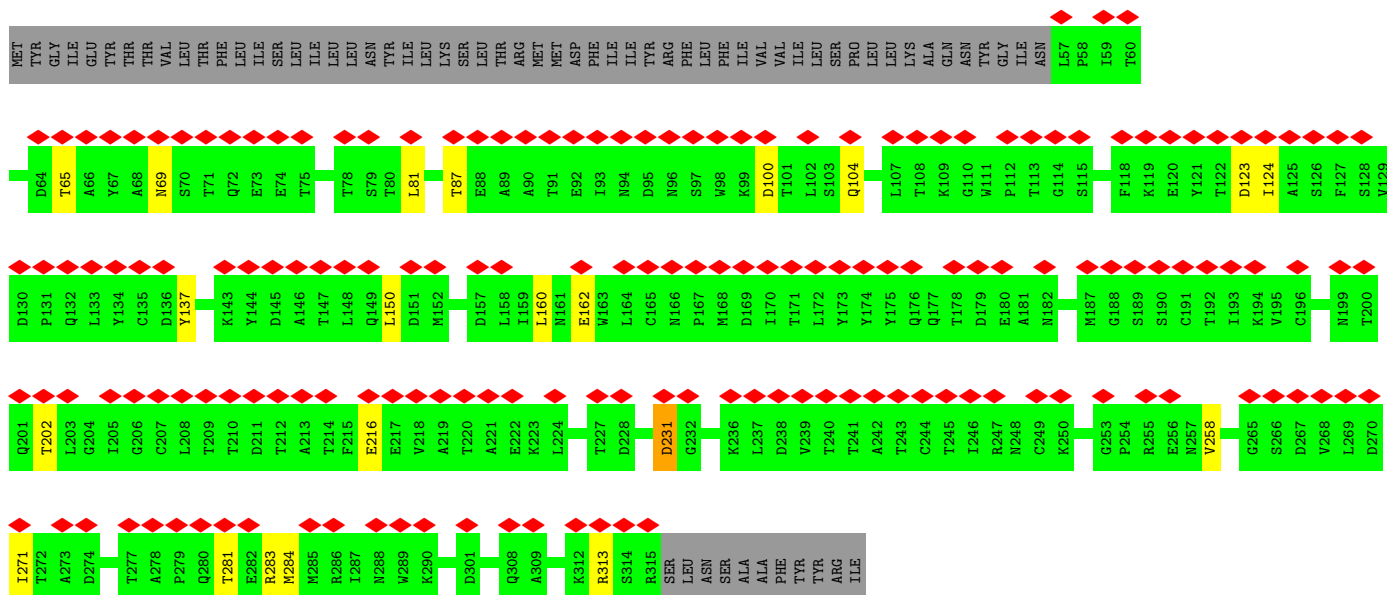
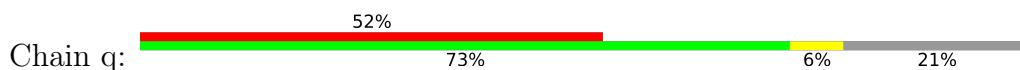
- Molecule 3: Outer capsid glycoprotein VP7



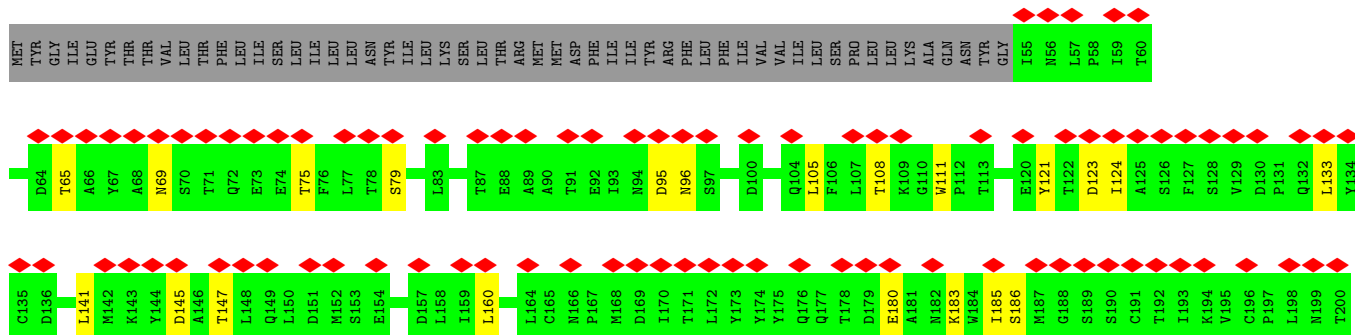
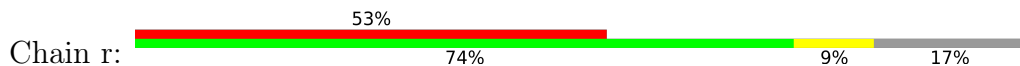
- Molecule 3: Outer capsid glycoprotein VP7

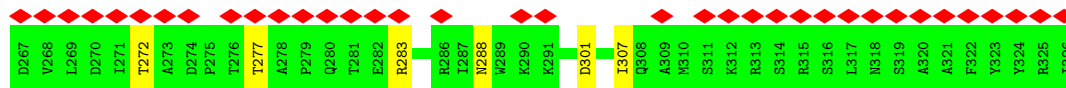


- Molecule 3: Outer capsid glycoprotein VP7



- Molecule 3: Outer capsid glycoprotein VP7





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 252548                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 33                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 40605                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.157                                   | Depositor |
| Minimum map value                    | -0.100                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.010                                   | Depositor |
| Recommended contour level            | 0.05                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 393.91998, 393.91998, 393.91998         | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.231, 1.231, 1.231                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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   | 1     | 0.19         | 0/2232      | 0.40        | 0/3032      |
| 1   | 2     | 0.19         | 0/2232      | 0.41        | 0/3032      |
| 1   | 3     | 0.21         | 0/2232      | 0.42        | 0/3032      |
| 2   | A     | 0.21         | 0/3233      | 0.48        | 0/4397      |
| 2   | B     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 2   | C     | 0.20         | 0/3233      | 0.46        | 0/4397      |
| 2   | D     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 2   | E     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 2   | F     | 0.22         | 0/3233      | 0.48        | 0/4397      |
| 2   | G     | 0.21         | 0/3233      | 0.48        | 0/4397      |
| 2   | H     | 0.22         | 0/3233      | 0.46        | 0/4397      |
| 2   | I     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 2   | J     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 2   | K     | 0.21         | 0/3233      | 0.46        | 0/4397      |
| 2   | L     | 0.21         | 0/3233      | 0.46        | 0/4397      |
| 2   | M     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 2   | N     | 0.20         | 0/3233      | 0.45        | 0/4397      |
| 2   | O     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 2   | P     | 0.21         | 0/3233      | 0.46        | 0/4397      |
| 2   | Q     | 0.21         | 0/3233      | 0.48        | 0/4397      |
| 2   | R     | 0.21         | 0/3233      | 0.47        | 0/4397      |
| 3   | a     | 0.19         | 0/2089      | 0.43        | 0/2854      |
| 3   | b     | 0.18         | 0/2200      | 0.44        | 0/3005      |
| 3   | c     | 0.19         | 0/2105      | 0.44        | 0/2876      |
| 3   | d     | 0.20         | 0/2139      | 0.44        | 0/2922      |
| 3   | e     | 0.20         | 0/2094      | 0.45        | 0/2862      |
| 3   | f     | 0.18         | 0/2139      | 0.43        | 0/2922      |
| 3   | g     | 0.19         | 0/2200      | 0.45        | 0/3005      |
| 3   | h     | 0.19         | 0/2089      | 0.42        | 0/2854      |
| 3   | i     | 0.20         | 0/2200      | 0.44        | 0/3005      |
| 3   | j     | 0.19         | 0/2200      | 0.45        | 0/3005      |
| 3   | k     | 0.19         | 0/2139      | 0.45        | 0/2922      |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 3   | l     | 0.19         | 0/2139   | 0.44        | 0/2922   |
| 3   | m     | 0.19         | 0/2200   | 0.45        | 0/3005   |
| 3   | n     | 0.18         | 0/2139   | 0.43        | 0/2922   |
| 3   | o     | 0.19         | 0/2139   | 0.44        | 0/2922   |
| 3   | p     | 0.19         | 0/2200   | 0.44        | 0/3005   |
| 3   | q     | 0.18         | 0/2089   | 0.43        | 0/2854   |
| 3   | r     | 0.18         | 0/2200   | 0.44        | 0/3005   |
| All | All   | 0.20         | 0/103590 | 0.45        | 0/141109 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | e     | 0                   | 1                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | e     | 311 | SER  | Peptide |

## 5.2 Too-close contacts [i](#)

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   | 1     | 2184  | 2107     | 2107     | 21      | 0            |
| 1   | 2     | 2184  | 2107     | 2107     | 14      | 0            |
| 1   | 3     | 2184  | 2107     | 2107     | 20      | 0            |
| 2   | A     | 3163  | 3112     | 3112     | 32      | 0            |
| 2   | B     | 3163  | 3112     | 3112     | 25      | 0            |
| 2   | C     | 3163  | 3112     | 3112     | 25      | 0            |
| 2   | D     | 3163  | 3112     | 3112     | 29      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | E     | 3163  | 3113     | 3112     | 33      | 0            |
| 2   | F     | 3163  | 3113     | 3112     | 31      | 0            |
| 2   | G     | 3163  | 3113     | 3112     | 30      | 0            |
| 2   | H     | 3163  | 3113     | 3112     | 24      | 0            |
| 2   | I     | 3163  | 3112     | 3112     | 27      | 0            |
| 2   | J     | 3163  | 3112     | 3112     | 29      | 0            |
| 2   | K     | 3163  | 3112     | 3112     | 28      | 0            |
| 2   | L     | 3163  | 3113     | 3112     | 29      | 0            |
| 2   | M     | 3163  | 3113     | 3112     | 27      | 0            |
| 2   | N     | 3163  | 3112     | 3112     | 22      | 0            |
| 2   | O     | 3163  | 3113     | 3112     | 25      | 0            |
| 2   | P     | 3163  | 3112     | 3112     | 34      | 0            |
| 2   | Q     | 3163  | 3113     | 3112     | 25      | 0            |
| 2   | R     | 3163  | 3112     | 3112     | 25      | 0            |
| 3   | a     | 2047  | 1994     | 1993     | 21      | 0            |
| 3   | b     | 2155  | 2099     | 2099     | 27      | 0            |
| 3   | c     | 2063  | 2011     | 2010     | 19      | 0            |
| 3   | d     | 2096  | 2037     | 2036     | 15      | 0            |
| 3   | e     | 2052  | 1998     | 1997     | 21      | 0            |
| 3   | f     | 2096  | 2037     | 2036     | 21      | 0            |
| 3   | g     | 2155  | 2099     | 2098     | 17      | 0            |
| 3   | h     | 2047  | 1994     | 1993     | 17      | 0            |
| 3   | i     | 2155  | 2099     | 2098     | 16      | 0            |
| 3   | j     | 2155  | 2099     | 2098     | 18      | 0            |
| 3   | k     | 2096  | 2037     | 2036     | 17      | 0            |
| 3   | l     | 2096  | 2037     | 2036     | 22      | 0            |
| 3   | m     | 2155  | 2099     | 2098     | 21      | 0            |
| 3   | n     | 2096  | 2037     | 2036     | 17      | 0            |
| 3   | o     | 2096  | 2037     | 2036     | 15      | 0            |
| 3   | p     | 2155  | 2099     | 2098     | 14      | 0            |
| 3   | q     | 2047  | 1994     | 1993     | 13      | 0            |
| 3   | r     | 2155  | 2099     | 2098     | 18      | 0            |
| 4   | a     | 14    | 14       | 13       | 1       | 0            |
| 4   | b     | 14    | 14       | 13       | 0       | 0            |
| 4   | c     | 14    | 14       | 13       | 1       | 0            |
| 4   | d     | 14    | 14       | 13       | 0       | 0            |
| 4   | e     | 14    | 14       | 13       | 0       | 0            |
| 4   | f     | 14    | 14       | 13       | 0       | 0            |
| 4   | g     | 14    | 14       | 13       | 0       | 0            |
| 4   | h     | 14    | 14       | 13       | 1       | 0            |
| 4   | i     | 14    | 14       | 13       | 1       | 0            |
| 4   | j     | 14    | 14       | 13       | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 4   | k     | 14     | 14       | 13       | 1       | 0            |
| 4   | l     | 14     | 14       | 13       | 0       | 0            |
| 4   | m     | 14     | 14       | 13       | 1       | 0            |
| 4   | n     | 14     | 14       | 13       | 0       | 0            |
| 4   | o     | 14     | 14       | 13       | 0       | 0            |
| 4   | p     | 14     | 14       | 13       | 1       | 0            |
| 4   | q     | 14     | 14       | 13       | 0       | 0            |
| 4   | r     | 14     | 14       | 13       | 1       | 0            |
| 5   | a     | 5      | 0        | 0        | 0       | 0            |
| 5   | b     | 3      | 0        | 0        | 0       | 0            |
| 5   | c     | 1      | 0        | 0        | 0       | 0            |
| 5   | d     | 5      | 0        | 0        | 0       | 0            |
| 5   | e     | 3      | 0        | 0        | 0       | 0            |
| 5   | f     | 1      | 0        | 0        | 0       | 0            |
| 5   | g     | 5      | 0        | 0        | 0       | 0            |
| 5   | h     | 3      | 0        | 0        | 0       | 0            |
| 5   | i     | 1      | 0        | 0        | 0       | 0            |
| 5   | j     | 5      | 0        | 0        | 0       | 0            |
| 5   | k     | 3      | 0        | 0        | 0       | 0            |
| 5   | l     | 1      | 0        | 0        | 0       | 0            |
| 5   | m     | 5      | 0        | 0        | 0       | 0            |
| 5   | n     | 3      | 0        | 0        | 0       | 0            |
| 5   | o     | 1      | 0        | 0        | 0       | 0            |
| 5   | p     | 5      | 0        | 0        | 0       | 0            |
| 5   | q     | 3      | 0        | 0        | 0       | 0            |
| 5   | r     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 101709 | 99503    | 99460    | 769     | 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 4.

All (769) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:1:485:THR:HG1 | 1:2:412:SER:HG | 1.26                     | 0.80              |
| 2:G:255:ARG:NH1 | 3:h:65:THR:O   | 2.18                     | 0.77              |
| 2:E:255:ARG:NH1 | 3:f:65:THR:O   | 2.19                     | 0.76              |
| 2:Q:255:ARG:NH1 | 3:r:65:THR:O   | 2.19                     | 0.75              |
| 2:H:255:ARG:NH1 | 3:i:65:THR:O   | 2.19                     | 0.74              |
| 2:B:255:ARG:NH1 | 3:a:65:THR:O   | 2.20                     | 0.74              |
| 2:O:141:LEU:O   | 2:O:144:ARG:C  | 2.31                     | 0.74              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:b:160:LEU:O   | 3:b:283:ARG:NH2  | 2.22                     | 0.72              |
| 1:3:270:ASP:OD1 | 1:3:467:ARG:NH1  | 2.23                     | 0.72              |
| 2:E:239:ASN:ND2 | 2:E:240:SER:O    | 2.23                     | 0.71              |
| 2:F:255:ARG:NH1 | 3:d:65:THR:O     | 2.22                     | 0.71              |
| 2:P:255:ARG:NH1 | 3:q:65:THR:O     | 2.23                     | 0.71              |
| 3:k:160:LEU:O   | 3:k:283:ARG:NH2  | 2.23                     | 0.71              |
| 2:K:141:LEU:O   | 2:K:144:ARG:O    | 2.09                     | 0.71              |
| 3:r:160:LEU:O   | 3:r:283:ARG:NH2  | 2.23                     | 0.71              |
| 3:f:142:MET:HE2 | 3:f:155:LEU:HD23 | 1.70                     | 0.71              |
| 2:F:239:ASN:ND2 | 2:F:240:SER:O    | 2.24                     | 0.70              |
| 2:K:239:ASN:ND2 | 2:K:240:SER:O    | 2.23                     | 0.70              |
| 2:B:141:LEU:O   | 2:B:144:ARG:O    | 2.09                     | 0.70              |
| 3:q:160:LEU:O   | 3:q:283:ARG:NH2  | 2.24                     | 0.70              |
| 2:K:255:ARG:NH1 | 3:l:65:THR:O     | 2.26                     | 0.69              |
| 2:O:239:ASN:ND2 | 2:O:240:SER:O    | 2.25                     | 0.69              |
| 2:I:239:ASN:ND2 | 2:I:240:SER:O    | 2.25                     | 0.69              |
| 3:i:160:LEU:O   | 3:i:283:ARG:NH2  | 2.26                     | 0.69              |
| 2:R:141:LEU:O   | 2:R:144:ARG:C    | 2.36                     | 0.69              |
| 2:I:255:ARG:NH1 | 3:g:65:THR:O     | 2.25                     | 0.69              |
| 2:R:141:LEU:O   | 2:R:144:ARG:O    | 2.11                     | 0.69              |
| 3:i:75:THR:O    | 3:i:79:SER:OG    | 2.11                     | 0.68              |
| 1:1:493:ASP:OD1 | 1:1:496:ARG:NH2  | 2.27                     | 0.68              |
| 2:G:342:MET:N   | 2:G:342:MET:SD   | 2.67                     | 0.68              |
| 2:A:255:ARG:NH1 | 3:c:65:THR:O     | 2.27                     | 0.68              |
| 2:C:230:GLU:O   | 2:C:233:SER:OG   | 2.10                     | 0.68              |
| 2:I:141:LEU:O   | 2:I:144:ARG:C    | 2.37                     | 0.68              |
| 2:N:57:ARG:NH1  | 2:N:94:ASN:OD1   | 2.27                     | 0.68              |
| 2:F:113:SER:O   | 2:F:116:LEU:N    | 2.27                     | 0.68              |
| 2:F:141:LEU:O   | 2:F:144:ARG:O    | 2.12                     | 0.68              |
| 2:H:141:LEU:O   | 2:H:144:ARG:C    | 2.37                     | 0.68              |
| 2:O:141:LEU:O   | 2:O:144:ARG:O    | 2.11                     | 0.68              |
| 3:m:272:THR:OG1 | 3:m:277:THR:OG1  | 2.11                     | 0.68              |
| 3:b:57:LEU:O    | 3:f:52:ASN:ND2   | 2.27                     | 0.67              |
| 3:e:160:LEU:O   | 3:e:283:ARG:NH2  | 2.26                     | 0.67              |
| 2:L:57:ARG:NH1  | 2:L:94:ASN:OD1   | 2.27                     | 0.67              |
| 2:I:334:VAL:O   | 2:I:374:TYR:OH   | 2.13                     | 0.67              |
| 1:1:485:THR:OG1 | 1:2:412:SER:OG   | 2.09                     | 0.67              |
| 2:B:103:GLU:OE2 | 2:B:350:ARG:NH2  | 2.28                     | 0.67              |
| 2:H:141:LEU:O   | 2:H:144:ARG:O    | 2.13                     | 0.67              |
| 2:I:229:ALA:O   | 2:I:233:SER:OG   | 2.13                     | 0.67              |
| 2:K:57:ARG:NH1  | 2:K:94:ASN:OD1   | 2.28                     | 0.67              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:m:160:LEU:O   | 3:m:283:ARG:NH2 | 2.27                     | 0.67              |
| 2:R:213:GLN:NE2 | 2:R:286:ASP:OD1 | 2.28                     | 0.67              |
| 3:b:176:GLN:NE2 | 3:b:234:ASN:OD1 | 2.28                     | 0.67              |
| 2:A:228:ASP:OD2 | 2:B:236:ARG:NH2 | 2.28                     | 0.67              |
| 2:B:57:ARG:NH1  | 2:B:94:ASN:OD1  | 2.27                     | 0.67              |
| 3:d:294:GLN:NE2 | 3:f:228:ASP:O   | 2.29                     | 0.66              |
| 2:I:90:ASP:OD1  | 2:I:94:ASN:ND2  | 2.29                     | 0.66              |
| 3:k:145:ASP:OD2 | 3:k:147:THR:OG1 | 2.14                     | 0.66              |
| 2:H:93:ASP:OD1  | 2:H:392:ARG:NE  | 2.28                     | 0.66              |
| 2:K:93:ASP:OD1  | 2:K:392:ARG:NE  | 2.28                     | 0.66              |
| 2:I:57:ARG:NH1  | 2:I:94:ASN:OD1  | 2.28                     | 0.66              |
| 2:O:93:ASP:OD1  | 2:O:392:ARG:NE  | 2.29                     | 0.66              |
| 2:P:113:SER:O   | 2:P:116:LEU:N   | 2.28                     | 0.66              |
| 3:e:187:MET:SD  | 3:e:247:ARG:NH2 | 2.69                     | 0.66              |
| 3:k:75:THR:O    | 3:k:79:SER:OG   | 2.12                     | 0.66              |
| 2:C:113:SER:O   | 2:C:116:LEU:N   | 2.29                     | 0.66              |
| 2:G:141:LEU:O   | 2:G:144:ARG:C   | 2.38                     | 0.66              |
| 2:R:334:VAL:O   | 2:R:374:TYR:OH  | 2.13                     | 0.66              |
| 3:h:160:LEU:O   | 3:h:283:ARG:NH2 | 2.29                     | 0.66              |
| 2:H:57:ARG:NH1  | 2:H:94:ASN:OD1  | 2.28                     | 0.66              |
| 2:I:93:ASP:OD1  | 2:I:392:ARG:NE  | 2.29                     | 0.66              |
| 3:l:51:GLN:N    | 3:m:55:ILE:O    | 2.29                     | 0.66              |
| 2:O:57:ARG:NH1  | 2:O:94:ASN:OD1  | 2.29                     | 0.65              |
| 3:a:160:LEU:O   | 3:a:283:ARG:NH2 | 2.29                     | 0.65              |
| 2:A:44:ASN:OD1  | 2:A:118:LYS:NZ  | 2.30                     | 0.65              |
| 2:D:213:GLN:OE1 | 2:D:287:THR:OG1 | 2.12                     | 0.65              |
| 2:N:103:GLU:OE2 | 2:N:350:ARG:NH2 | 2.29                     | 0.65              |
| 2:B:147:ARG:NH1 | 2:B:332:GLU:OE2 | 2.29                     | 0.65              |
| 2:F:93:ASP:OD1  | 2:F:392:ARG:NE  | 2.29                     | 0.65              |
| 1:1:491:ARG:NH2 | 1:2:492:GLN:OE1 | 2.30                     | 0.65              |
| 2:I:141:LEU:O   | 2:I:144:ARG:O   | 2.15                     | 0.65              |
| 1:1:360:GLN:OE1 | 1:1:363:ARG:NH1 | 2.30                     | 0.64              |
| 2:F:57:ARG:NH1  | 2:F:94:ASN:OD1  | 2.29                     | 0.64              |
| 3:d:160:LEU:O   | 3:d:283:ARG:NH2 | 2.29                     | 0.64              |
| 3:j:294:GLN:NE2 | 3:l:228:ASP:O   | 2.30                     | 0.64              |
| 3:p:160:LEU:O   | 3:p:283:ARG:NH2 | 2.30                     | 0.64              |
| 2:M:33:GLN:NE2  | 2:M:127:ILE:O   | 2.29                     | 0.64              |
| 2:O:113:SER:O   | 2:O:116:LEU:N   | 2.29                     | 0.64              |
| 2:E:141:LEU:O   | 2:E:144:ARG:O   | 2.16                     | 0.64              |
| 2:J:141:LEU:O   | 2:J:144:ARG:C   | 2.41                     | 0.64              |
| 2:P:141:LEU:O   | 2:P:144:ARG:C   | 2.41                     | 0.64              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:D:342:MET:SD  | 2:D:342:MET:N   | 2.71                     | 0.64              |
| 2:K:44:ASN:OD1  | 2:K:118:LYS:NZ  | 2.31                     | 0.64              |
| 2:K:113:SER:O   | 2:K:116:LEU:N   | 2.28                     | 0.64              |
| 3:r:145:ASP:OD2 | 3:r:147:THR:OG1 | 2.16                     | 0.64              |
| 2:D:216:ARG:NH2 | 2:D:374:TYR:O   | 2.31                     | 0.64              |
| 2:D:141:LEU:O   | 2:D:144:ARG:O   | 2.14                     | 0.64              |
| 2:A:57:ARG:NH1  | 2:A:94:ASN:OD1  | 2.31                     | 0.63              |
| 2:F:141:LEU:O   | 2:F:144:ARG:C   | 2.41                     | 0.63              |
| 2:L:255:ARG:NH1 | 3:j:65:THR:O    | 2.32                     | 0.63              |
| 2:M:103:GLU:OE2 | 2:M:350:ARG:NH2 | 2.31                     | 0.63              |
| 2:P:33:GLN:NE2  | 2:P:127:ILE:O   | 2.31                     | 0.63              |
| 3:l:160:LEU:O   | 3:l:283:ARG:NH2 | 2.31                     | 0.63              |
| 2:Q:57:ARG:NH1  | 2:Q:94:ASN:OD1  | 2.31                     | 0.63              |
| 2:R:230:GLU:O   | 2:R:233:SER:OG  | 2.13                     | 0.63              |
| 2:K:141:LEU:O   | 2:K:144:ARG:C   | 2.41                     | 0.63              |
| 2:H:342:MET:SD  | 2:H:342:MET:N   | 2.71                     | 0.63              |
| 2:E:57:ARG:NH1  | 2:E:94:ASN:OD1  | 2.31                     | 0.63              |
| 2:P:236:ARG:NH2 | 2:R:228:ASP:OD2 | 2.32                     | 0.63              |
| 2:B:93:ASP:OD1  | 2:B:392:ARG:NE  | 2.32                     | 0.63              |
| 2:B:141:LEU:O   | 2:B:144:ARG:C   | 2.41                     | 0.63              |
| 3:c:160:LEU:O   | 3:c:283:ARG:NH2 | 2.32                     | 0.62              |
| 3:q:162:GLU:OE2 | 3:q:313:ARG:NH1 | 2.32                     | 0.62              |
| 2:L:33:GLN:NE2  | 2:L:127:ILE:O   | 2.32                     | 0.62              |
| 3:n:52:ASN:ND2  | 3:p:57:LEU:O    | 2.32                     | 0.62              |
| 2:K:230:GLU:O   | 2:K:233:SER:OG  | 2.17                     | 0.62              |
| 2:A:141:LEU:O   | 2:A:144:ARG:C   | 2.42                     | 0.62              |
| 3:p:165:CYS:SG  | 3:p:247:ARG:NH1 | 2.73                     | 0.62              |
| 2:P:103:GLU:OE2 | 2:P:350:ARG:NH2 | 2.33                     | 0.62              |
| 2:P:44:ASN:OD1  | 2:P:118:LYS:NZ  | 2.33                     | 0.61              |
| 2:M:230:GLU:O   | 2:M:233:SER:OG  | 2.12                     | 0.61              |
| 2:A:239:ASN:ND2 | 2:A:240:SER:O   | 2.33                     | 0.61              |
| 2:L:215:ARG:O   | 2:L:216:ARG:NH1 | 2.33                     | 0.61              |
| 2:M:57:ARG:NH1  | 2:M:94:ASN:OD1  | 2.32                     | 0.61              |
| 2:P:153:HIS:N   | 2:P:337:ASP:OD1 | 2.33                     | 0.61              |
| 2:E:216:ARG:NH2 | 2:E:374:TYR:O   | 2.34                     | 0.60              |
| 3:c:183:LYS:NZ  | 3:c:228:ASP:OD2 | 2.34                     | 0.60              |
| 2:N:44:ASN:OD1  | 2:N:118:LYS:NZ  | 2.34                     | 0.60              |
| 3:n:228:ASP:O   | 3:o:294:GLN:NE2 | 2.34                     | 0.60              |
| 2:J:236:ARG:NH2 | 2:L:228:ASP:OD2 | 2.34                     | 0.60              |
| 2:L:141:LEU:O   | 2:L:144:ARG:O   | 2.20                     | 0.60              |
| 2:G:57:ARG:NH1  | 2:G:94:ASN:OD1  | 2.35                     | 0.60              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:F:230:GLU:O   | 2:F:233:SER:OG   | 2.13                     | 0.60              |
| 1:1:502:ARG:NH2 | 1:2:283:LYS:O    | 2.35                     | 0.60              |
| 3:m:294:GLN:NE2 | 3:o:228:ASP:O    | 2.35                     | 0.59              |
| 3:j:160:LEU:O   | 3:j:283:ARG:NH2  | 2.35                     | 0.59              |
| 2:C:44:ASN:OD1  | 2:C:118:LYS:NZ   | 2.35                     | 0.59              |
| 2:I:142:GLN:HG3 | 2:I:148:THR:HG21 | 1.83                     | 0.59              |
| 3:p:267:ASP:OD2 | 3:p:280:GLN:NE2  | 2.35                     | 0.59              |
| 1:2:485:THR:OG1 | 1:3:412:SER:OG   | 2.17                     | 0.59              |
| 2:D:74:ASP:N    | 2:D:74:ASP:OD2   | 2.34                     | 0.59              |
| 2:M:147:ARG:NH1 | 2:M:332:GLU:OE2  | 2.36                     | 0.59              |
| 1:1:270:ASP:OD1 | 1:1:467:ARG:NH1  | 2.35                     | 0.59              |
| 2:F:342:MET:SD  | 2:F:342:MET:N    | 2.76                     | 0.59              |
| 3:n:187:MET:SD  | 3:n:247:ARG:NH2  | 2.76                     | 0.59              |
| 2:E:141:LEU:O   | 2:E:144:ARG:C    | 2.45                     | 0.58              |
| 2:J:228:ASP:OD2 | 2:K:236:ARG:NH2  | 2.36                     | 0.58              |
| 2:R:57:ARG:NH1  | 2:R:94:ASN:OD1   | 2.35                     | 0.58              |
| 3:g:272:THR:OG1 | 3:g:277:THR:OG1  | 2.18                     | 0.58              |
| 2:M:44:ASN:OD1  | 2:M:118:LYS:NZ   | 2.36                     | 0.58              |
| 2:D:57:ARG:NH1  | 2:D:94:ASN:OD1   | 2.37                     | 0.58              |
| 2:I:342:MET:SD  | 2:I:342:MET:N    | 2.76                     | 0.58              |
| 2:M:239:ASN:OD1 | 2:O:255:ARG:NH1  | 2.36                     | 0.58              |
| 3:f:274:ASP:OD2 | 3:f:276:THR:OG1  | 2.20                     | 0.58              |
| 2:H:230:GLU:O   | 2:H:233:SER:OG   | 2.13                     | 0.58              |
| 2:C:103:GLU:OE2 | 2:C:350:ARG:NH2  | 2.37                     | 0.58              |
| 2:I:299:ASN:ND2 | 3:g:69:ASN:O     | 2.36                     | 0.58              |
| 2:J:230:GLU:OE1 | 2:J:230:GLU:N    | 2.37                     | 0.58              |
| 2:R:93:ASP:OD1  | 2:R:392:ARG:NE   | 2.37                     | 0.58              |
| 3:r:183:LYS:NZ  | 3:r:228:ASP:OD2  | 2.36                     | 0.58              |
| 3:a:121:TYR:OH  | 3:a:141:LEU:O    | 2.19                     | 0.58              |
| 3:g:57:LEU:O    | 3:k:52:ASN:ND2   | 2.37                     | 0.58              |
| 1:3:300:ASN:ND2 | 1:3:317:THR:OG1  | 2.37                     | 0.57              |
| 2:A:334:VAL:O   | 2:A:374:TYR:OH   | 2.20                     | 0.57              |
| 2:D:141:LEU:O   | 2:D:144:ARG:C    | 2.47                     | 0.57              |
| 3:a:75:THR:O    | 3:a:79:SER:OG    | 2.17                     | 0.57              |
| 2:L:141:LEU:O   | 2:L:144:ARG:C    | 2.48                     | 0.57              |
| 2:M:141:LEU:O   | 2:M:144:ARG:C    | 2.47                     | 0.57              |
| 3:m:121:TYR:OH  | 3:m:141:LEU:O    | 2.21                     | 0.57              |
| 2:E:230:GLU:O   | 2:E:233:SER:OG   | 2.20                     | 0.57              |
| 2:G:33:GLN:NE2  | 2:G:127:ILE:O    | 2.38                     | 0.57              |
| 2:P:228:ASP:OD2 | 2:Q:236:ARG:NH2  | 2.38                     | 0.57              |
| 2:A:103:GLU:OE2 | 2:A:350:ARG:NH2  | 2.37                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:103:GLU:OE2  | 2:J:350:ARG:NH2  | 2.38                     | 0.57              |
| 3:e:75:THR:O     | 3:e:79:SER:OG    | 2.13                     | 0.57              |
| 2:B:230:GLU:OE2  | 2:C:231:ARG:NH2  | 2.38                     | 0.56              |
| 2:Q:261:VAL:HG13 | 2:Q:290:LEU:HD23 | 1.87                     | 0.56              |
| 2:E:99:GLU:OE2   | 2:E:384:ARG:NH1  | 2.37                     | 0.56              |
| 3:m:165:CYS:SG   | 3:m:247:ARG:NH1  | 2.79                     | 0.56              |
| 2:D:134:GLU:O    | 2:D:138:ASN:ND2  | 2.37                     | 0.56              |
| 2:P:93:ASP:OD1   | 2:P:392:ARG:NE   | 2.37                     | 0.56              |
| 1:3:403:SER:OG   | 1:3:433:GLU:OE2  | 2.23                     | 0.56              |
| 2:J:57:ARG:NH1   | 2:J:94:ASN:OD1   | 2.38                     | 0.56              |
| 2:C:57:ARG:NH1   | 2:C:94:ASN:OD1   | 2.38                     | 0.56              |
| 3:e:272:THR:OG1  | 3:e:277:THR:OG1  | 2.23                     | 0.56              |
| 2:O:41:MET:HE1   | 2:O:119:LEU:HD21 | 1.88                     | 0.56              |
| 2:J:338:ALA:O    | 2:L:153:HIS:ND1  | 2.39                     | 0.56              |
| 3:d:121:TYR:OH   | 3:d:141:LEU:O    | 2.21                     | 0.56              |
| 3:m:183:LYS:NZ   | 3:m:228:ASP:OD2  | 2.39                     | 0.56              |
| 2:Q:153:HIS:ND1  | 2:R:338:ALA:O    | 2.38                     | 0.56              |
| 2:D:33:GLN:NE2   | 2:D:127:ILE:O    | 2.39                     | 0.56              |
| 2:G:236:ARG:NH2  | 2:I:228:ASP:OD2  | 2.39                     | 0.56              |
| 2:I:2:ASP:O      | 2:I:6:SER:OG     | 2.21                     | 0.56              |
| 3:o:216:GLU:N    | 3:o:216:GLU:OE1  | 2.39                     | 0.56              |
| 2:N:141:LEU:O    | 2:N:144:ARG:C    | 2.50                     | 0.55              |
| 3:f:160:LEU:O    | 3:f:283:ARG:NH2  | 2.38                     | 0.55              |
| 3:r:121:TYR:OH   | 3:r:141:LEU:O    | 2.24                     | 0.55              |
| 2:F:103:GLU:OE2  | 2:F:350:ARG:NH2  | 2.39                     | 0.55              |
| 2:K:216:ARG:NH2  | 2:K:374:TYR:O    | 2.38                     | 0.55              |
| 2:A:153:HIS:ND1  | 2:B:338:ALA:O    | 2.39                     | 0.55              |
| 2:O:83:ASN:OD1   | 2:P:122:ILE:HD13 | 2.06                     | 0.55              |
| 3:g:176:GLN:NE2  | 3:g:234:ASN:OD1  | 2.39                     | 0.55              |
| 2:E:334:VAL:O    | 2:E:374:TYR:OH   | 2.16                     | 0.55              |
| 2:E:342:MET:SD   | 2:E:342:MET:N    | 2.79                     | 0.55              |
| 2:O:99:GLU:OE2   | 2:O:384:ARG:NH1  | 2.38                     | 0.55              |
| 3:j:228:ASP:O    | 3:k:294:GLN:NE2  | 2.40                     | 0.55              |
| 3:p:316:SER:OG   | 3:p:317:LEU:N    | 2.40                     | 0.55              |
| 1:2:416:THR:OG1  | 1:2:419:VAL:O    | 2.22                     | 0.55              |
| 3:l:142:MET:HE2  | 3:l:155:LEU:HD23 | 1.88                     | 0.55              |
| 3:l:274:ASP:OD2  | 3:l:276:THR:OG1  | 2.23                     | 0.55              |
| 2:M:338:ALA:O    | 2:O:153:HIS:ND1  | 2.39                     | 0.55              |
| 3:d:216:GLU:OE1  | 3:d:216:GLU:N    | 2.40                     | 0.55              |
| 3:h:142:MET:HE2  | 3:h:155:LEU:HD23 | 1.88                     | 0.55              |
| 2:A:338:ALA:O    | 2:C:153:HIS:ND1  | 2.39                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:141:LEU:O    | 2:J:144:ARG:O    | 2.25                     | 0.55              |
| 2:C:342:MET:SD   | 2:C:342:MET:N    | 2.79                     | 0.55              |
| 2:F:99:GLU:OE2   | 2:F:384:ARG:NH1  | 2.40                     | 0.55              |
| 2:G:112:GLN:OE1  | 2:G:117:ARG:NH2  | 2.40                     | 0.55              |
| 2:L:134:GLU:O    | 2:L:138:ASN:ND2  | 2.40                     | 0.55              |
| 2:P:388:VAL:HA   | 2:P:391:ILE:HD12 | 1.89                     | 0.54              |
| 3:n:274:ASP:OD2  | 3:n:276:THR:OG1  | 2.25                     | 0.54              |
| 2:J:33:GLN:NE2   | 2:J:127:ILE:O    | 2.40                     | 0.54              |
| 2:L:257:ASN:ND2  | 2:L:293:GLN:OE1  | 2.40                     | 0.54              |
| 2:R:260:GLU:OE2  | 2:R:272:THR:OG1  | 2.25                     | 0.54              |
| 3:l:216:GLU:OE1  | 3:l:216:GLU:N    | 2.41                     | 0.54              |
| 3:b:217:GLU:OE2  | 3:b:220:THR:OG1  | 2.17                     | 0.54              |
| 2:A:2:ASP:O      | 2:A:6:SER:OG     | 2.24                     | 0.54              |
| 2:A:260:GLU:OE2  | 2:A:272:THR:OG1  | 2.26                     | 0.54              |
| 2:N:141:LEU:O    | 2:N:144:ARG:O    | 2.25                     | 0.54              |
| 2:D:333:SER:OG   | 2:D:379:GLU:OE2  | 2.23                     | 0.54              |
| 3:f:105:LEU:O    | 3:f:108:THR:OG1  | 2.24                     | 0.54              |
| 3:p:272:THR:HG1  | 3:p:277:THR:HG1  | 1.55                     | 0.54              |
| 3:b:138:ASN:HB2  | 3:b:258:VAL:HG12 | 1.90                     | 0.54              |
| 2:G:375:SER:OG   | 2:K:266:ASN:OD1  | 2.11                     | 0.54              |
| 2:H:33:GLN:NE2   | 2:H:127:ILE:O    | 2.41                     | 0.54              |
| 2:E:153:HIS:ND1  | 2:F:338:ALA:O    | 2.41                     | 0.53              |
| 2:K:156:ASN:O    | 2:K:367:TRP:NE1  | 2.41                     | 0.53              |
| 3:p:216:GLU:N    | 3:p:216:GLU:OE1  | 2.41                     | 0.53              |
| 2:Q:147:ARG:NH1  | 2:Q:332:GLU:OE2  | 2.41                     | 0.53              |
| 3:j:211:ASP:O    | 3:j:214:THR:OG1  | 2.25                     | 0.53              |
| 2:E:230:GLU:OE1  | 2:E:230:GLU:N    | 2.41                     | 0.53              |
| 3:a:294:GLN:NE2  | 3:c:228:ASP:O    | 2.41                     | 0.53              |
| 2:R:225:LEU:HD13 | 2:R:324:LEU:HD12 | 1.88                     | 0.53              |
| 2:B:328:SER:OG   | 2:C:338:ALA:O    | 2.26                     | 0.53              |
| 2:B:342:MET:SD   | 2:B:342:MET:N    | 2.81                     | 0.53              |
| 2:I:33:GLN:NE2   | 2:I:127:ILE:O    | 2.41                     | 0.53              |
| 2:M:23:LEU:HD13  | 2:O:36:GLN:OE1   | 2.08                     | 0.53              |
| 2:M:156:ASN:O    | 2:M:367:TRP:NE1  | 2.41                     | 0.53              |
| 3:m:216:GLU:N    | 3:m:216:GLU:OE1  | 2.42                     | 0.53              |
| 2:E:366:ASN:ND2  | 2:E:369:ASP:OD2  | 2.41                     | 0.53              |
| 3:c:165:CYS:SG   | 3:c:247:ARG:NH1  | 2.82                     | 0.53              |
| 3:j:216:GLU:N    | 3:j:216:GLU:OE1  | 2.41                     | 0.53              |
| 2:A:366:ASN:ND2  | 2:A:369:ASP:OD2  | 2.41                     | 0.53              |
| 2:C:33:GLN:NE2   | 2:C:127:ILE:O    | 2.40                     | 0.53              |
| 1:1:502:ARG:NH1  | 1:3:504:GLU:OE1  | 2.40                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:99:GLU:OE2   | 2:G:384:ARG:NH1  | 2.42                     | 0.53              |
| 2:H:186:SER:OG   | 2:H:326:ILE:O    | 2.27                     | 0.53              |
| 2:M:199:ILE:HD13 | 2:M:296:ARG:CZ   | 2.38                     | 0.53              |
| 2:P:230:GLU:OE2  | 2:Q:231:ARG:NH2  | 2.42                     | 0.53              |
| 3:b:99:LYS:HB3   | 3:f:172:LEU:HD21 | 1.90                     | 0.53              |
| 2:N:255:ARG:NH1  | 3:o:65:THR:O     | 2.41                     | 0.53              |
| 3:a:272:THR:HG1  | 3:a:277:THR:HG1  | 1.54                     | 0.53              |
| 3:b:55:ILE:N     | 3:f:52:ASN:O     | 2.42                     | 0.53              |
| 3:g:117:TYR:HH   | 3:k:175:TYR:HH   | 1.55                     | 0.53              |
| 2:O:230:GLU:O    | 2:O:233:SER:OG   | 2.26                     | 0.52              |
| 3:b:99:LYS:CB    | 3:f:172:LEU:HD21 | 2.39                     | 0.52              |
| 3:j:130:ASP:OD1  | 3:j:132:GLN:NE2  | 2.42                     | 0.52              |
| 3:l:138:ASN:HB2  | 3:l:258:VAL:HG12 | 1.92                     | 0.52              |
| 3:n:75:THR:O     | 3:n:79:SER:OG    | 2.19                     | 0.52              |
| 1:3:360:GLN:NE2  | 1:3:478:ASP:OD1  | 2.42                     | 0.52              |
| 2:G:141:LEU:O    | 2:G:144:ARG:O    | 2.27                     | 0.52              |
| 2:K:153:HIS:ND1  | 2:L:338:ALA:O    | 2.43                     | 0.52              |
| 3:a:216:GLU:N    | 3:a:216:GLU:OE1  | 2.42                     | 0.52              |
| 3:b:268:VAL:O    | 3:c:286:ARG:NH1  | 2.41                     | 0.52              |
| 3:e:228:ASP:O    | 3:f:294:GLN:NE2  | 2.41                     | 0.52              |
| 2:D:388:VAL:HA   | 2:D:391:ILE:HD12 | 1.91                     | 0.52              |
| 2:E:134:GLU:O    | 2:E:138:ASN:ND2  | 2.43                     | 0.52              |
| 2:K:368:THR:O    | 2:K:372:THR:OG1  | 2.21                     | 0.52              |
| 3:f:144:TYR:HD2  | 3:f:152:MET:HE1  | 1.74                     | 0.52              |
| 3:p:301:ASP:CG   | 3:r:231:ASP:OD1  | 2.52                     | 0.52              |
| 2:C:261:VAL:HG13 | 2:C:290:LEU:HD23 | 1.90                     | 0.52              |
| 2:P:99:GLU:OE2   | 2:P:384:ARG:NH1  | 2.42                     | 0.52              |
| 2:R:388:VAL:HA   | 2:R:391:ILE:HD12 | 1.92                     | 0.52              |
| 3:j:121:TYR:OH   | 3:j:141:LEU:O    | 2.24                     | 0.52              |
| 3:n:268:VAL:O    | 3:o:286:ARG:NH1  | 2.43                     | 0.52              |
| 3:a:187:MET:SD   | 3:a:247:ARG:NH2  | 2.83                     | 0.52              |
| 3:h:306:ILE:HG22 | 3:h:310:MET:HE2  | 1.92                     | 0.52              |
| 2:Q:186:SER:OG   | 2:Q:326:ILE:O    | 2.27                     | 0.52              |
| 3:o:160:LEU:HD23 | 3:o:258:VAL:HG23 | 1.92                     | 0.52              |
| 1:3:281:ILE:HG21 | 1:3:385:TYR:OH   | 2.10                     | 0.51              |
| 2:C:93:ASP:OD1   | 2:C:392:ARG:NE   | 2.40                     | 0.51              |
| 2:H:153:HIS:ND1  | 2:I:338:ALA:O    | 2.43                     | 0.51              |
| 2:J:388:VAL:HA   | 2:J:391:ILE:HD12 | 1.92                     | 0.51              |
| 3:e:216:GLU:N    | 3:e:216:GLU:OE1  | 2.42                     | 0.51              |
| 3:i:81:LEU:HD13  | 3:i:307:ILE:HD11 | 1.91                     | 0.51              |
| 2:P:57:ARG:NH1   | 2:P:94:ASN:OD1   | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:33:GLN:NE2   | 2:Q:127:ILE:O    | 2.43                     | 0.51              |
| 3:e:142:MET:HE2  | 3:e:155:LEU:HD23 | 1.92                     | 0.51              |
| 3:n:216:GLU:OE1  | 3:n:216:GLU:N    | 2.43                     | 0.51              |
| 3:q:231:ASP:OD1  | 3:q:231:ASP:N    | 2.43                     | 0.51              |
| 1:1:416:THR:OG1  | 1:1:419:VAL:O    | 2.27                     | 0.51              |
| 1:2:485:THR:HG1  | 1:3:412:SER:HG   | 1.56                     | 0.51              |
| 2:J:230:GLU:OE2  | 2:K:231:ARG:NH2  | 2.44                     | 0.51              |
| 2:M:342:MET:O    | 2:M:346:VAL:HG23 | 2.10                     | 0.51              |
| 3:e:306:ILE:HG22 | 3:e:310:MET:HE2  | 1.93                     | 0.51              |
| 3:r:69:ASN:OD1   | 4:r:401:NAG:N2   | 2.43                     | 0.51              |
| 2:A:231:ARG:NH2  | 2:C:230:GLU:OE2  | 2.44                     | 0.51              |
| 2:B:388:VAL:HA   | 2:B:391:ILE:HD12 | 1.92                     | 0.51              |
| 2:D:163:SER:OG   | 2:D:181:TRP:NE1  | 2.44                     | 0.51              |
| 2:I:230:GLU:N    | 2:I:230:GLU:OE1  | 2.44                     | 0.51              |
| 3:a:266:SER:HB3  | 3:c:268:VAL:HG12 | 1.93                     | 0.51              |
| 3:h:187:MET:SD   | 3:h:247:ARG:NH2  | 2.83                     | 0.51              |
| 2:N:255:ARG:NH2  | 2:O:239:ASN:OD1  | 2.43                     | 0.51              |
| 2:P:338:ALA:O    | 2:R:153:HIS:ND1  | 2.44                     | 0.51              |
| 3:r:216:GLU:N    | 3:r:216:GLU:OE1  | 2.44                     | 0.51              |
| 2:E:342:MET:O    | 2:E:346:VAL:HG23 | 2.10                     | 0.51              |
| 3:j:138:ASN:HB2  | 3:j:258:VAL:HG12 | 1.93                     | 0.51              |
| 2:J:176:LEU:HD12 | 2:J:195:TYR:CZ   | 2.45                     | 0.51              |
| 1:1:490:VAL:O    | 1:3:491:ARG:NE   | 2.40                     | 0.51              |
| 2:F:176:LEU:HD12 | 2:F:195:TYR:CZ   | 2.45                     | 0.51              |
| 2:H:1:MET:HE1    | 2:H:384:ARG:HG3  | 1.93                     | 0.51              |
| 2:N:153:HIS:ND1  | 2:O:338:ALA:O    | 2.42                     | 0.51              |
| 1:3:253:ASP:OD1  | 1:3:253:ASP:N    | 2.44                     | 0.50              |
| 2:D:239:ASN:O    | 2:D:247:TRP:NE1  | 2.44                     | 0.50              |
| 2:G:153:HIS:ND1  | 2:H:338:ALA:O    | 2.44                     | 0.50              |
| 2:J:334:VAL:O    | 2:J:374:TYR:OH   | 2.21                     | 0.50              |
| 2:K:342:MET:O    | 2:K:346:VAL:HG23 | 2.11                     | 0.50              |
| 2:P:366:ASN:ND2  | 2:P:369:ASP:OD2  | 2.44                     | 0.50              |
| 3:g:228:ASP:O    | 3:h:294:GLN:NE2  | 2.43                     | 0.50              |
| 2:L:7:LEU:HD23   | 2:L:37:MET:SD    | 2.50                     | 0.50              |
| 2:R:230:GLU:N    | 2:R:230:GLU:OE1  | 2.45                     | 0.50              |
| 3:r:272:THR:OG1  | 3:r:277:THR:OG1  | 2.28                     | 0.50              |
| 2:G:36:GLN:OE1   | 2:H:23:LEU:HD22  | 2.12                     | 0.50              |
| 2:H:230:GLU:N    | 2:H:230:GLU:OE1  | 2.43                     | 0.50              |
| 2:H:368:THR:O    | 2:H:372:THR:OG1  | 2.17                     | 0.50              |
| 3:i:111:TRP:HZ2  | 3:i:307:ILE:HD13 | 1.76                     | 0.50              |
| 2:I:239:ASN:O    | 2:I:247:TRP:NE1  | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:215:ARG:O    | 2:O:216:ARG:NH1  | 2.43                     | 0.50              |
| 3:b:216:GLU:OE1  | 3:b:216:GLU:N    | 2.44                     | 0.50              |
| 1:1:450:LEU:HD12 | 1:1:451:PRO:HD2  | 1.94                     | 0.50              |
| 2:C:186:SER:OG   | 2:C:326:ILE:O    | 2.28                     | 0.50              |
| 2:Q:1:MET:HE2    | 2:Q:388:VAL:CG1  | 2.41                     | 0.50              |
| 3:q:81:LEU:HD12  | 3:q:137:TYR:O    | 2.11                     | 0.50              |
| 3:q:160:LEU:HD23 | 3:q:258:VAL:HG23 | 1.93                     | 0.50              |
| 2:P:141:LEU:O    | 2:P:144:ARG:O    | 2.29                     | 0.50              |
| 3:b:165:CYS:SG   | 3:b:247:ARG:NH1  | 2.85                     | 0.50              |
| 3:d:176:GLN:NE2  | 3:d:234:ASN:OD1  | 2.44                     | 0.50              |
| 2:E:1:MET:HE2    | 2:E:388:VAL:CG1  | 2.42                     | 0.50              |
| 2:F:2:ASP:O      | 2:F:6:SER:OG     | 2.27                     | 0.50              |
| 3:h:261:ILE:HG21 | 3:h:287:ILE:HD12 | 1.94                     | 0.50              |
| 3:m:138:ASN:HB2  | 3:m:258:VAL:HG12 | 1.94                     | 0.50              |
| 1:3:466:GLY:HA2  | 3:a:210:THR:HG21 | 1.94                     | 0.49              |
| 3:a:268:VAL:O    | 3:b:286:ARG:NH1  | 2.44                     | 0.49              |
| 3:b:111:TRP:HZ2  | 3:b:307:ILE:HD13 | 1.77                     | 0.49              |
| 3:l:172:LEU:HD21 | 3:m:99:LYS:CB    | 2.42                     | 0.49              |
| 1:1:383:GLY:N    | 1:1:454:ASN:O    | 2.44                     | 0.49              |
| 2:A:176:LEU:HD12 | 2:A:195:TYR:CZ   | 2.46                     | 0.49              |
| 2:A:370:LEU:HD23 | 2:A:370:LEU:O    | 2.12                     | 0.49              |
| 2:E:7:LEU:HD23   | 2:E:37:MET:SD    | 2.52                     | 0.49              |
| 2:G:366:ASN:ND2  | 2:G:369:ASP:OD2  | 2.46                     | 0.49              |
| 2:O:230:GLU:OE1  | 2:O:230:GLU:N    | 2.45                     | 0.49              |
| 2:R:33:GLN:NE2   | 2:R:127:ILE:O    | 2.46                     | 0.49              |
| 3:m:81:LEU:HD12  | 3:m:137:TYR:O    | 2.12                     | 0.49              |
| 2:A:33:GLN:NE2   | 2:A:127:ILE:O    | 2.45                     | 0.49              |
| 2:F:333:SER:OG   | 2:F:379:GLU:OE2  | 2.23                     | 0.49              |
| 3:k:228:ASP:O    | 3:l:294:GLN:NE2  | 2.44                     | 0.49              |
| 3:o:123:ASP:OD1  | 3:o:124:ILE:N    | 2.46                     | 0.49              |
| 3:o:144:TYR:HD2  | 3:o:152:MET:HE1  | 1.78                     | 0.49              |
| 2:I:213:GLN:NE2  | 2:I:286:ASP:OD1  | 2.45                     | 0.49              |
| 2:O:163:SER:OG   | 2:O:181:TRP:NE1  | 2.46                     | 0.49              |
| 1:1:253:ASP:OD1  | 1:1:253:ASP:N    | 2.45                     | 0.49              |
| 2:B:180:MET:HE2  | 2:B:232:PHE:CD1  | 2.47                     | 0.49              |
| 2:M:388:VAL:HA   | 2:M:391:ILE:HD12 | 1.93                     | 0.49              |
| 2:G:122:ILE:HD13 | 2:L:83:ASN:OD1   | 2.13                     | 0.49              |
| 3:i:187:MET:SD   | 3:i:247:ARG:NH2  | 2.86                     | 0.49              |
| 3:k:111:TRP:HZ2  | 3:k:307:ILE:HD13 | 1.78                     | 0.49              |
| 3:r:160:LEU:HD23 | 3:r:258:VAL:HG23 | 1.94                     | 0.49              |
| 1:3:418:PHE:O    | 1:3:486:ASN:N    | 2.44                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:93:ASP:OD1   | 2:G:392:ARG:NE   | 2.40                     | 0.49              |
| 2:N:214:LEU:HD11 | 2:N:285:PHE:CE1  | 2.48                     | 0.49              |
| 2:Q:1:MET:HE1    | 2:Q:384:ARG:HG3  | 1.95                     | 0.49              |
| 3:q:100:ASP:OD2  | 3:q:104:GLN:NE2  | 2.44                     | 0.49              |
| 2:A:388:VAL:HA   | 2:A:391:ILE:HD12 | 1.95                     | 0.49              |
| 2:G:176:LEU:HD12 | 2:G:195:TYR:CZ   | 2.48                     | 0.49              |
| 2:P:1:MET:HE1    | 2:P:384:ARG:HG3  | 1.95                     | 0.49              |
| 2:Q:7:LEU:HD23   | 2:Q:37:MET:SD    | 2.52                     | 0.49              |
| 2:Q:93:ASP:OD1   | 2:Q:392:ARG:NE   | 2.46                     | 0.49              |
| 3:f:138:ASN:HB2  | 3:f:258:VAL:HG12 | 1.95                     | 0.49              |
| 2:D:230:GLU:N    | 2:D:230:GLU:OE1  | 2.46                     | 0.49              |
| 3:b:313:ARG:NH2  | 3:b:323:TYR:OH   | 2.46                     | 0.49              |
| 2:C:99:GLU:OE2   | 2:C:384:ARG:NH1  | 2.46                     | 0.48              |
| 2:E:215:ARG:O    | 2:E:216:ARG:NH1  | 2.46                     | 0.48              |
| 2:I:388:VAL:HA   | 2:I:391:ILE:HD12 | 1.95                     | 0.48              |
| 2:L:93:ASP:OD1   | 2:L:392:ARG:NE   | 2.43                     | 0.48              |
| 3:h:231:ASP:OD1  | 3:h:231:ASP:N    | 2.44                     | 0.48              |
| 3:r:231:ASP:OD1  | 3:r:231:ASP:N    | 2.46                     | 0.48              |
| 2:E:186:SER:OG   | 2:E:326:ILE:O    | 2.30                     | 0.48              |
| 2:M:370:LEU:O    | 2:M:370:LEU:HD23 | 2.13                     | 0.48              |
| 2:P:146:GLN:O    | 2:P:148:THR:HG23 | 2.13                     | 0.48              |
| 3:a:69:ASN:OD1   | 4:a:401:NAG:N2   | 2.45                     | 0.48              |
| 3:d:228:ASP:O    | 3:e:294:GLN:NE2  | 2.44                     | 0.48              |
| 2:I:216:ARG:NH2  | 2:I:374:TYR:O    | 2.46                     | 0.48              |
| 2:J:351:GLN:OE1  | 2:L:271:ASN:ND2  | 2.46                     | 0.48              |
| 1:2:329:ASN:HA   | 1:2:338:VAL:HG23 | 1.95                     | 0.48              |
| 1:3:270:ASP:OD1  | 1:3:270:ASP:N    | 2.45                     | 0.48              |
| 2:J:231:ARG:NH2  | 2:L:230:GLU:OE2  | 2.45                     | 0.48              |
| 2:Q:366:ASN:ND2  | 2:Q:369:ASP:OD2  | 2.45                     | 0.48              |
| 3:h:261:ILE:CG2  | 3:h:287:ILE:HD12 | 2.43                     | 0.48              |
| 3:h:274:ASP:OD2  | 3:h:276:THR:OG1  | 2.31                     | 0.48              |
| 1:1:289:TYR:OH   | 1:1:391:VAL:O    | 2.24                     | 0.48              |
| 2:J:153:HIS:N    | 2:J:337:ASP:OD1  | 2.46                     | 0.48              |
| 2:N:1:MET:HE2    | 2:N:388:VAL:CG1  | 2.44                     | 0.48              |
| 2:R:1:MET:HE2    | 2:R:388:VAL:CG1  | 2.43                     | 0.48              |
| 3:c:180:GLU:OE1  | 3:c:180:GLU:N    | 2.46                     | 0.48              |
| 3:d:142:MET:HE2  | 3:d:155:LEU:HD23 | 1.94                     | 0.48              |
| 3:j:183:LYS:NZ   | 3:j:228:ASP:OD2  | 2.47                     | 0.48              |
| 3:q:216:GLU:N    | 3:q:216:GLU:OE1  | 2.46                     | 0.48              |
| 2:D:153:HIS:ND1  | 2:E:338:ALA:O    | 2.47                     | 0.48              |
| 2:G:230:GLU:O    | 2:G:233:SER:OG   | 2.31                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:1:MET:HE2    | 2:P:388:VAL:CG1  | 2.44                     | 0.48              |
| 3:g:183:LYS:NZ   | 3:g:228:ASP:OD2  | 2.47                     | 0.48              |
| 3:h:69:ASN:OD1   | 4:h:401:NAG:N2   | 2.46                     | 0.48              |
| 2:C:141:LEU:O    | 2:C:144:ARG:C    | 2.57                     | 0.48              |
| 3:e:81:LEU:HD13  | 3:e:307:ILE:HD11 | 1.96                     | 0.48              |
| 1:1:345:ILE:HD12 | 1:1:450:LEU:HD23 | 1.94                     | 0.48              |
| 2:B:230:GLU:OE1  | 2:B:230:GLU:N    | 2.47                     | 0.48              |
| 2:P:141:LEU:HB3  | 2:P:148:THR:HG22 | 1.96                     | 0.48              |
| 3:e:138:ASN:HB2  | 3:e:258:VAL:HG12 | 1.94                     | 0.48              |
| 3:p:183:LYS:NZ   | 3:p:228:ASP:OD2  | 2.47                     | 0.48              |
| 3:r:111:TRP:HZ2  | 3:r:307:ILE:HD13 | 1.79                     | 0.48              |
| 2:A:141:LEU:O    | 2:A:144:ARG:O    | 2.32                     | 0.48              |
| 2:E:253:ILE:HD13 | 2:E:319:THR:OG1  | 2.14                     | 0.48              |
| 3:c:216:GLU:N    | 3:c:216:GLU:OE1  | 2.47                     | 0.48              |
| 1:2:331:GLY:N    | 1:2:336:ASP:OD2  | 2.47                     | 0.47              |
| 1:3:329:ASN:HA   | 1:3:338:VAL:HG23 | 1.96                     | 0.47              |
| 2:C:334:VAL:O    | 2:C:374:TYR:OH   | 2.22                     | 0.47              |
| 2:E:93:ASP:OD1   | 2:E:392:ARG:NE   | 2.45                     | 0.47              |
| 2:G:207:GLN:OE1  | 2:G:293:GLN:NE2  | 2.47                     | 0.47              |
| 2:J:1:MET:HE2    | 2:J:388:VAL:CG1  | 2.44                     | 0.47              |
| 2:K:228:ASP:OD2  | 2:L:236:ARG:NH2  | 2.47                     | 0.47              |
| 2:Q:388:VAL:HA   | 2:Q:391:ILE:HD12 | 1.96                     | 0.47              |
| 3:k:183:LYS:NZ   | 3:k:228:ASP:OD2  | 2.47                     | 0.47              |
| 2:A:36:GLN:OE1   | 2:B:23:LEU:HD13  | 2.14                     | 0.47              |
| 2:D:1:MET:HE2    | 2:D:388:VAL:CG1  | 2.44                     | 0.47              |
| 2:E:388:VAL:HA   | 2:E:391:ILE:HD12 | 1.94                     | 0.47              |
| 2:K:186:SER:OG   | 2:K:326:ILE:O    | 2.29                     | 0.47              |
| 2:M:113:SER:OG   | 2:M:113:SER:O    | 2.31                     | 0.47              |
| 3:b:228:ASP:O    | 3:c:294:GLN:NE2  | 2.47                     | 0.47              |
| 3:f:216:GLU:N    | 3:f:216:GLU:OE1  | 2.47                     | 0.47              |
| 3:l:160:LEU:HD21 | 3:l:260:VAL:HG23 | 1.96                     | 0.47              |
| 2:F:131:ASN:OD1  | 2:F:131:ASN:N    | 2.47                     | 0.47              |
| 3:f:199:ASN:ND2  | 3:f:201:GLN:OE1  | 2.46                     | 0.47              |
| 1:1:438:SER:OG   | 1:1:444:VAL:O    | 2.32                     | 0.47              |
| 2:A:1:MET:HE1    | 2:A:384:ARG:HG3  | 1.97                     | 0.47              |
| 2:C:1:MET:HE2    | 2:C:388:VAL:HG13 | 1.96                     | 0.47              |
| 2:E:1:MET:HE1    | 2:E:384:ARG:HG3  | 1.97                     | 0.47              |
| 2:G:375:SER:HG   | 2:K:266:ASN:CG   | 2.15                     | 0.47              |
| 3:i:69:ASN:OD1   | 4:i:401:NAG:N2   | 2.47                     | 0.47              |
| 3:k:216:GLU:N    | 3:k:216:GLU:OE1  | 2.46                     | 0.47              |
| 2:A:163:SER:OG   | 2:A:181:TRP:NE1  | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:216:ARG:NH2  | 2:J:374:TYR:O    | 2.48                     | 0.47              |
| 2:M:228:ASP:OD2  | 2:N:236:ARG:NH2  | 2.47                     | 0.47              |
| 3:n:267:ASP:OD2  | 3:n:280:GLN:NE2  | 2.48                     | 0.47              |
| 2:N:199:ILE:HD13 | 2:N:296:ARG:CZ   | 2.45                     | 0.47              |
| 1:2:270:ASP:OD1  | 1:2:467:ARG:NH1  | 2.47                     | 0.47              |
| 2:A:186:SER:OG   | 2:A:186:SER:O    | 2.31                     | 0.47              |
| 2:F:1:MET:HE2    | 2:F:388:VAL:CG1  | 2.45                     | 0.47              |
| 2:H:1:MET:HE2    | 2:H:388:VAL:CG1  | 2.44                     | 0.47              |
| 3:e:144:TYR:CD2  | 3:e:152:MET:HE1  | 2.49                     | 0.47              |
| 3:g:216:GLU:OE1  | 3:g:216:GLU:N    | 2.47                     | 0.47              |
| 3:h:259:ALA:HB1  | 3:h:285:MET:HE3  | 1.97                     | 0.47              |
| 3:m:170:ILE:HD11 | 3:m:246:ILE:HG21 | 1.96                     | 0.47              |
| 3:r:95:ASP:OD1   | 3:r:96:ASN:N     | 2.48                     | 0.47              |
| 2:N:33:GLN:NE2   | 2:N:127:ILE:O    | 2.47                     | 0.47              |
| 2:Q:215:ARG:O    | 2:Q:216:ARG:NH1  | 2.48                     | 0.47              |
| 2:G:259:VAL:HG11 | 2:G:277:PHE:CZ   | 2.49                     | 0.47              |
| 2:G:388:VAL:HA   | 2:G:391:ILE:HD12 | 1.96                     | 0.47              |
| 2:J:370:LEU:O    | 2:J:370:LEU:HD23 | 2.15                     | 0.47              |
| 3:n:180:GLU:OE1  | 3:n:180:GLU:N    | 2.48                     | 0.47              |
| 2:K:199:ILE:HD13 | 2:K:296:ARG:CZ   | 2.45                     | 0.47              |
| 2:D:367:TRP:O    | 2:D:371:ILE:HG22 | 2.15                     | 0.46              |
| 2:F:90:ASP:O     | 2:F:94:ASN:ND2   | 2.48                     | 0.46              |
| 2:F:260:GLU:OE2  | 2:F:272:THR:OG1  | 2.33                     | 0.46              |
| 2:G:225:LEU:HD13 | 2:G:324:LEU:HD12 | 1.98                     | 0.46              |
| 3:c:69:ASN:OD1   | 4:c:401:NAG:N2   | 2.49                     | 0.46              |
| 3:j:286:ARG:NH1  | 3:l:268:VAL:O    | 2.47                     | 0.46              |
| 2:A:216:ARG:NH2  | 2:A:374:TYR:O    | 2.49                     | 0.46              |
| 3:m:313:ARG:NH2  | 3:m:316:SER:O    | 2.47                     | 0.46              |
| 3:o:183:LYS:NZ   | 3:o:228:ASP:OD2  | 2.48                     | 0.46              |
| 2:C:230:GLU:N    | 2:C:230:GLU:OE1  | 2.49                     | 0.46              |
| 2:D:23:LEU:HD13  | 2:F:36:GLN:OE1   | 2.15                     | 0.46              |
| 2:P:7:LEU:HD12   | 2:P:127:ILE:HG21 | 1.97                     | 0.46              |
| 3:g:301:ASP:CG   | 3:i:231:ASP:OD1  | 2.39                     | 0.46              |
| 3:h:95:ASP:OD1   | 3:h:96:ASN:N     | 2.45                     | 0.46              |
| 1:1:329:ASN:HA   | 1:1:338:VAL:HG23 | 1.98                     | 0.46              |
| 3:b:55:ILE:O     | 3:f:52:ASN:N     | 2.49                     | 0.46              |
| 3:k:69:ASN:OD1   | 4:k:401:NAG:N2   | 2.49                     | 0.46              |
| 3:q:231:ASP:OD1  | 3:r:301:ASP:CG   | 2.58                     | 0.46              |
| 2:P:253:ILE:C    | 2:P:254:LEU:HD12 | 2.40                     | 0.46              |
| 3:n:267:ASP:OD1  | 3:n:286:ARG:NE   | 2.49                     | 0.46              |
| 2:H:388:VAL:HA   | 2:H:391:ILE:HD12 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:1:MET:HE2    | 2:L:388:VAL:CG1  | 2.45                     | 0.46              |
| 2:L:239:ASN:ND2  | 2:L:240:SER:O    | 2.48                     | 0.46              |
| 2:M:333:SER:OG   | 2:M:379:GLU:OE2  | 2.30                     | 0.46              |
| 2:Q:141:LEU:O    | 2:Q:144:ARG:C    | 2.59                     | 0.46              |
| 2:A:230:GLU:N    | 2:A:230:GLU:OE1  | 2.49                     | 0.46              |
| 2:J:23:LEU:HD13  | 2:L:36:GLN:OE1   | 2.15                     | 0.46              |
| 2:K:33:GLN:NE2   | 2:K:127:ILE:O    | 2.48                     | 0.46              |
| 3:q:150:LEU:HD13 | 3:r:288:ASN:O    | 2.15                     | 0.46              |
| 2:E:14:ALA:HB1   | 2:E:85:ILE:HD11  | 1.98                     | 0.46              |
| 3:f:304:ASN:OD1  | 3:f:305:GLN:N    | 2.49                     | 0.46              |
| 3:i:316:SER:OG   | 3:i:317:LEU:N    | 2.49                     | 0.46              |
| 2:F:33:GLN:NE2   | 2:F:127:ILE:O    | 2.49                     | 0.46              |
| 3:g:165:CYS:SG   | 3:g:247:ARG:NH1  | 2.88                     | 0.46              |
| 2:L:180:MET:HE2  | 2:L:232:PHE:CD1  | 2.50                     | 0.45              |
| 3:m:304:ASN:OD1  | 3:m:305:GLN:N    | 2.49                     | 0.45              |
| 2:G:338:ALA:O    | 2:I:153:HIS:ND1  | 2.49                     | 0.45              |
| 3:e:183:LYS:NZ   | 3:e:228:ASP:OD2  | 2.49                     | 0.45              |
| 3:i:121:TYR:OH   | 3:i:141:LEU:O    | 2.28                     | 0.45              |
| 1:2:386:SER:HA   | 1:2:396:VAL:HG12 | 1.99                     | 0.45              |
| 2:G:1:MET:HE2    | 2:G:388:VAL:HG13 | 1.99                     | 0.45              |
| 2:D:156:ASN:O    | 2:D:367:TRP:NE1  | 2.46                     | 0.45              |
| 2:F:112:GLN:OE1  | 2:F:117:ARG:NH2  | 2.49                     | 0.45              |
| 2:R:1:MET:HE1    | 2:R:384:ARG:HG3  | 1.98                     | 0.45              |
| 3:e:271:ILE:HD11 | 3:e:284:MET:SD   | 2.56                     | 0.45              |
| 3:j:160:LEU:HD21 | 3:j:260:VAL:HG23 | 1.99                     | 0.45              |
| 3:g:160:LEU:O    | 3:g:283:ARG:NH2  | 2.49                     | 0.45              |
| 3:k:142:MET:HE2  | 3:k:155:LEU:HD23 | 1.97                     | 0.45              |
| 2:I:1:MET:HE2    | 2:I:388:VAL:CG1  | 2.47                     | 0.45              |
| 3:h:160:LEU:HD23 | 3:h:258:VAL:HG23 | 1.99                     | 0.45              |
| 2:D:113:SER:O    | 2:D:113:SER:OG   | 2.34                     | 0.45              |
| 2:J:255:ARG:NH2  | 2:K:239:ASN:OD1  | 2.47                     | 0.45              |
| 2:M:230:GLU:N    | 2:M:230:GLU:OE1  | 2.49                     | 0.45              |
| 2:P:239:ASN:ND2  | 2:P:240:SER:O    | 2.48                     | 0.45              |
| 3:b:183:LYS:NZ   | 3:b:228:ASP:OD2  | 2.49                     | 0.45              |
| 3:i:274:ASP:OD2  | 3:i:276:THR:OG1  | 2.35                     | 0.45              |
| 2:J:48:THR:HG21  | 2:J:94:ASN:HB3   | 1.98                     | 0.45              |
| 2:J:154:LYS:N    | 2:J:327:GLU:O    | 2.48                     | 0.45              |
| 3:a:255:ARG:O    | 3:a:283:ARG:NH2  | 2.49                     | 0.45              |
| 3:l:172:LEU:HD21 | 3:m:99:LYS:HB3   | 1.98                     | 0.45              |
| 2:G:300:MET:HB3  | 2:G:304:VAL:HG13 | 1.99                     | 0.44              |
| 2:O:7:LEU:HD23   | 2:O:37:MET:SD    | 2.57                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:113:SER:OG   | 2:Q:113:SER:O    | 2.34                     | 0.44              |
| 2:R:186:SER:OG   | 2:R:326:ILE:O    | 2.35                     | 0.44              |
| 3:r:123:ASP:OD1  | 3:r:124:ILE:N    | 2.50                     | 0.44              |
| 2:K:134:GLU:O    | 2:K:138:ASN:ND2  | 2.46                     | 0.44              |
| 2:M:99:GLU:OE2   | 2:M:384:ARG:NH1  | 2.50                     | 0.44              |
| 2:M:260:GLU:OE2  | 2:M:272:THR:OG1  | 2.35                     | 0.44              |
| 2:R:134:GLU:O    | 2:R:138:ASN:ND2  | 2.50                     | 0.44              |
| 3:f:187:MET:SD   | 3:f:247:ARG:NH2  | 2.90                     | 0.44              |
| 1:1:339:ILE:HD12 | 1:1:342:TYR:CD2  | 2.52                     | 0.44              |
| 1:3:416:THR:OG1  | 1:3:419:VAL:O    | 2.34                     | 0.44              |
| 2:N:134:GLU:O    | 2:N:138:ASN:ND2  | 2.49                     | 0.44              |
| 2:Q:141:LEU:O    | 2:Q:144:ARG:O    | 2.35                     | 0.44              |
| 3:b:180:GLU:OE1  | 3:b:180:GLU:N    | 2.49                     | 0.44              |
| 3:c:217:GLU:OE2  | 3:c:220:THR:OG1  | 2.31                     | 0.44              |
| 2:B:186:SER:OG   | 2:B:326:ILE:O    | 2.35                     | 0.44              |
| 2:G:41:MET:HE1   | 2:G:119:LEU:HD21 | 1.99                     | 0.44              |
| 3:a:123:ASP:OD1  | 3:a:124:ILE:N    | 2.49                     | 0.44              |
| 3:c:267:ASP:OD2  | 3:c:280:GLN:NE2  | 2.51                     | 0.44              |
| 3:g:303:VAL:HA   | 3:g:306:ILE:HD12 | 1.99                     | 0.44              |
| 3:n:272:THR:OG1  | 3:n:277:THR:OG1  | 2.34                     | 0.44              |
| 3:r:75:THR:O     | 3:r:79:SER:OG    | 2.22                     | 0.44              |
| 2:A:141:LEU:HB3  | 2:A:148:THR:HG22 | 1.98                     | 0.44              |
| 2:B:169:SER:O    | 3:c:55:ILE:N     | 2.51                     | 0.44              |
| 3:a:144:TYR:CD2  | 3:a:152:MET:HE1  | 2.52                     | 0.44              |
| 3:a:183:LYS:NZ   | 3:a:228:ASP:OD2  | 2.50                     | 0.44              |
| 3:b:160:LEU:HD21 | 3:b:260:VAL:HG23 | 1.99                     | 0.44              |
| 3:c:160:LEU:HD23 | 3:c:258:VAL:HG23 | 2.00                     | 0.44              |
| 3:c:266:SER:O    | 3:c:268:VAL:HG13 | 2.18                     | 0.44              |
| 3:g:138:ASN:HB2  | 3:g:258:VAL:HG12 | 2.00                     | 0.44              |
| 3:l:169:ASP:OD2  | 3:l:172:LEU:HD22 | 2.17                     | 0.44              |
| 3:m:142:MET:HE2  | 3:m:155:LEU:HD23 | 1.98                     | 0.44              |
| 2:C:380:ASP:OD1  | 2:Q:106:ARG:NH1  | 2.50                     | 0.44              |
| 3:p:69:ASN:OD1   | 4:p:401:NAG:N2   | 2.51                     | 0.44              |
| 3:p:272:THR:OG1  | 3:p:277:THR:OG1  | 2.31                     | 0.44              |
| 2:D:154:LYS:N    | 2:D:327:GLU:O    | 2.47                     | 0.44              |
| 2:D:228:ASP:OD2  | 2:E:236:ARG:NH2  | 2.49                     | 0.44              |
| 2:F:225:LEU:HD13 | 2:F:324:LEU:HD12 | 2.00                     | 0.44              |
| 2:L:156:ASN:O    | 2:L:367:TRP:NE1  | 2.49                     | 0.44              |
| 2:M:153:HIS:ND1  | 2:N:338:ALA:O    | 2.51                     | 0.44              |
| 2:M:176:LEU:HD12 | 2:M:195:TYR:CZ   | 2.52                     | 0.44              |
| 2:R:199:ILE:HD13 | 2:R:296:ARG:CZ   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:i:123:ASP:OD1  | 3:i:124:ILE:N    | 2.49                     | 0.44              |
| 3:i:183:LYS:NZ   | 3:i:228:ASP:OD2  | 2.50                     | 0.44              |
| 3:n:227:THR:HG23 | 3:o:294:GLN:OE1  | 2.18                     | 0.44              |
| 2:D:338:ALA:O    | 2:F:153:HIS:ND1  | 2.51                     | 0.44              |
| 2:L:214:LEU:HD11 | 2:L:285:PHE:CE1  | 2.53                     | 0.44              |
| 3:b:304:ASN:OD1  | 3:b:305:GLN:N    | 2.50                     | 0.44              |
| 3:d:187:MET:SD   | 3:d:247:ARG:NH2  | 2.91                     | 0.44              |
| 3:n:160:LEU:HD23 | 3:n:258:VAL:HG23 | 1.99                     | 0.44              |
| 2:A:1:MET:HE2    | 2:A:388:VAL:CG1  | 2.48                     | 0.44              |
| 2:F:1:MET:HE1    | 2:F:384:ARG:HG3  | 2.00                     | 0.44              |
| 2:H:113:SER:OG   | 2:H:113:SER:O    | 2.36                     | 0.44              |
| 2:H:134:GLU:O    | 2:H:138:ASN:ND2  | 2.48                     | 0.44              |
| 2:O:1:MET:HE2    | 2:O:388:VAL:HG13 | 2.00                     | 0.44              |
| 2:C:299:ASN:ND2  | 3:b:69:ASN:O     | 2.50                     | 0.43              |
| 3:c:211:ASP:O    | 3:c:214:THR:OG1  | 2.34                     | 0.43              |
| 3:p:95:ASP:OD1   | 3:p:96:ASN:N     | 2.51                     | 0.43              |
| 1:3:488:VAL:HG12 | 1:3:490:VAL:H    | 1.82                     | 0.43              |
| 2:N:230:GLU:N    | 2:N:230:GLU:OE1  | 2.51                     | 0.43              |
| 3:b:285:MET:HE1  | 3:b:306:ILE:HG23 | 1.98                     | 0.43              |
| 3:e:111:TRP:HZ2  | 3:e:307:ILE:HD13 | 1.84                     | 0.43              |
| 2:D:22:THR:CG2   | 2:D:73:LEU:HD22  | 2.48                     | 0.43              |
| 2:J:1:MET:HE1    | 2:J:384:ARG:HG3  | 2.00                     | 0.43              |
| 2:J:299:ASN:ND2  | 3:k:69:ASN:O     | 2.51                     | 0.43              |
| 2:L:1:MET:HE1    | 2:L:384:ARG:HG3  | 2.01                     | 0.43              |
| 3:j:74:GLU:O     | 3:j:78:THR:HG22  | 2.18                     | 0.43              |
| 2:A:154:LYS:N    | 2:A:327:GLU:O    | 2.48                     | 0.43              |
| 2:D:231:ARG:NH2  | 2:F:230:GLU:OE2  | 2.50                     | 0.43              |
| 2:D:342:MET:O    | 2:D:346:VAL:HG23 | 2.17                     | 0.43              |
| 2:E:36:GLN:OE1   | 2:F:23:LEU:HD13  | 2.19                     | 0.43              |
| 2:E:257:ASN:ND2  | 2:E:293:GLN:OE1  | 2.52                     | 0.43              |
| 2:M:366:ASN:ND2  | 2:M:369:ASP:OD2  | 2.51                     | 0.43              |
| 2:N:156:ASN:O    | 2:N:367:TRP:NE1  | 2.49                     | 0.43              |
| 3:m:69:ASN:OD1   | 4:m:401:NAG:N2   | 2.50                     | 0.43              |
| 2:P:100:MET:SD   | 2:P:346:VAL:HG22 | 2.58                     | 0.43              |
| 3:a:304:ASN:OD1  | 3:a:305:GLN:N    | 2.51                     | 0.43              |
| 3:h:144:TYR:CD2  | 3:h:152:MET:HE1  | 2.53                     | 0.43              |
| 3:m:286:ARG:NH1  | 3:o:268:VAL:O    | 2.50                     | 0.43              |
| 3:o:138:ASN:HB2  | 3:o:258:VAL:HG12 | 1.99                     | 0.43              |
| 2:A:239:ASN:O    | 2:A:247:TRP:NE1  | 2.48                     | 0.43              |
| 2:B:156:ASN:O    | 2:B:367:TRP:NE1  | 2.50                     | 0.43              |
| 2:R:216:ARG:NH2  | 2:R:374:TYR:O    | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:d:182:ASN:OD1  | 3:d:248:ASN:ND2  | 2.50                     | 0.43              |
| 3:q:123:ASP:OD1  | 3:q:124:ILE:N    | 2.51                     | 0.43              |
| 2:G:368:THR:O    | 2:G:372:THR:OG1  | 2.27                     | 0.43              |
| 2:J:186:SER:OG   | 2:J:326:ILE:O    | 2.36                     | 0.43              |
| 2:M:141:LEU:O    | 2:M:144:ARG:O    | 2.36                     | 0.43              |
| 3:b:303:VAL:HG22 | 3:b:307:ILE:HD12 | 1.99                     | 0.43              |
| 3:c:123:ASP:OD1  | 3:c:124:ILE:N    | 2.50                     | 0.43              |
| 3:n:123:ASP:OD1  | 3:n:124:ILE:N    | 2.50                     | 0.43              |
| 2:Q:228:ASP:OD2  | 2:R:236:ARG:NH2  | 2.49                     | 0.43              |
| 3:j:219:ALA:HB2  | 3:j:225:VAL:HG11 | 2.00                     | 0.43              |
| 3:o:75:THR:HA    | 3:o:78:THR:HG22  | 2.01                     | 0.43              |
| 3:p:180:GLU:OE1  | 3:p:180:GLU:N    | 2.49                     | 0.43              |
| 2:J:153:HIS:ND1  | 2:K:338:ALA:O    | 2.51                     | 0.43              |
| 3:b:123:ASP:OD1  | 3:b:124:ILE:N    | 2.51                     | 0.43              |
| 3:d:306:ILE:HG22 | 3:d:310:MET:HE2  | 2.00                     | 0.43              |
| 3:g:304:ASN:OD1  | 3:g:305:GLN:N    | 2.52                     | 0.43              |
| 1:2:418:PHE:O    | 1:2:486:ASN:N    | 2.50                     | 0.43              |
| 2:E:228:ASP:OD2  | 2:F:236:ARG:NH2  | 2.52                     | 0.43              |
| 1:2:488:VAL:HG13 | 1:2:490:VAL:HG23 | 2.01                     | 0.42              |
| 2:B:230:GLU:O    | 2:B:233:SER:OG   | 2.34                     | 0.42              |
| 2:K:18:ILE:HG23  | 2:K:73:LEU:HD23  | 2.01                     | 0.42              |
| 2:N:1:MET:HE1    | 2:N:384:ARG:HG3  | 2.01                     | 0.42              |
| 3:e:303:VAL:HG22 | 3:e:307:ILE:HD12 | 2.00                     | 0.42              |
| 1:2:375:LEU:HD11 | 1:2:426:PHE:CD1  | 2.54                     | 0.42              |
| 2:A:23:LEU:HD13  | 2:C:36:GLN:NE2   | 2.35                     | 0.42              |
| 2:D:260:GLU:OE2  | 2:D:272:THR:OG1  | 2.33                     | 0.42              |
| 2:N:225:LEU:HD13 | 2:N:324:LEU:HD12 | 2.01                     | 0.42              |
| 2:Q:333:SER:OG   | 2:Q:379:GLU:OE2  | 2.23                     | 0.42              |
| 3:j:285:MET:HE1  | 3:j:306:ILE:HG23 | 2.00                     | 0.42              |
| 2:D:230:GLU:OE2  | 2:E:231:ARG:NH2  | 2.52                     | 0.42              |
| 2:H:269:ILE:HD11 | 2:H:272:THR:HB   | 1.99                     | 0.42              |
| 2:R:29:ASP:OD1   | 2:R:30:LEU:N     | 2.52                     | 0.42              |
| 3:o:160:LEU:HD21 | 3:o:260:VAL:HG23 | 2.01                     | 0.42              |
| 2:N:228:ASP:OD2  | 2:O:236:ARG:NH2  | 2.51                     | 0.42              |
| 2:Q:99:GLU:OE2   | 2:Q:384:ARG:NH1  | 2.52                     | 0.42              |
| 3:h:304:ASN:OD1  | 3:h:305:GLN:N    | 2.51                     | 0.42              |
| 2:F:158:PHE:CZ   | 2:F:188:ILE:HD11 | 2.53                     | 0.42              |
| 3:b:169:ASP:OD2  | 3:b:172:LEU:HD13 | 2.19                     | 0.42              |
| 2:I:224:THR:OG1  | 2:I:327:GLU:OE2  | 2.36                     | 0.42              |
| 3:l:158:LEU:HD21 | 3:l:187:MET:CE   | 2.50                     | 0.42              |
| 2:H:367:TRP:CZ3  | 2:H:370:LEU:HD22 | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:156:ASN:O    | 2:G:367:TRP:NE1  | 2.49                     | 0.42              |
| 2:N:388:VAL:HA   | 2:N:391:ILE:HD12 | 2.01                     | 0.42              |
| 3:d:54:GLY:C     | 3:d:55:ILE:HD13  | 2.45                     | 0.42              |
| 3:e:255:ARG:O    | 3:e:283:ARG:NH2  | 2.51                     | 0.42              |
| 3:l:172:LEU:HD21 | 3:m:99:LYS:HB2   | 2.02                     | 0.42              |
| 2:E:156:ASN:O    | 2:E:367:TRP:NE1  | 2.49                     | 0.42              |
| 2:L:230:GLU:OE1  | 2:L:230:GLU:N    | 2.52                     | 0.42              |
| 3:d:304:ASN:OD1  | 3:d:305:GLN:N    | 2.51                     | 0.42              |
| 3:g:160:LEU:HD21 | 3:g:260:VAL:HG23 | 2.02                     | 0.42              |
| 3:n:144:TYR:CD2  | 3:n:152:MET:HE1  | 2.55                     | 0.42              |
| 3:n:144:TYR:HD2  | 3:n:152:MET:HE1  | 1.84                     | 0.42              |
| 2:A:146:GLN:O    | 2:A:148:THR:HG23 | 2.20                     | 0.42              |
| 2:L:233:SER:O    | 2:L:233:SER:OG   | 2.34                     | 0.42              |
| 2:P:176:LEU:HD12 | 2:P:195:TYR:CZ   | 2.55                     | 0.42              |
| 3:l:144:TYR:HD2  | 3:l:152:MET:HE1  | 1.85                     | 0.42              |
| 3:l:158:LEU:HD21 | 3:l:187:MET:HE2  | 2.01                     | 0.42              |
| 1:l:375:LEU:HD11 | 1:l:426:PHE:CD1  | 2.55                     | 0.41              |
| 3:e:180:GLU:OE1  | 3:e:180:GLU:N    | 2.50                     | 0.41              |
| 3:f:266:SER:O    | 3:f:268:VAL:HG13 | 2.20                     | 0.41              |
| 3:j:125:ALA:HB1  | 3:j:223:LYS:HD2  | 2.02                     | 0.41              |
| 3:k:261:ILE:CG2  | 3:k:287:ILE:HD12 | 2.50                     | 0.41              |
| 3:l:123:ASP:OD1  | 3:l:124:ILE:N    | 2.50                     | 0.41              |
| 2:H:29:ASP:OD1   | 2:H:30:LEU:N     | 2.52                     | 0.41              |
| 2:J:199:ILE:HD13 | 2:J:296:ARG:CZ   | 2.49                     | 0.41              |
| 2:L:186:SER:OG   | 2:L:326:ILE:O    | 2.36                     | 0.41              |
| 2:P:7:LEU:HD21   | 2:P:41:MET:HE3   | 2.02                     | 0.41              |
| 3:f:179:ASP:OD1  | 3:f:179:ASP:N    | 2.53                     | 0.41              |
| 3:h:183:LYS:NZ   | 3:h:228:ASP:OD2  | 2.54                     | 0.41              |
| 3:k:268:VAL:O    | 3:l:286:ARG:NH1  | 2.52                     | 0.41              |
| 3:m:316:SER:OG   | 3:m:317:LEU:N    | 2.53                     | 0.41              |
| 2:F:188:ILE:HD12 | 2:F:324:LEU:HD22 | 2.02                     | 0.41              |
| 2:F:388:VAL:HA   | 2:F:391:ILE:HD12 | 2.03                     | 0.41              |
| 2:G:186:SER:OG   | 2:G:326:ILE:O    | 2.38                     | 0.41              |
| 2:K:183:ASN:OD1  | 2:K:188:ILE:HG23 | 2.20                     | 0.41              |
| 2:N:93:ASP:OD1   | 2:N:392:ARG:NE   | 2.48                     | 0.41              |
| 3:e:266:SER:O    | 3:e:268:VAL:HG13 | 2.20                     | 0.41              |
| 3:f:123:ASP:OD1  | 3:f:124:ILE:N    | 2.51                     | 0.41              |
| 2:A:215:ARG:O    | 2:A:216:ARG:NH1  | 2.51                     | 0.41              |
| 2:B:225:LEU:HD22 | 2:B:261:VAL:HG21 | 2.02                     | 0.41              |
| 2:G:113:SER:OG   | 2:G:113:SER:O    | 2.37                     | 0.41              |
| 2:I:186:SER:OG   | 2:I:326:ILE:O    | 2.38                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:134:GLU:O    | 2:Q:138:ASN:ND2  | 2.51                     | 0.41              |
| 2:E:189:GLN:HG2  | 2:E:323:THR:HG23 | 2.01                     | 0.41              |
| 2:K:100:MET:HG3  | 2:K:388:VAL:HG23 | 2.03                     | 0.41              |
| 3:l:170:ILE:HD11 | 3:l:246:ILE:HG21 | 2.02                     | 0.41              |
| 1:1:270:ASP:OD1  | 1:1:270:ASP:N    | 2.54                     | 0.41              |
| 2:B:33:GLN:NE2   | 2:B:127:ILE:O    | 2.53                     | 0.41              |
| 2:B:158:PHE:CZ   | 2:B:188:ILE:HD11 | 2.56                     | 0.41              |
| 2:I:1:MET:HE1    | 2:I:384:ARG:HG3  | 2.02                     | 0.41              |
| 2:L:366:ASN:ND2  | 2:L:369:ASP:OD2  | 2.53                     | 0.41              |
| 2:O:103:GLU:OE2  | 2:O:350:ARG:NH2  | 2.54                     | 0.41              |
| 2:O:186:SER:O    | 2:O:186:SER:OG   | 2.38                     | 0.41              |
| 3:a:133:LEU:HD13 | 3:a:258:VAL:HG11 | 2.02                     | 0.41              |
| 3:i:216:GLU:OE1  | 3:i:216:GLU:N    | 2.53                     | 0.41              |
| 3:i:272:THR:OG1  | 3:i:277:THR:OG1  | 2.34                     | 0.41              |
| 3:l:285:MET:HE1  | 3:l:306:ILE:HG23 | 2.02                     | 0.41              |
| 2:C:225:LEU:HD13 | 2:C:324:LEU:HD12 | 2.03                     | 0.41              |
| 2:H:22:THR:CG2   | 2:H:73:LEU:HD22  | 2.51                     | 0.41              |
| 2:P:85:ILE:O     | 2:P:89:VAL:HG23  | 2.21                     | 0.41              |
| 2:P:230:GLU:N    | 2:P:230:GLU:OE1  | 2.53                     | 0.41              |
| 3:e:176:GLN:NE2  | 3:e:234:ASN:OD1  | 2.52                     | 0.41              |
| 3:g:123:ASP:OD1  | 3:g:124:ILE:N    | 2.53                     | 0.41              |
| 3:r:105:LEU:O    | 3:r:108:THR:OG1  | 2.26                     | 0.41              |
| 1:1:488:VAL:HG11 | 1:3:490:VAL:CG2  | 2.51                     | 0.41              |
| 3:a:138:ASN:HB2  | 3:a:258:VAL:HG12 | 2.02                     | 0.41              |
| 3:c:306:ILE:HG22 | 3:c:310:MET:HE2  | 2.01                     | 0.41              |
| 3:j:313:ARG:NH2  | 3:j:316:SER:O    | 2.54                     | 0.41              |
| 3:q:271:ILE:HD11 | 3:q:284:MET:SD   | 2.61                     | 0.41              |
| 1:3:423:SER:OG   | 1:3:424:LEU:N    | 2.54                     | 0.41              |
| 2:D:261:VAL:HG13 | 2:D:290:LEU:HD23 | 2.03                     | 0.41              |
| 2:J:22:THR:CG2   | 2:J:73:LEU:HD22  | 2.51                     | 0.41              |
| 2:L:239:ASN:O    | 2:L:247:TRP:NE1  | 2.52                     | 0.41              |
| 2:P:299:ASN:ND2  | 3:q:69:ASN:O     | 2.53                     | 0.41              |
| 2:R:85:ILE:O     | 2:R:89:VAL:HG23  | 2.20                     | 0.41              |
| 3:a:185:ILE:HG22 | 3:a:226:ILE:HG12 | 2.03                     | 0.41              |
| 3:b:144:TYR:CD2  | 3:b:152:MET:HE1  | 2.56                     | 0.41              |
| 3:d:271:ILE:HD11 | 3:d:284:MET:SD   | 2.61                     | 0.41              |
| 2:B:1:MET:HE2    | 2:B:388:VAL:CG1  | 2.51                     | 0.41              |
| 2:B:214:LEU:HD11 | 2:B:285:PHE:CE1  | 2.56                     | 0.41              |
| 3:e:136:ASP:OD1  | 3:e:313:ARG:NH1  | 2.53                     | 0.41              |
| 3:j:123:ASP:OD1  | 3:j:124:ILE:N    | 2.53                     | 0.41              |
| 2:E:199:ILE:HD13 | 2:E:296:ARG:CZ   | 2.51                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:1:MET:HE2    | 2:M:388:VAL:HG13 | 2.02                     | 0.40              |
| 3:b:144:TYR:HD2  | 3:b:152:MET:HE1  | 1.86                     | 0.40              |
| 1:3:502:ARG:O    | 1:3:506:ASN:ND2  | 2.53                     | 0.40              |
| 2:C:154:LYS:N    | 2:C:327:GLU:O    | 2.50                     | 0.40              |
| 2:M:108:GLY:O    | 2:M:384:ARG:NE   | 2.54                     | 0.40              |
| 2:O:163:SER:HG   | 2:O:181:TRP:NE1  | 2.19                     | 0.40              |
| 2:P:169:SER:HA   | 2:P:176:LEU:HD23 | 2.03                     | 0.40              |
| 3:d:123:ASP:OD1  | 3:d:124:ILE:N    | 2.54                     | 0.40              |
| 3:i:160:LEU:HD13 | 3:i:271:ILE:HD11 | 2.04                     | 0.40              |
| 3:o:185:ILE:HG22 | 3:o:226:ILE:HG12 | 2.04                     | 0.40              |
| 1:3:354:ASP:N    | 1:3:354:ASP:OD1  | 2.53                     | 0.40              |
| 2:I:134:GLU:O    | 2:I:138:ASN:ND2  | 2.52                     | 0.40              |
| 2:P:14:ALA:HB1   | 2:P:85:ILE:HD11  | 2.04                     | 0.40              |
| 2:C:106:ARG:NH1  | 2:Q:380:ASP:OD1  | 2.55                     | 0.40              |
| 2:H:170:GLN:NE2  | 2:H:175:ASN:O    | 2.51                     | 0.40              |
| 3:a:199:ASN:OD1  | 3:a:203:LEU:N    | 2.49                     | 0.40              |
| 3:k:111:TRP:CZ2  | 3:k:307:ILE:HD13 | 2.57                     | 0.40              |
| 3:k:271:ILE:HD11 | 3:k:284:MET:SD   | 2.62                     | 0.40              |
| 3:m:74:GLU:O     | 3:m:78:THR:HG22  | 2.22                     | 0.40              |
| 3:n:306:ILE:HG22 | 3:n:310:MET:HE2  | 2.02                     | 0.40              |
| 2:O:133:SER:OG   | 2:O:136:ILE:HG22 | 2.22                     | 0.40              |
| 2:P:41:MET:HE1   | 2:P:119:LEU:CD2  | 2.50                     | 0.40              |
| 2:R:141:LEU:HB3  | 2:R:148:THR:HG22 | 2.02                     | 0.40              |
| 3:p:144:TYR:CD2  | 3:p:152:MET:HE1  | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles           |
|-----|-------|---------------|------------|---------|----------|-----------------------|
| 1   | 1     | 273/776 (35%) | 273 (100%) | 0       | 0        | <b>100</b> <b>100</b> |

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| Mol | Chain | Analysed       | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|------------|---------|----------|-------------|-----|
| 1   | 2     | 273/776 (35%)  | 273 (100%) | 0       | 0        | 100         | 100 |
| 1   | 3     | 273/776 (35%)  | 273 (100%) | 0       | 0        | 100         | 100 |
| 2   | A     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | B     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | C     | 395/397 (100%) | 393 (100%) | 2 (0%)  | 0        | 100         | 100 |
| 2   | D     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | E     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | F     | 395/397 (100%) | 391 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 2   | G     | 395/397 (100%) | 393 (100%) | 2 (0%)  | 0        | 100         | 100 |
| 2   | H     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | I     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | J     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | K     | 395/397 (100%) | 391 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 2   | L     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | M     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | N     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | O     | 395/397 (100%) | 393 (100%) | 2 (0%)  | 0        | 100         | 100 |
| 2   | P     | 395/397 (100%) | 392 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 2   | Q     | 395/397 (100%) | 393 (100%) | 2 (0%)  | 0        | 100         | 100 |
| 2   | R     | 395/397 (100%) | 393 (100%) | 2 (0%)  | 0        | 100         | 100 |
| 3   | a     | 257/326 (79%)  | 257 (100%) | 0       | 0        | 100         | 100 |
| 3   | b     | 270/326 (83%)  | 269 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 3   | c     | 259/326 (79%)  | 258 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 3   | d     | 263/326 (81%)  | 263 (100%) | 0       | 0        | 100         | 100 |
| 3   | e     | 258/326 (79%)  | 257 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 3   | f     | 263/326 (81%)  | 263 (100%) | 0       | 0        | 100         | 100 |
| 3   | g     | 270/326 (83%)  | 269 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 3   | h     | 257/326 (79%)  | 257 (100%) | 0       | 0        | 100         | 100 |
| 3   | i     | 270/326 (83%)  | 270 (100%) | 0       | 0        | 100         | 100 |
| 3   | j     | 270/326 (83%)  | 268 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 3   | k     | 263/326 (81%)  | 263 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured     | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|---------|----------|-------------|-----|
| 3   | l     | 263/326 (81%)     | 263 (100%)   | 0       | 0        | 100         | 100 |
| 3   | m     | 270/326 (83%)     | 269 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| 3   | n     | 263/326 (81%)     | 263 (100%)   | 0       | 0        | 100         | 100 |
| 3   | o     | 263/326 (81%)     | 263 (100%)   | 0       | 0        | 100         | 100 |
| 3   | p     | 270/326 (83%)     | 270 (100%)   | 0       | 0        | 100         | 100 |
| 3   | q     | 257/326 (79%)     | 257 (100%)   | 0       | 0        | 100         | 100 |
| 3   | r     | 270/326 (83%)     | 269 (100%)   | 1 (0%)  | 0        | 100         | 100 |
| All | All   | 12685/15342 (83%) | 12626 (100%) | 59 (0%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | 1     | 241/688 (35%)  | 234 (97%) | 7 (3%)   | 37          | 62 |
| 1   | 2     | 241/688 (35%)  | 235 (98%) | 6 (2%)   | 42          | 64 |
| 1   | 3     | 241/688 (35%)  | 232 (96%) | 9 (4%)   | 30          | 58 |
| 2   | A     | 350/350 (100%) | 345 (99%) | 5 (1%)   | 59          | 73 |
| 2   | B     | 350/350 (100%) | 344 (98%) | 6 (2%)   | 53          | 71 |
| 2   | C     | 350/350 (100%) | 344 (98%) | 6 (2%)   | 53          | 71 |
| 2   | D     | 350/350 (100%) | 344 (98%) | 6 (2%)   | 53          | 71 |
| 2   | E     | 350/350 (100%) | 346 (99%) | 4 (1%)   | 65          | 76 |
| 2   | F     | 350/350 (100%) | 341 (97%) | 9 (3%)   | 40          | 64 |
| 2   | G     | 350/350 (100%) | 346 (99%) | 4 (1%)   | 65          | 76 |
| 2   | H     | 350/350 (100%) | 343 (98%) | 7 (2%)   | 48          | 68 |
| 2   | I     | 350/350 (100%) | 346 (99%) | 4 (1%)   | 65          | 76 |
| 2   | J     | 350/350 (100%) | 346 (99%) | 4 (1%)   | 65          | 76 |
| 2   | K     | 350/350 (100%) | 346 (99%) | 4 (1%)   | 65          | 76 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 2   | L     | 350/350 (100%)    | 345 (99%)   | 5 (1%)   | 59          | 73 |
| 2   | M     | 350/350 (100%)    | 347 (99%)   | 3 (1%)   | 70          | 78 |
| 2   | N     | 350/350 (100%)    | 346 (99%)   | 4 (1%)   | 65          | 76 |
| 2   | O     | 350/350 (100%)    | 344 (98%)   | 6 (2%)   | 53          | 71 |
| 2   | P     | 350/350 (100%)    | 345 (99%)   | 5 (1%)   | 59          | 73 |
| 2   | Q     | 350/350 (100%)    | 347 (99%)   | 3 (1%)   | 70          | 78 |
| 2   | R     | 350/350 (100%)    | 347 (99%)   | 3 (1%)   | 70          | 78 |
| 3   | a     | 233/295 (79%)     | 231 (99%)   | 2 (1%)   | 70          | 78 |
| 3   | b     | 244/295 (83%)     | 238 (98%)   | 6 (2%)   | 42          | 64 |
| 3   | c     | 235/295 (80%)     | 232 (99%)   | 3 (1%)   | 61          | 74 |
| 3   | d     | 238/295 (81%)     | 233 (98%)   | 5 (2%)   | 47          | 67 |
| 3   | e     | 234/295 (79%)     | 229 (98%)   | 5 (2%)   | 47          | 67 |
| 3   | f     | 238/295 (81%)     | 234 (98%)   | 4 (2%)   | 53          | 71 |
| 3   | g     | 244/295 (83%)     | 239 (98%)   | 5 (2%)   | 48          | 68 |
| 3   | h     | 233/295 (79%)     | 230 (99%)   | 3 (1%)   | 61          | 74 |
| 3   | i     | 244/295 (83%)     | 239 (98%)   | 5 (2%)   | 48          | 68 |
| 3   | j     | 244/295 (83%)     | 238 (98%)   | 6 (2%)   | 42          | 64 |
| 3   | k     | 238/295 (81%)     | 233 (98%)   | 5 (2%)   | 47          | 67 |
| 3   | l     | 238/295 (81%)     | 230 (97%)   | 8 (3%)   | 32          | 59 |
| 3   | m     | 244/295 (83%)     | 241 (99%)   | 3 (1%)   | 63          | 75 |
| 3   | n     | 238/295 (81%)     | 235 (99%)   | 3 (1%)   | 61          | 74 |
| 3   | o     | 238/295 (81%)     | 231 (97%)   | 7 (3%)   | 37          | 62 |
| 3   | p     | 244/295 (83%)     | 238 (98%)   | 6 (2%)   | 42          | 64 |
| 3   | q     | 233/295 (79%)     | 229 (98%)   | 4 (2%)   | 53          | 71 |
| 3   | r     | 244/295 (83%)     | 239 (98%)   | 5 (2%)   | 48          | 68 |
| All | All   | 11327/13674 (83%) | 11132 (98%) | 195 (2%) | 52          | 71 |

All (195) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 312 | VAL  |
| 1   | 1     | 323 | MET  |
| 1   | 1     | 339 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 413 | THR  |
| 1   | 1     | 423 | SER  |
| 1   | 1     | 424 | LEU  |
| 1   | 1     | 473 | LEU  |
| 1   | 2     | 312 | VAL  |
| 1   | 2     | 335 | THR  |
| 1   | 2     | 345 | ILE  |
| 1   | 2     | 349 | SER  |
| 1   | 2     | 423 | SER  |
| 1   | 2     | 477 | ASN  |
| 1   | 3     | 270 | ASP  |
| 1   | 3     | 312 | VAL  |
| 1   | 3     | 323 | MET  |
| 1   | 3     | 354 | ASP  |
| 1   | 3     | 413 | THR  |
| 1   | 3     | 423 | SER  |
| 1   | 3     | 424 | LEU  |
| 1   | 3     | 473 | LEU  |
| 1   | 3     | 477 | ASN  |
| 2   | A     | 6   | SER  |
| 2   | A     | 7   | LEU  |
| 2   | A     | 207 | GLN  |
| 2   | A     | 238 | ILE  |
| 2   | A     | 342 | MET  |
| 2   | B     | 7   | LEU  |
| 2   | B     | 231 | ARG  |
| 2   | B     | 264 | LEU  |
| 2   | B     | 301 | THR  |
| 2   | B     | 312 | GLN  |
| 2   | B     | 342 | MET  |
| 2   | C     | 7   | LEU  |
| 2   | C     | 179 | THR  |
| 2   | C     | 207 | GLN  |
| 2   | C     | 239 | ASN  |
| 2   | C     | 319 | THR  |
| 2   | C     | 342 | MET  |
| 2   | D     | 7   | LEU  |
| 2   | D     | 74  | ASP  |
| 2   | D     | 83  | ASN  |
| 2   | D     | 179 | THR  |
| 2   | D     | 207 | GLN  |
| 2   | D     | 319 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 301 | THR  |
| 2   | E     | 319 | THR  |
| 2   | E     | 337 | ASP  |
| 2   | E     | 342 | MET  |
| 2   | F     | 6   | SER  |
| 2   | F     | 7   | LEU  |
| 2   | F     | 86  | ASP  |
| 2   | F     | 131 | ASN  |
| 2   | F     | 207 | GLN  |
| 2   | F     | 238 | ILE  |
| 2   | F     | 255 | ARG  |
| 2   | F     | 312 | GLN  |
| 2   | F     | 342 | MET  |
| 2   | G     | 7   | LEU  |
| 2   | G     | 69  | THR  |
| 2   | G     | 272 | THR  |
| 2   | G     | 342 | MET  |
| 2   | H     | 6   | SER  |
| 2   | H     | 7   | LEU  |
| 2   | H     | 207 | GLN  |
| 2   | H     | 239 | ASN  |
| 2   | H     | 264 | LEU  |
| 2   | H     | 272 | THR  |
| 2   | H     | 342 | MET  |
| 2   | I     | 6   | SER  |
| 2   | I     | 7   | LEU  |
| 2   | I     | 323 | THR  |
| 2   | I     | 342 | MET  |
| 2   | J     | 7   | LEU  |
| 2   | J     | 207 | GLN  |
| 2   | J     | 239 | ASN  |
| 2   | J     | 337 | ASP  |
| 2   | K     | 7   | LEU  |
| 2   | K     | 207 | GLN  |
| 2   | K     | 238 | ILE  |
| 2   | K     | 264 | LEU  |
| 2   | L     | 62  | ASP  |
| 2   | L     | 207 | GLN  |
| 2   | L     | 264 | LEU  |
| 2   | L     | 315 | GLU  |
| 2   | L     | 319 | THR  |
| 2   | M     | 7   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 238 | ILE  |
| 2   | M     | 239 | ASN  |
| 2   | N     | 7   | LEU  |
| 2   | N     | 212 | VAL  |
| 2   | N     | 238 | ILE  |
| 2   | N     | 264 | LEU  |
| 2   | O     | 7   | LEU  |
| 2   | O     | 69  | THR  |
| 2   | O     | 186 | SER  |
| 2   | O     | 207 | GLN  |
| 2   | O     | 239 | ASN  |
| 2   | O     | 342 | MET  |
| 2   | P     | 264 | LEU  |
| 2   | P     | 272 | THR  |
| 2   | P     | 315 | GLU  |
| 2   | P     | 337 | ASP  |
| 2   | P     | 370 | LEU  |
| 2   | Q     | 207 | GLN  |
| 2   | Q     | 239 | ASN  |
| 2   | Q     | 301 | THR  |
| 2   | R     | 7   | LEU  |
| 2   | R     | 264 | LEU  |
| 2   | R     | 286 | ASP  |
| 3   | a     | 186 | SER  |
| 3   | a     | 281 | THR  |
| 3   | b     | 73  | GLU  |
| 3   | b     | 149 | GLN  |
| 3   | b     | 202 | THR  |
| 3   | b     | 208 | LEU  |
| 3   | b     | 281 | THR  |
| 3   | b     | 284 | MET  |
| 3   | c     | 179 | ASP  |
| 3   | c     | 281 | THR  |
| 3   | c     | 284 | MET  |
| 3   | d     | 73  | GLU  |
| 3   | d     | 87  | THR  |
| 3   | d     | 149 | GLN  |
| 3   | d     | 185 | ILE  |
| 3   | d     | 281 | THR  |
| 3   | e     | 55  | ILE  |
| 3   | e     | 202 | THR  |
| 3   | e     | 209 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | e     | 225 | VAL  |
| 3   | e     | 281 | THR  |
| 3   | f     | 150 | LEU  |
| 3   | f     | 220 | THR  |
| 3   | f     | 281 | THR  |
| 3   | f     | 314 | SER  |
| 3   | g     | 180 | GLU  |
| 3   | g     | 225 | VAL  |
| 3   | g     | 281 | THR  |
| 3   | g     | 318 | ASN  |
| 3   | g     | 324 | TYR  |
| 3   | h     | 231 | ASP  |
| 3   | h     | 281 | THR  |
| 3   | h     | 287 | ILE  |
| 3   | i     | 87  | THR  |
| 3   | i     | 176 | GLN  |
| 3   | i     | 186 | SER  |
| 3   | i     | 281 | THR  |
| 3   | i     | 324 | TYR  |
| 3   | j     | 176 | GLN  |
| 3   | j     | 185 | ILE  |
| 3   | j     | 225 | VAL  |
| 3   | j     | 277 | THR  |
| 3   | j     | 281 | THR  |
| 3   | j     | 284 | MET  |
| 3   | k     | 60  | THR  |
| 3   | k     | 74  | GLU  |
| 3   | k     | 149 | GLN  |
| 3   | k     | 208 | LEU  |
| 3   | k     | 281 | THR  |
| 3   | l     | 162 | GLU  |
| 3   | l     | 186 | SER  |
| 3   | l     | 202 | THR  |
| 3   | l     | 209 | THR  |
| 3   | l     | 225 | VAL  |
| 3   | l     | 274 | ASP  |
| 3   | l     | 281 | THR  |
| 3   | l     | 283 | ARG  |
| 3   | m     | 151 | ASP  |
| 3   | m     | 185 | ILE  |
| 3   | m     | 281 | THR  |
| 3   | n     | 169 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | n     | 207 | CYS  |
| 3   | n     | 281 | THR  |
| 3   | o     | 73  | GLU  |
| 3   | o     | 74  | GLU  |
| 3   | o     | 133 | LEU  |
| 3   | o     | 209 | THR  |
| 3   | o     | 225 | VAL  |
| 3   | o     | 281 | THR  |
| 3   | o     | 284 | MET  |
| 3   | p     | 133 | LEU  |
| 3   | p     | 185 | ILE  |
| 3   | p     | 209 | THR  |
| 3   | p     | 237 | LEU  |
| 3   | p     | 281 | THR  |
| 3   | p     | 284 | MET  |
| 3   | q     | 87  | THR  |
| 3   | q     | 202 | THR  |
| 3   | q     | 231 | ASP  |
| 3   | q     | 281 | THR  |
| 3   | r     | 133 | LEU  |
| 3   | r     | 180 | GLU  |
| 3   | r     | 185 | ILE  |
| 3   | r     | 186 | SER  |
| 3   | r     | 231 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 506 | ASN  |
| 1   | 2     | 321 | ASN  |
| 1   | 2     | 516 | GLN  |
| 2   | A     | 32  | GLN  |
| 2   | A     | 146 | GLN  |
| 2   | A     | 175 | ASN  |
| 2   | A     | 257 | ASN  |
| 2   | A     | 345 | ASN  |
| 2   | B     | 26  | ASN  |
| 2   | B     | 47  | GLN  |
| 2   | B     | 183 | ASN  |
| 2   | B     | 206 | GLN  |
| 2   | B     | 210 | HIS  |
| 2   | C     | 131 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 175 | ASN  |
| 2   | D     | 72  | ASN  |
| 2   | D     | 128 | ASN  |
| 2   | D     | 200 | ASN  |
| 2   | D     | 257 | ASN  |
| 2   | E     | 146 | GLN  |
| 2   | E     | 167 | ASN  |
| 2   | E     | 206 | GLN  |
| 2   | E     | 310 | ASN  |
| 2   | F     | 26  | ASN  |
| 2   | F     | 175 | ASN  |
| 2   | F     | 206 | GLN  |
| 2   | F     | 317 | HIS  |
| 2   | G     | 60  | ASN  |
| 2   | G     | 146 | GLN  |
| 2   | G     | 206 | GLN  |
| 2   | G     | 310 | ASN  |
| 2   | H     | 131 | ASN  |
| 2   | H     | 167 | ASN  |
| 2   | H     | 173 | HIS  |
| 2   | H     | 257 | ASN  |
| 2   | H     | 293 | GLN  |
| 2   | I     | 146 | GLN  |
| 2   | I     | 189 | GLN  |
| 2   | J     | 32  | GLN  |
| 2   | J     | 36  | GLN  |
| 2   | J     | 72  | ASN  |
| 2   | J     | 146 | GLN  |
| 2   | K     | 26  | ASN  |
| 2   | K     | 72  | ASN  |
| 2   | K     | 112 | GLN  |
| 2   | K     | 173 | HIS  |
| 2   | K     | 206 | GLN  |
| 2   | K     | 345 | ASN  |
| 2   | L     | 173 | HIS  |
| 2   | L     | 257 | ASN  |
| 2   | L     | 293 | GLN  |
| 2   | L     | 383 | GLN  |
| 2   | M     | 47  | GLN  |
| 2   | M     | 58  | ASN  |
| 2   | M     | 60  | ASN  |
| 2   | M     | 72  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 146 | GLN  |
| 2   | M     | 257 | ASN  |
| 2   | N     | 47  | GLN  |
| 2   | N     | 183 | ASN  |
| 2   | N     | 210 | HIS  |
| 2   | O     | 44  | ASN  |
| 2   | O     | 146 | GLN  |
| 2   | O     | 257 | ASN  |
| 2   | P     | 32  | GLN  |
| 2   | P     | 183 | ASN  |
| 2   | P     | 210 | HIS  |
| 2   | Q     | 167 | ASN  |
| 2   | Q     | 257 | ASN  |
| 2   | Q     | 293 | GLN  |
| 2   | Q     | 345 | ASN  |
| 2   | Q     | 383 | GLN  |
| 3   | a     | 94  | ASN  |
| 3   | a     | 132 | GLN  |
| 3   | a     | 262 | GLN  |
| 3   | c     | 132 | GLN  |
| 3   | c     | 280 | GLN  |
| 3   | d     | 132 | GLN  |
| 3   | d     | 149 | GLN  |
| 3   | d     | 176 | GLN  |
| 3   | d     | 234 | ASN  |
| 3   | e     | 104 | GLN  |
| 3   | e     | 138 | ASN  |
| 3   | e     | 305 | GLN  |
| 3   | e     | 308 | GLN  |
| 3   | f     | 149 | GLN  |
| 3   | f     | 166 | ASN  |
| 3   | f     | 176 | GLN  |
| 3   | f     | 235 | HIS  |
| 3   | g     | 176 | GLN  |
| 3   | g     | 308 | GLN  |
| 3   | h     | 149 | GLN  |
| 3   | h     | 308 | GLN  |
| 3   | i     | 182 | ASN  |
| 3   | i     | 305 | GLN  |
| 3   | i     | 308 | GLN  |
| 3   | j     | 234 | ASN  |
| 3   | j     | 248 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | k     | 72  | GLN  |
| 3   | k     | 262 | GLN  |
| 3   | l     | 149 | GLN  |
| 3   | l     | 305 | GLN  |
| 3   | n     | 149 | GLN  |
| 3   | n     | 280 | GLN  |
| 3   | n     | 288 | ASN  |
| 3   | o     | 94  | ASN  |
| 3   | o     | 305 | GLN  |
| 3   | p     | 132 | GLN  |
| 3   | p     | 149 | GLN  |
| 3   | p     | 166 | ASN  |
| 3   | p     | 235 | HIS  |
| 3   | p     | 308 | GLN  |
| 3   | q     | 305 | 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](#)

Of 72 ligands modelled in this entry, 54 are monoatomic - leaving 18 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | m     | 401 | 3    | 14,14,15     | 0.62 | 1 (7%)   | 17,19,21    | 0.73 | 1 (5%)   |
| 4   | NAG  | e     | 401 | 3    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.57 | 0        |
| 4   | NAG  | a     | 401 | 3    | 14,14,15     | 0.67 | 1 (7%)   | 17,19,21    | 0.78 | 1 (5%)   |
| 4   | NAG  | c     | 401 | 3    | 14,14,15     | 0.62 | 1 (7%)   | 17,19,21    | 0.72 | 1 (5%)   |
| 4   | NAG  | b     | 401 | -    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.50 | 0        |
| 4   | NAG  | g     | 401 | 3    | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.46 | 0        |
| 4   | NAG  | j     | 401 | 3    | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.37 | 0        |
| 4   | NAG  | n     | 401 | 3    | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.36 | 0        |
| 4   | NAG  | q     | 401 | 3    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 4   | NAG  | d     | 401 | 3    | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.40 | 0        |
| 4   | NAG  | o     | 401 | 3    | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | NAG  | f     | 401 | 3    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.45 | 0        |
| 4   | NAG  | h     | 401 | 3    | 14,14,15     | 0.64 | 1 (7%)   | 17,19,21    | 0.74 | 1 (5%)   |
| 4   | NAG  | l     | 401 | 3    | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.47 | 0        |
| 4   | NAG  | p     | 401 | 3    | 14,14,15     | 0.55 | 0        | 17,19,21    | 0.76 | 1 (5%)   |
| 4   | NAG  | r     | 401 | 3    | 14,14,15     | 0.65 | 1 (7%)   | 17,19,21    | 0.78 | 1 (5%)   |
| 4   | NAG  | k     | 401 | 3    | 14,14,15     | 0.64 | 1 (7%)   | 17,19,21    | 0.81 | 1 (5%)   |
| 4   | NAG  | i     | 401 | 3    | 14,14,15     | 0.64 | 1 (7%)   | 17,19,21    | 0.75 | 1 (5%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | m     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | e     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | a     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | c     | 401 | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | b     | 401 | -    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | g     | 401 | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | j     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | n     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | q     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | d     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | o     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | f     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | h     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | l     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | p     | 401 | 3    | -       | 2/6/23/26 | 0/1/1/1 |

Continued on next page...



*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | r     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | k     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | i     | 401 | 3    | -       | 0/6/23/26 | 0/1/1/1 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | a     | 401 | NAG  | C1-C2 | 2.30 | 1.55        | 1.52     |
| 4   | r     | 401 | NAG  | C1-C2 | 2.22 | 1.55        | 1.52     |
| 4   | h     | 401 | NAG  | C1-C2 | 2.21 | 1.55        | 1.52     |
| 4   | k     | 401 | NAG  | C1-C2 | 2.21 | 1.55        | 1.52     |
| 4   | i     | 401 | NAG  | C1-C2 | 2.19 | 1.55        | 1.52     |
| 4   | c     | 401 | NAG  | C1-C2 | 2.16 | 1.55        | 1.52     |
| 4   | m     | 401 | NAG  | C1-C2 | 2.16 | 1.55        | 1.52     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 4   | k     | 401 | NAG  | C1-O5-C5 | 2.88 | 116.04      | 112.19   |
| 4   | r     | 401 | NAG  | C1-O5-C5 | 2.75 | 115.88      | 112.19   |
| 4   | a     | 401 | NAG  | C1-O5-C5 | 2.72 | 115.83      | 112.19   |
| 4   | p     | 401 | NAG  | C1-O5-C5 | 2.61 | 115.68      | 112.19   |
| 4   | i     | 401 | NAG  | C1-O5-C5 | 2.59 | 115.65      | 112.19   |
| 4   | h     | 401 | NAG  | C1-O5-C5 | 2.57 | 115.64      | 112.19   |
| 4   | m     | 401 | NAG  | C1-O5-C5 | 2.53 | 115.58      | 112.19   |
| 4   | c     | 401 | NAG  | C1-O5-C5 | 2.46 | 115.48      | 112.19   |
| 4   | q     | 401 | NAG  | C1-O5-C5 | 2.41 | 115.41      | 112.19   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | c     | 401 | NAG  | C4-C5-C6-O6 |
| 4   | c     | 401 | NAG  | O5-C5-C6-O6 |
| 4   | p     | 401 | NAG  | O5-C5-C6-O6 |
| 4   | p     | 401 | NAG  | C4-C5-C6-O6 |
| 4   | g     | 401 | NAG  | C1-C2-N2-C7 |

There are no ring outliers.

8 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | m     | 401 | NAG  | 1       | 0            |
| 4   | a     | 401 | NAG  | 1       | 0            |
| 4   | c     | 401 | NAG  | 1       | 0            |
| 4   | h     | 401 | NAG  | 1       | 0            |
| 4   | p     | 401 | NAG  | 1       | 0            |
| 4   | r     | 401 | NAG  | 1       | 0            |
| 4   | k     | 401 | NAG  | 1       | 0            |
| 4   | i     | 401 | NAG  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

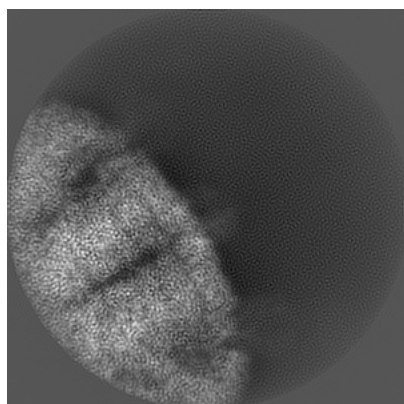
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21957. These allow visual inspection of the internal detail of the map and identification of artifacts.

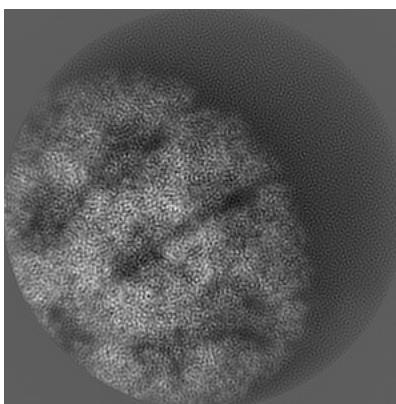
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

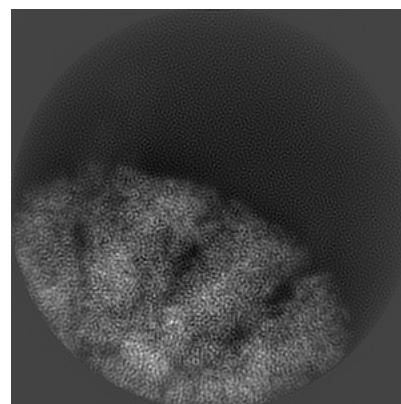
#### 6.1.1 Primary map



X

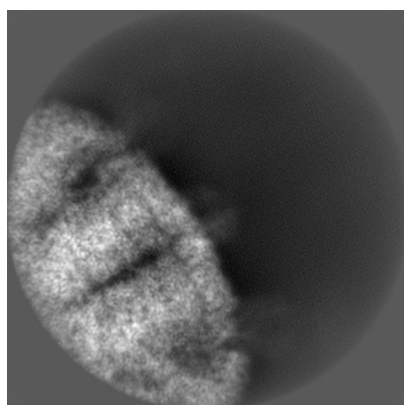


Y

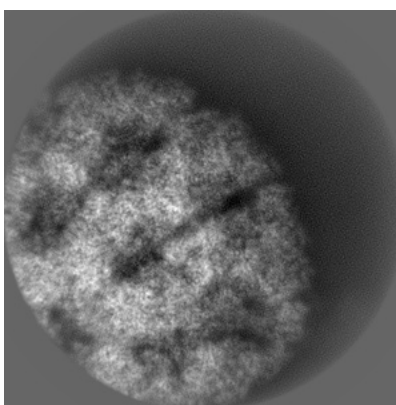


Z

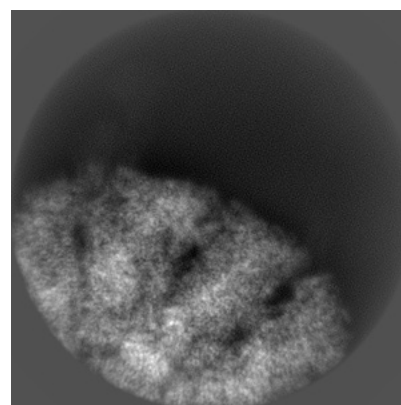
#### 6.1.2 Raw map



X



Y

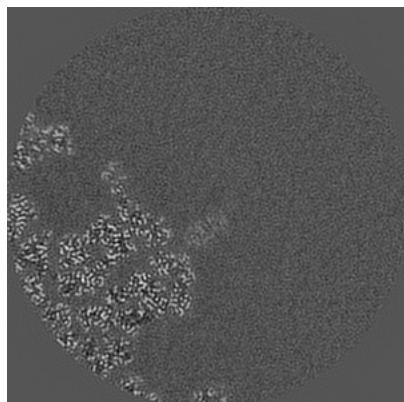


Z

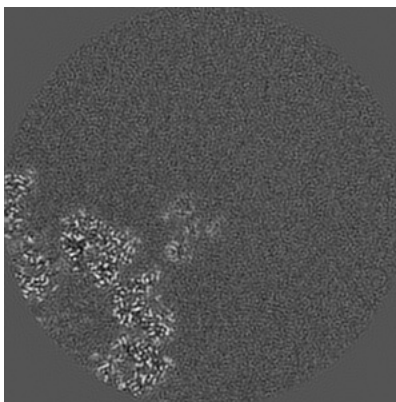
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

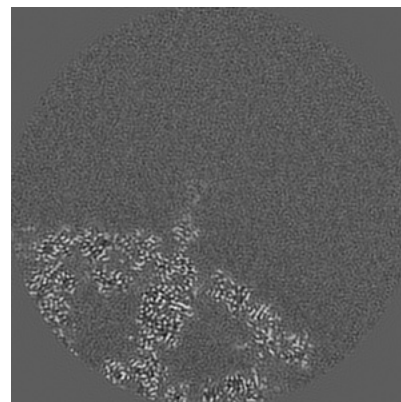
### 6.2.1 Primary map



X Index: 160

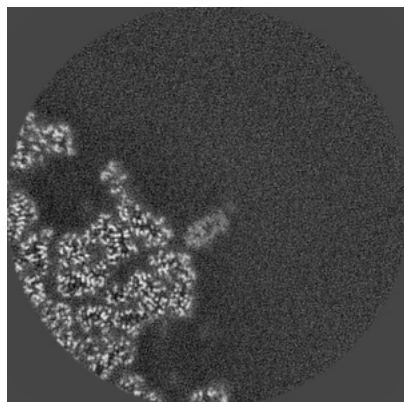


Y Index: 160

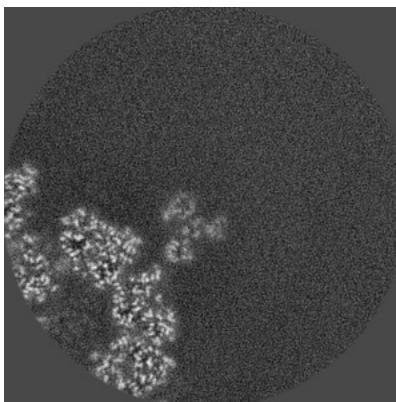


Z Index: 160

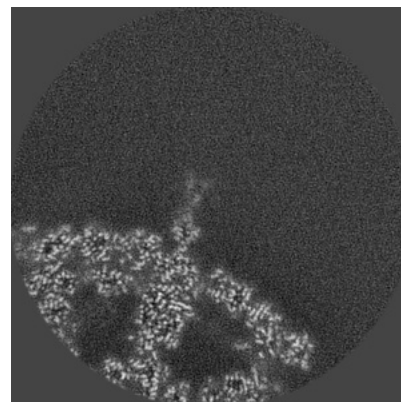
### 6.2.2 Raw map



X Index: 160



Y Index: 160

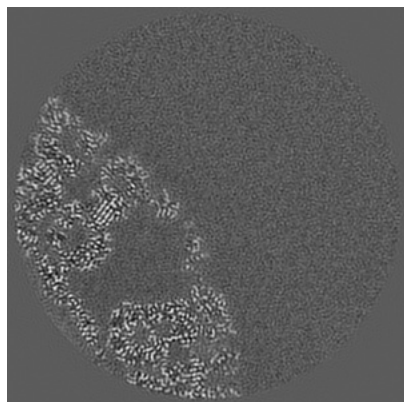


Z Index: 160

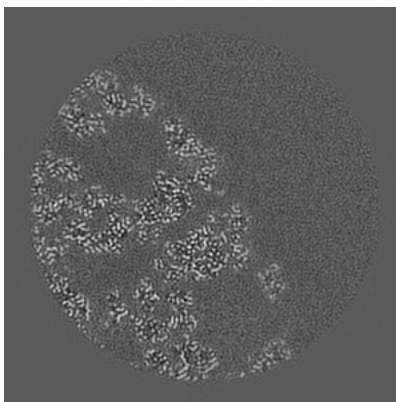
The images above show central slices of the map in three orthogonal directions.

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

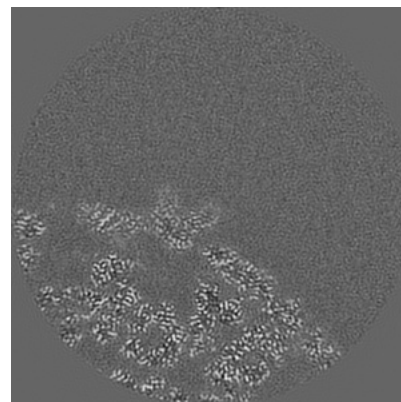
### 6.3.1 Primary map



X Index: 112

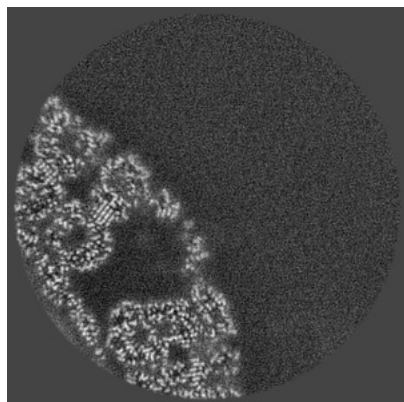


Y Index: 79

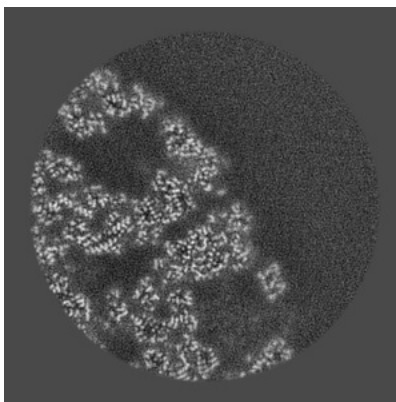


Z Index: 135

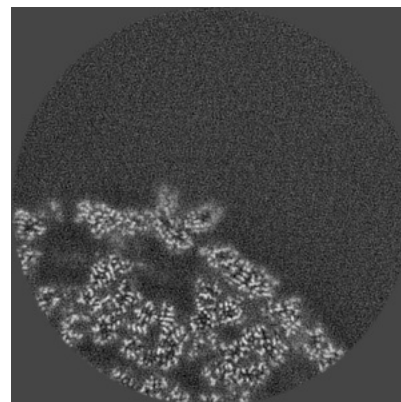
### 6.3.2 Raw map



X Index: 112



Y Index: 79



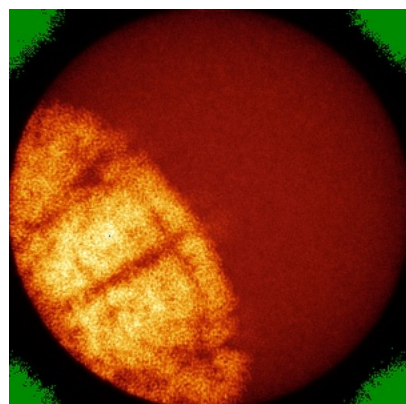
Z Index: 134

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

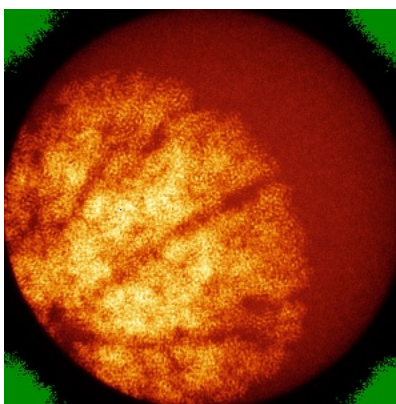


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

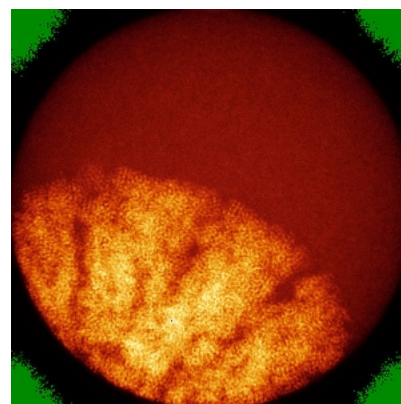
### 6.4.1 Primary map



X

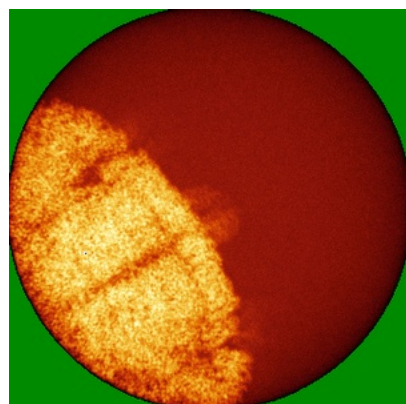


Y

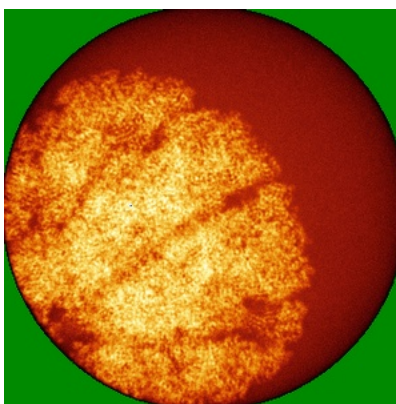


Z

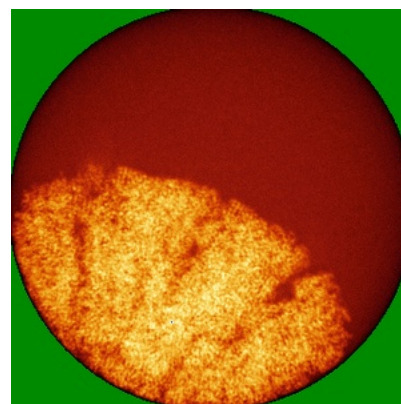
### 6.4.2 Raw map



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](#)

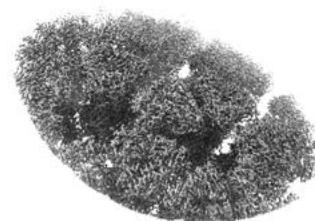
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

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

## 6.6 Mask visualisation [i](#)

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

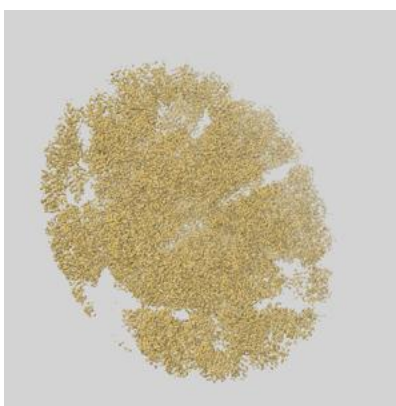
A mask typically either:

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

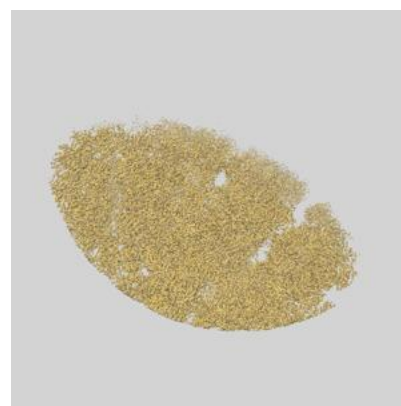
### 6.6.1 emd\_21957\_msk\_1.map [i](#)



X



Y



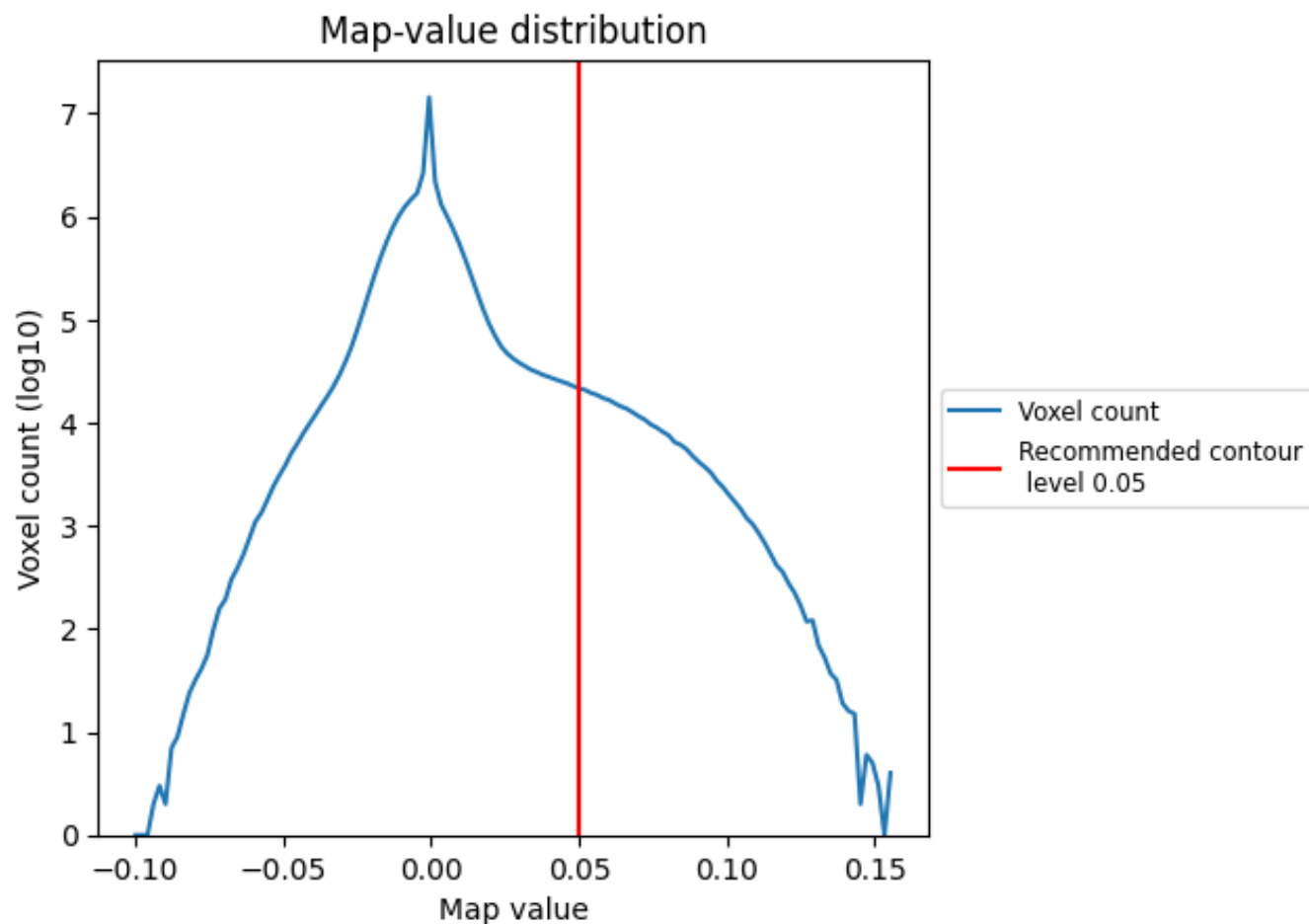
Z



## 7 Map analysis [i](#)

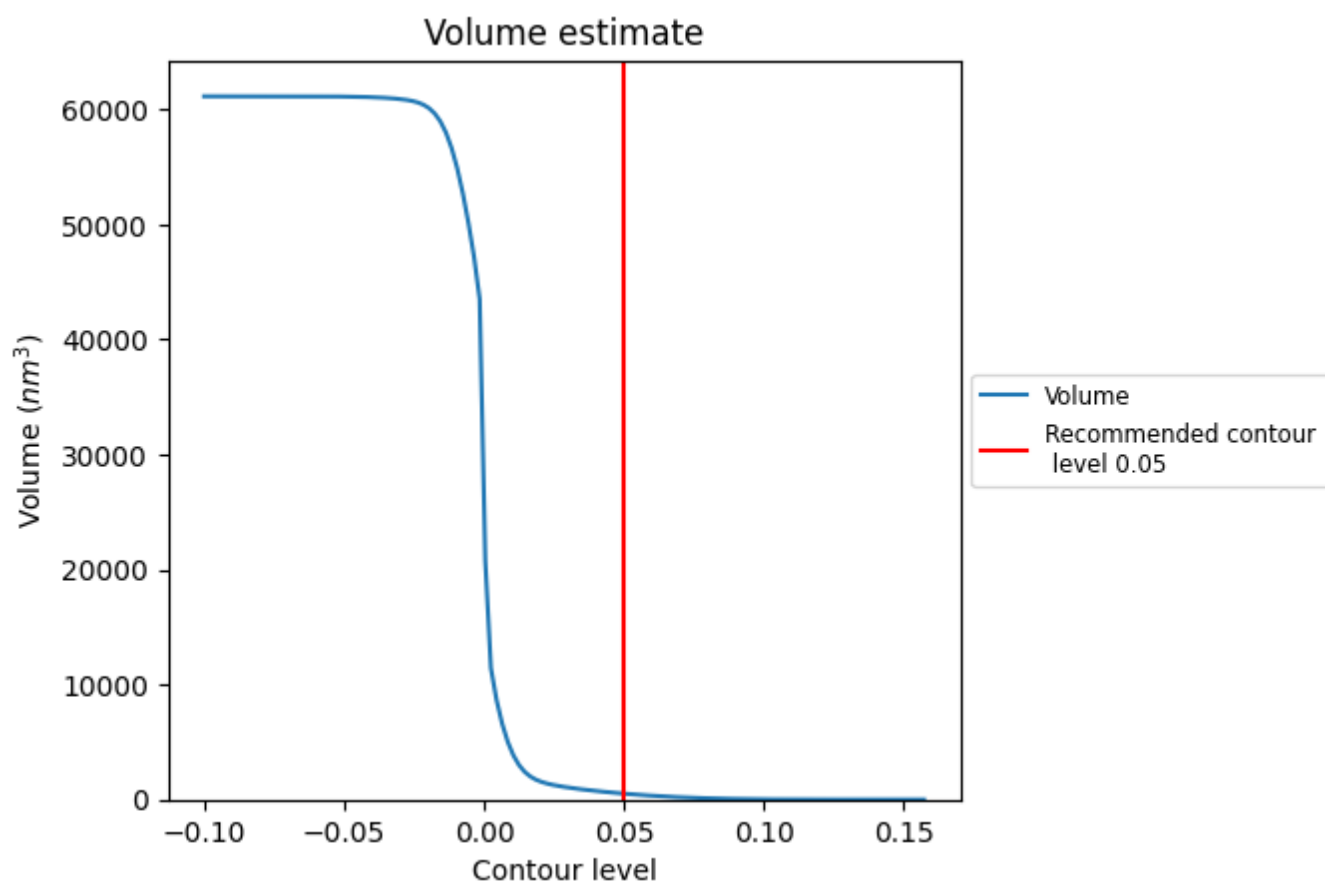
This section contains the results of statistical analysis of the map.

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



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

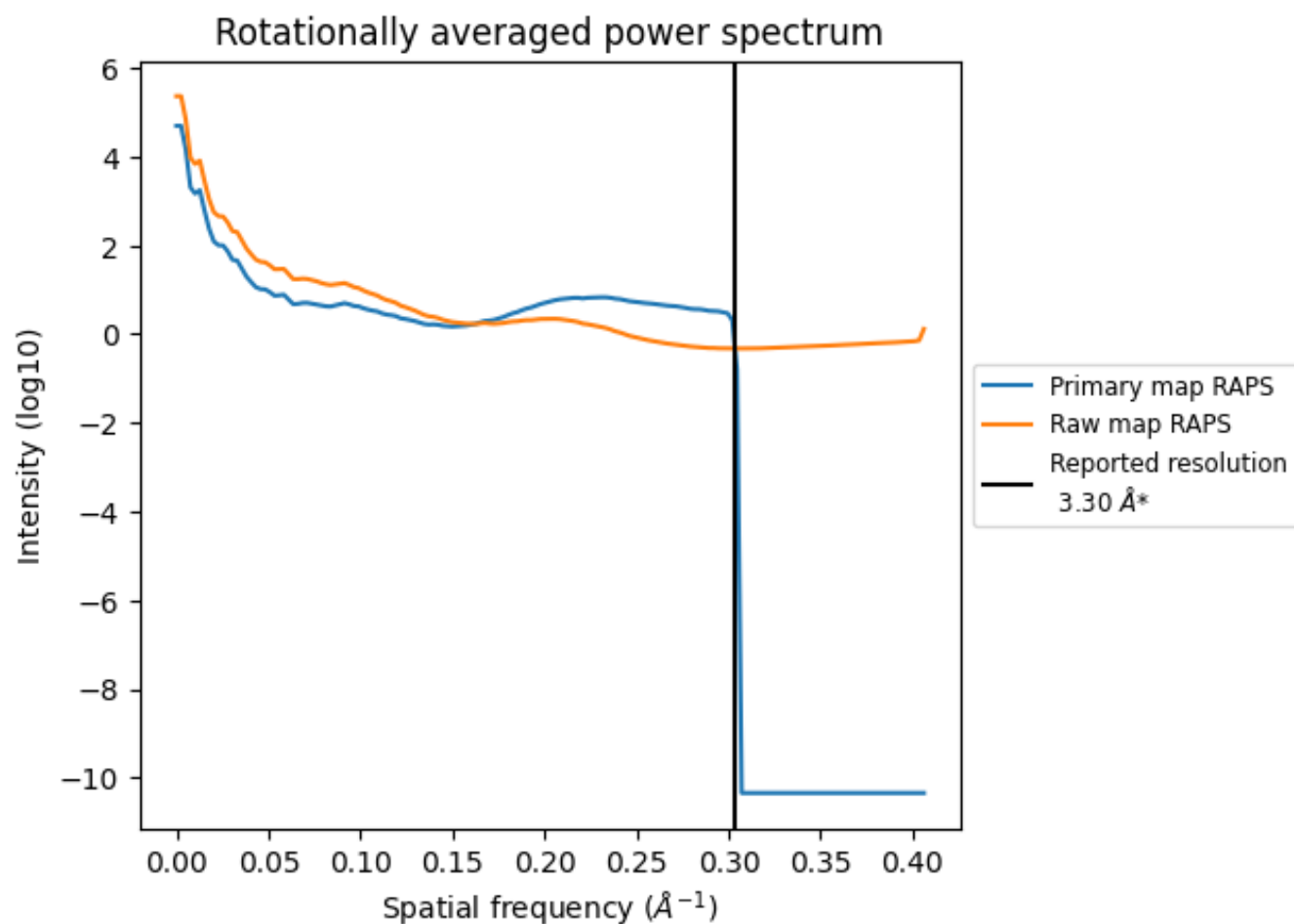
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm<sup>3</sup>; this corresponds to an approximate mass of 466 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 ⓘ

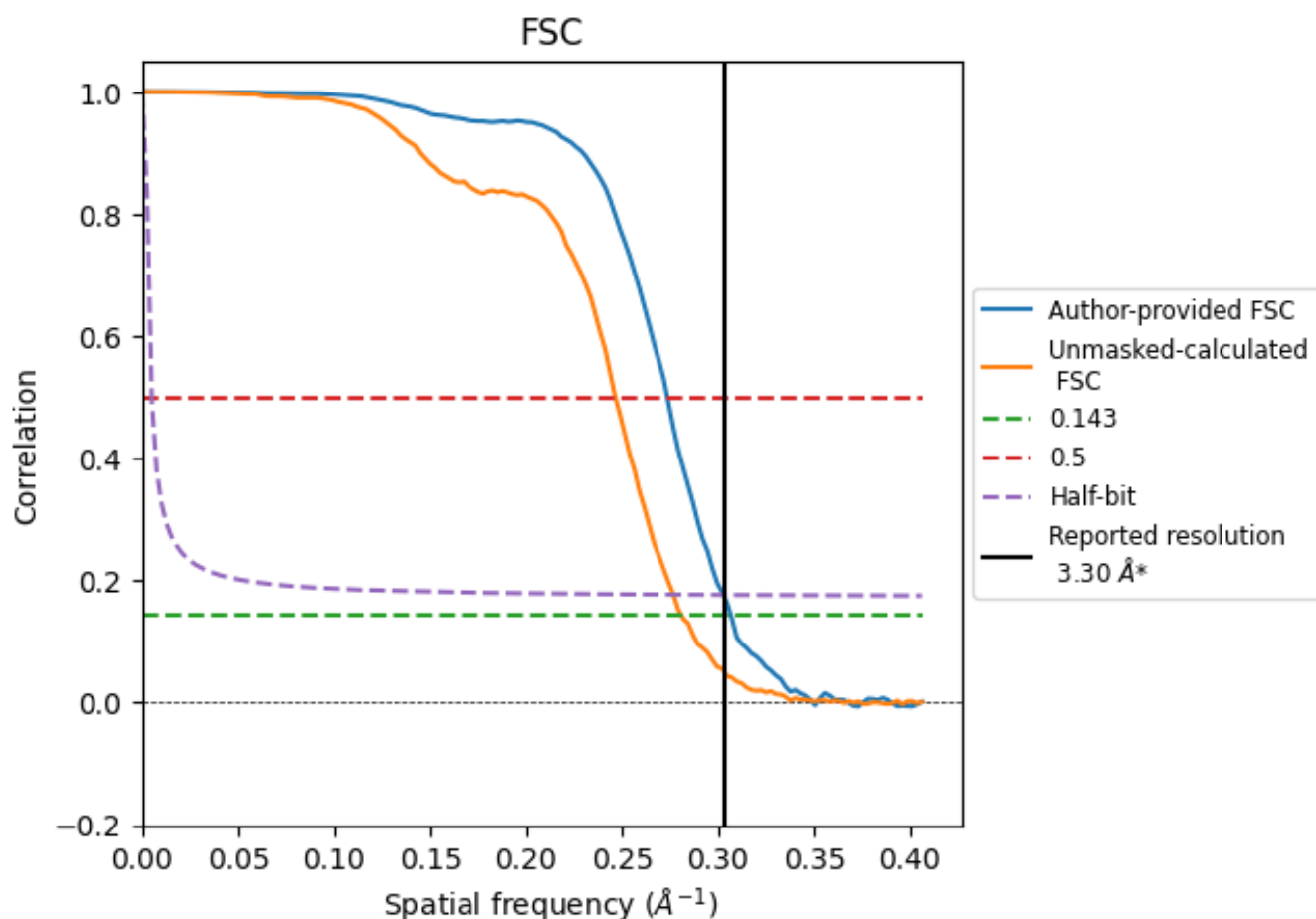


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

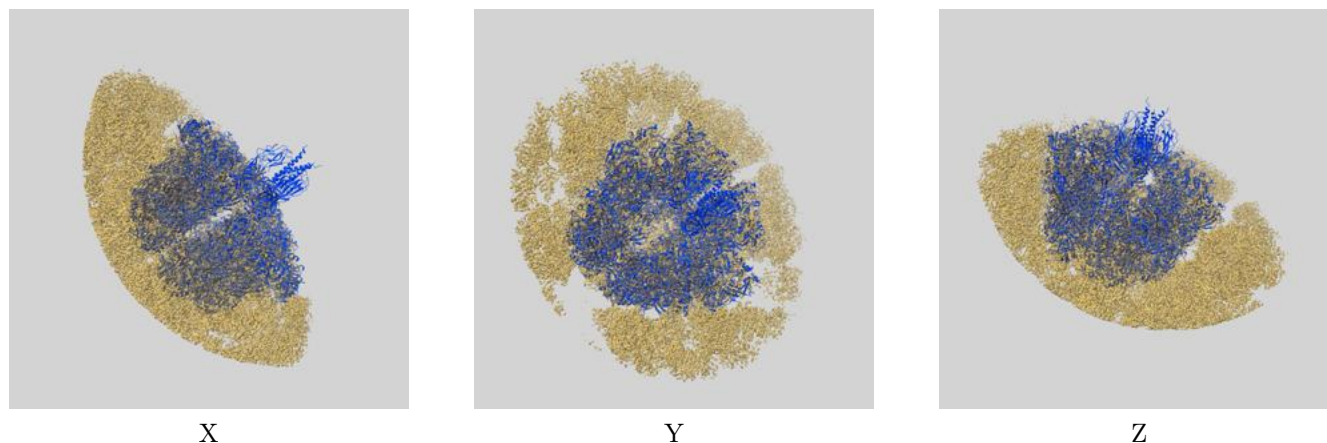
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.30                               | -    | -        |
| Author-provided FSC curve | 3.26                               | 3.66 | 3.30     |
| Unmasked-calculated*      | 3.56                               | 4.06 | 3.61     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

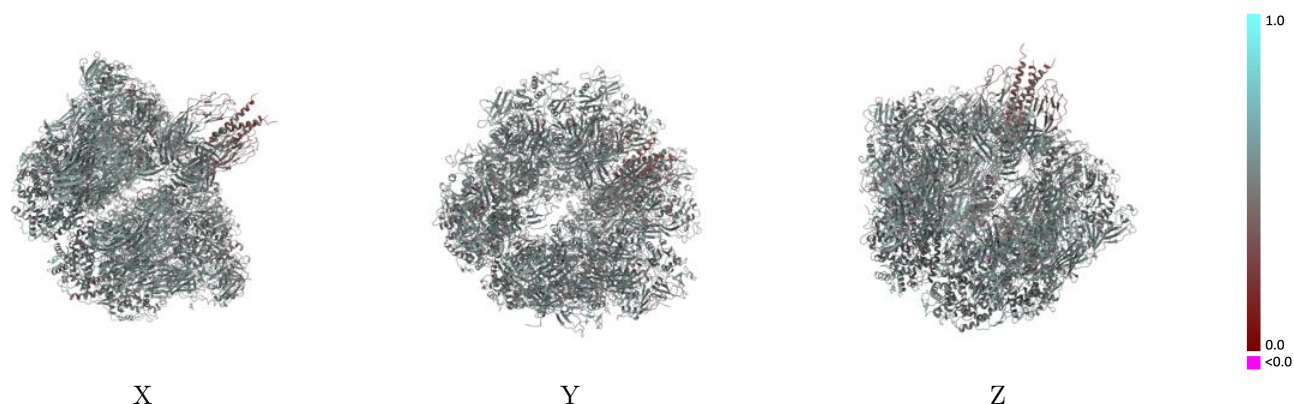
This section contains information regarding the fit between EMDB map EMD-21957 and PDB model 6WXG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



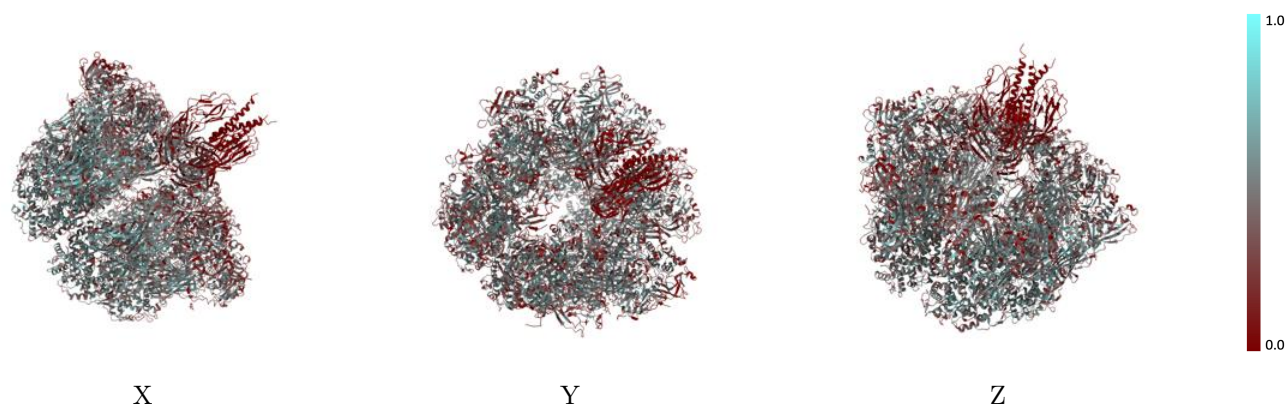
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



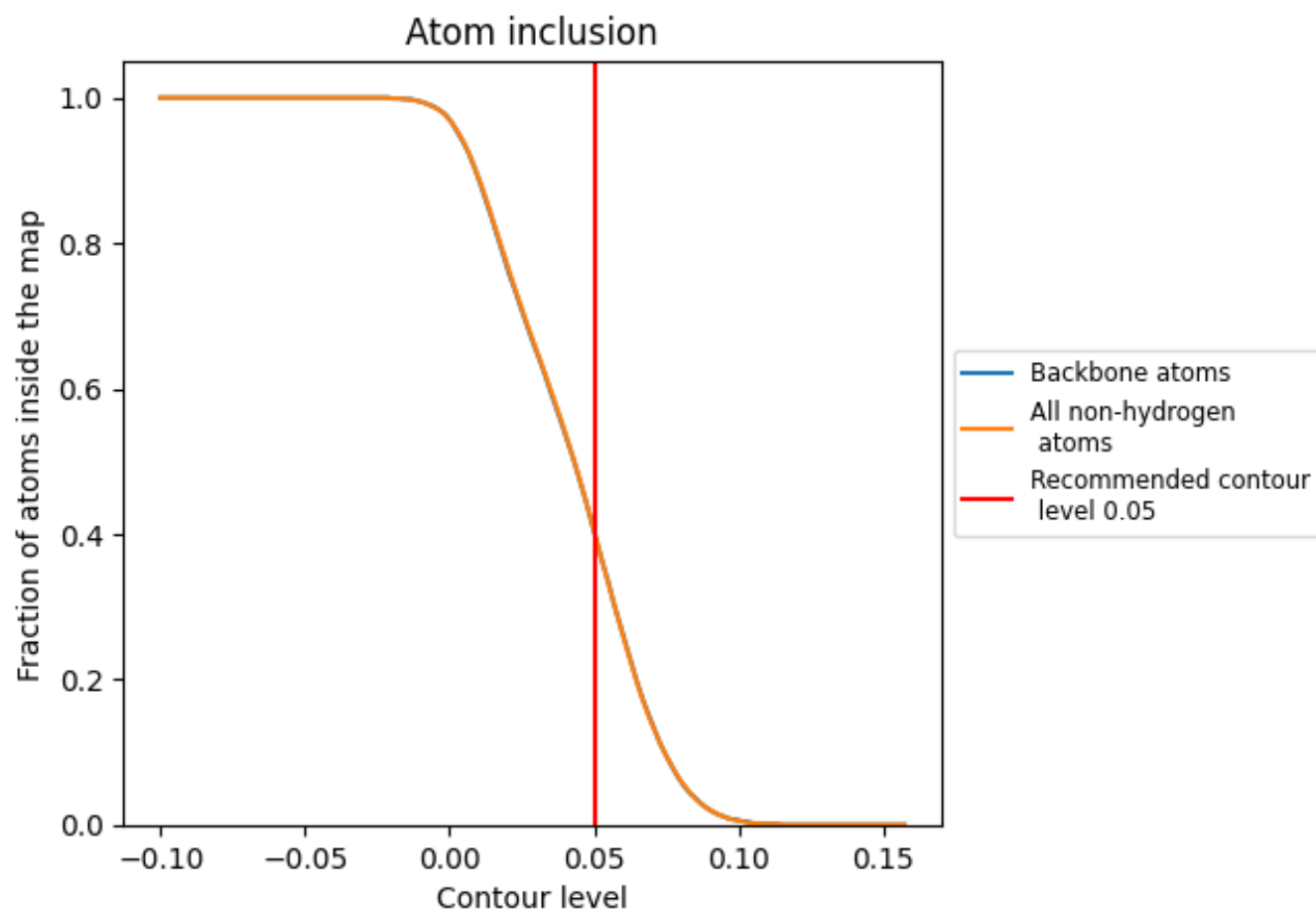
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 40% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.4040   |  0.5090   |
| 1     |  0.0880   |  0.4590   |
| 2     |  0.1000   |  0.4570   |
| 3     |  0.1000   |  0.4490   |
| A     |  0.5210   |  0.5290   |
| B     |  0.4960   |  0.5150   |
| C     |  0.5130   |  0.5250   |
| D     |  0.5190   |  0.5280   |
| E     |  0.5100   |  0.5220   |
| F     |  0.5070   |  0.5260   |
| G     |  0.5100   |  0.5220   |
| H     |  0.4900   |  0.5220   |
| I     |  0.5020   |  0.5280   |
| J     |  0.4770   |  0.5180   |
| K     |  0.4730  |  0.5200  |
| L     |  0.4750 |  0.5190 |
| M     |  0.4800 |  0.5200 |
| N     |  0.4770 |  0.5230 |
| O     |  0.4580 |  0.5190 |
| P     |  0.4820 |  0.5230 |
| Q     |  0.4910 |  0.5220 |
| R     |  0.4660 |  0.5170 |
| a     |  0.3450 |  0.5060 |
| b     |  0.3500 |  0.4970 |
| c     |  0.3600 |  0.5020 |
| d     |  0.3950 |  0.5090 |
| e     |  0.4000 |  0.5100 |
| f     |  0.3760 |  0.5070 |
| g     |  0.3240 |  0.4960 |
| h     |  0.3180 |  0.5000 |
| i     |  0.3640 |  0.4970 |
| j     |  0.3280 |  0.4920 |
| k     |  0.3170 |  0.4960 |
| l     |  0.3630 |  0.5110 |
| m     |  0.3470 |  0.4960 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| n     |  0.3270 |  0.5000 |
| o     |  0.3480 |  0.5000 |
| p     |  0.2940 |  0.4930 |
| q     |  0.3140 |  0.4980 |
| r     |  0.3220 |  0.4930 |