



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 09:11 PM EDT

PDB ID : 7TR9  
EMDB ID : EMD-26083  
Title : Cascade complex from type I-A CRISPR-Cas system  
Authors : Hu, C.; Ni, D.; Nam, K.H.; Majumdar, S.; McLean, J.; Stahlberg, H.; Terns, M.; Ke, A.  
Deposited on : 2022-01-28  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

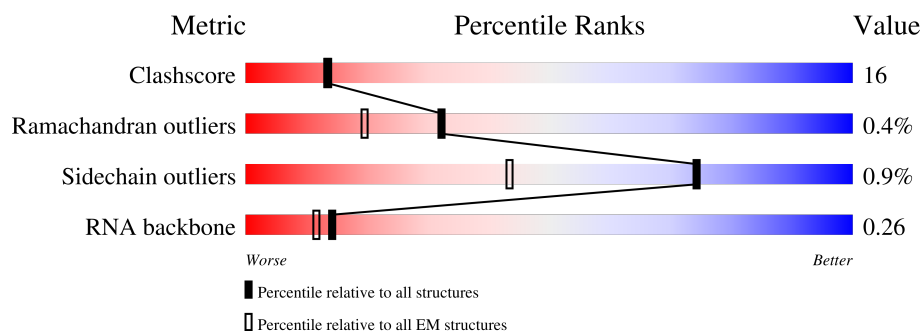
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 Å.

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



| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 210492                   | 15764                    |
| Ramachandran outliers | 207382                   | 16835                    |
| Sidechain outliers    | 206894                   | 16415                    |
| RNA backbone          | 6643                     | 2191                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | C     | 341    | <div> <div>10%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>  |
| 2   | D     | 108    | <div> <div>11%</div> <div>71%</div> <div>24%</div> <div>..</div> </div> |
| 2   | E     | 108    | <div> <div>7%</div> <div>64%</div> <div>35%</div> <div>.</div> </div>   |
| 2   | F     | 108    | <div> <div>13%</div> <div>65%</div> <div>33%</div> <div>..</div> </div> |
| 2   | G     | 108    | <div> <div>20%</div> <div>65%</div> <div>33%</div> <div>..</div> </div> |
| 2   | H     | 108    | <div> <div>44%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>  |
| 3   | I     | 336    | <div> <div>9%</div> <div>65%</div> <div>34%</div> </div>                |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | J     | 336    |                  |
| 3   | K     | 336    |                  |
| 3   | L     | 336    |                  |
| 3   | M     | 336    |                  |
| 3   | N     | 336    |                  |
| 3   | O     | 336    |                  |
| 4   | P     | 256    |                  |
| 5   | R     | 45     |                  |
| 6   | A     | 572    |                  |
| 7   | Q     | 237    |                  |
| 8   | S     | 22     |                  |
| 9   | T     | 8      |                  |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 34208 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cas8a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | C     | 333      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2662  | 1730 | 439 | 484 | 9 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 24      | VAL      | GLU    | conflict | UNP Q8U338 |
| C     | 64      | SER      | GLU    | conflict | UNP Q8U338 |
| C     | 110     | LEU      | VAL    | conflict | UNP Q8U338 |
| C     | ?       | -        | SER    | deletion | UNP Q8U338 |
| C     | ?       | -        | LEU    | deletion | UNP Q8U338 |
| C     | ?       | -        | GLY    | deletion | UNP Q8U338 |

- Molecule 2 is a protein called Cas11a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | D     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 856   | 550 | 144 | 160 | 2 |         |       |
| 2   | E     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 860   | 552 | 145 | 161 | 2 |         |       |
| 2   | F     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 856   | 550 | 144 | 160 | 2 |         |       |
| 2   | G     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 856   | 550 | 144 | 160 | 2 |         |       |
| 2   | H     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 856   | 550 | 144 | 160 | 2 |         |       |

- Molecule 3 is a protein called Cas7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | I     | 335      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2597  | 1655 | 450 | 487 | 5 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | J     | 336      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2603  | 1659 | 451 | 488 | 5 |         |       |
| 3   | K     | 336      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2596  | 1656 | 448 | 487 | 5 |         |       |
| 3   | L     | 336      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2597  | 1656 | 448 | 488 | 5 |         |       |
| 3   | M     | 336      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2597  | 1656 | 448 | 488 | 5 |         |       |
| 3   | N     | 321      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2494  | 1595 | 431 | 463 | 5 |         |       |
| 3   | O     | 274      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2134  | 1370 | 364 | 396 | 4 |         |       |

- Molecule 4 is a protein called Cas5a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | P     | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1936  | 1266 | 315 | 349 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| P     | ?       | -        | THR    | deletion | UNP A0A5C0XNV9 |

- Molecule 5 is a RNA chain called crRNA (45-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5   | R     | 45       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 949   | 427 | 166 | 312 | 44 |         |       |

- Molecule 6 is a protein called CRISPR-associated helicase Cas3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | A     | 572      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 4307  | 2752 | 745 | 802 | 8 |         |       |

- Molecule 7 is a protein called CRISPR-associated endonuclease Cas3-HD.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | Q     | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1823  | 1167 | 314 | 329 | 13 |         |       |

- Molecule 8 is a DNA chain called Target strand DNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 8   | S     | 22       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 464   | 217 | 92 | 133 | 22 |         |       |

- Molecule 9 is a DNA chain called Non-Target strand DNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 9   | T     | 8        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 163   | 77 | 31 | 47 | 8 |         |       |

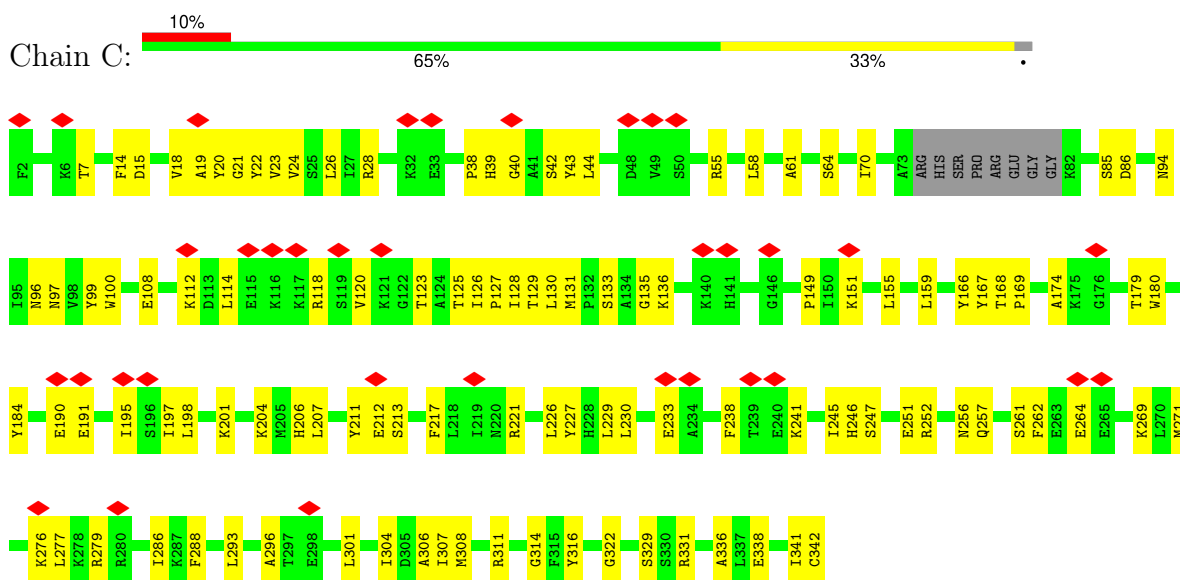
- Molecule 10 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 10  | Q     | 2        | Total | Ni | 0       |
|     |       |          | 2     | 2  |         |

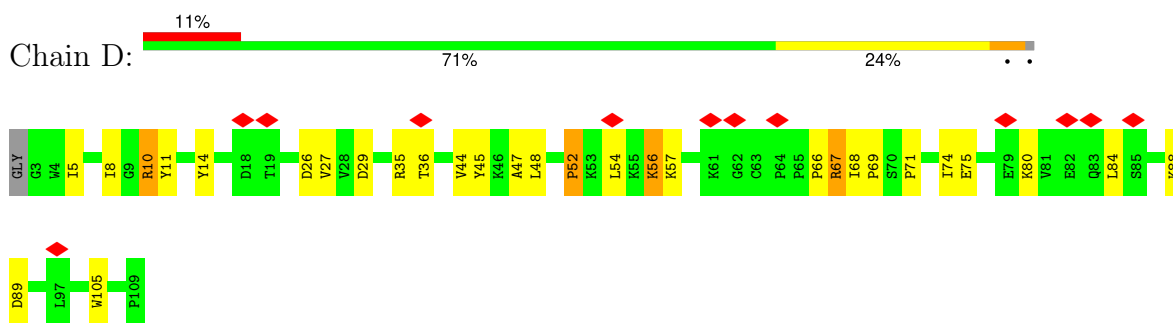
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

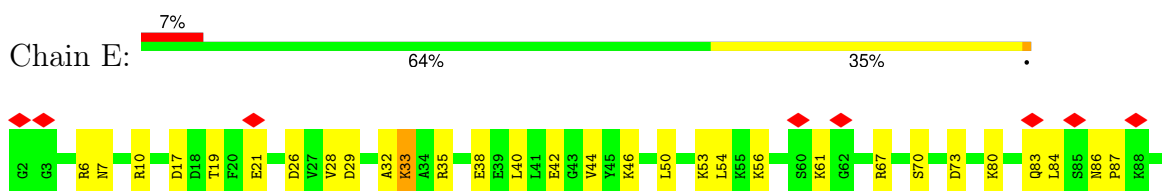
#### • Molecule 1: Cas8a

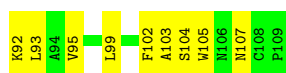


#### • Molecule 2: Cas11a

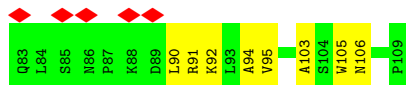
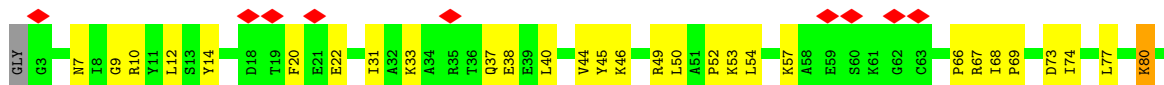


#### • Molecule 2: Cas11a

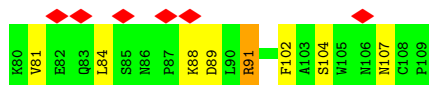
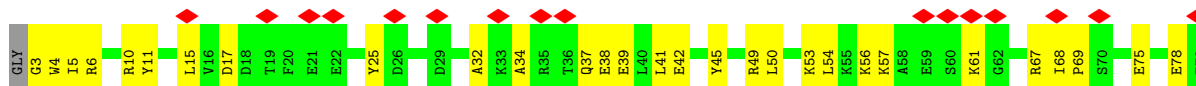




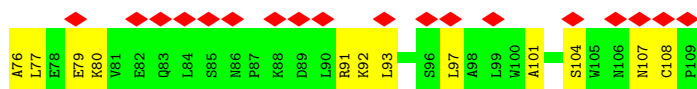
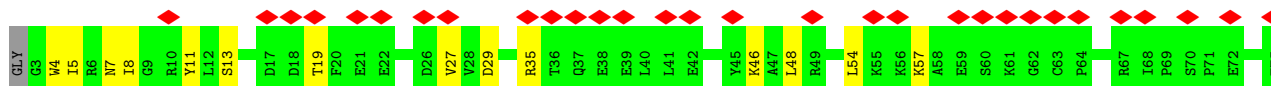
• Molecule 2: Cas11a



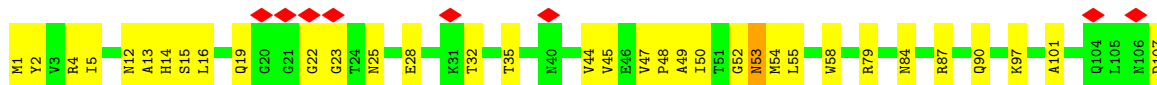
• Molecule 2: Cas11a

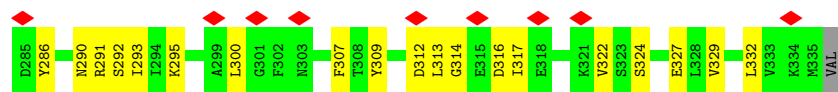


• Molecule 2: Cas11a

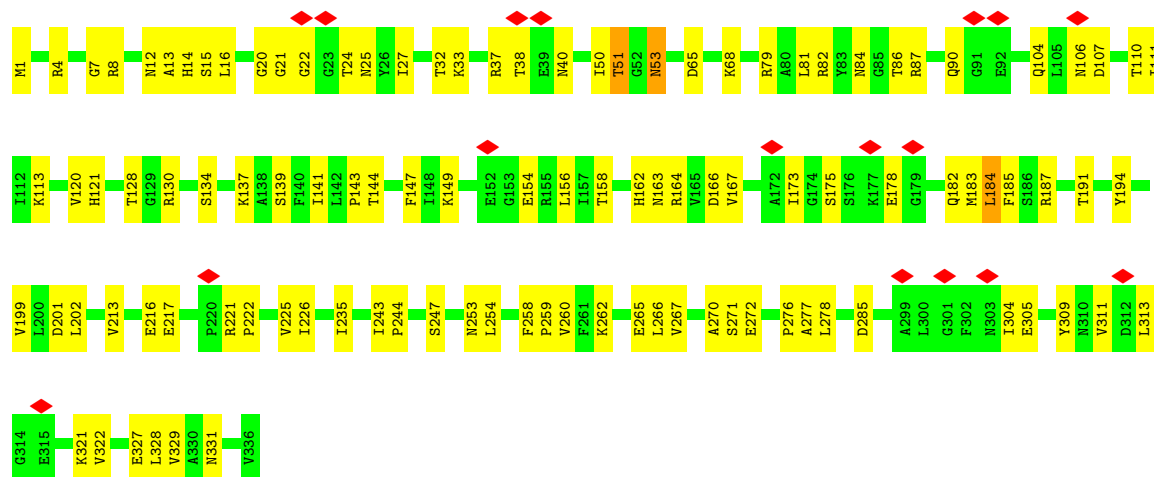


• Molecule 3: Cas7a

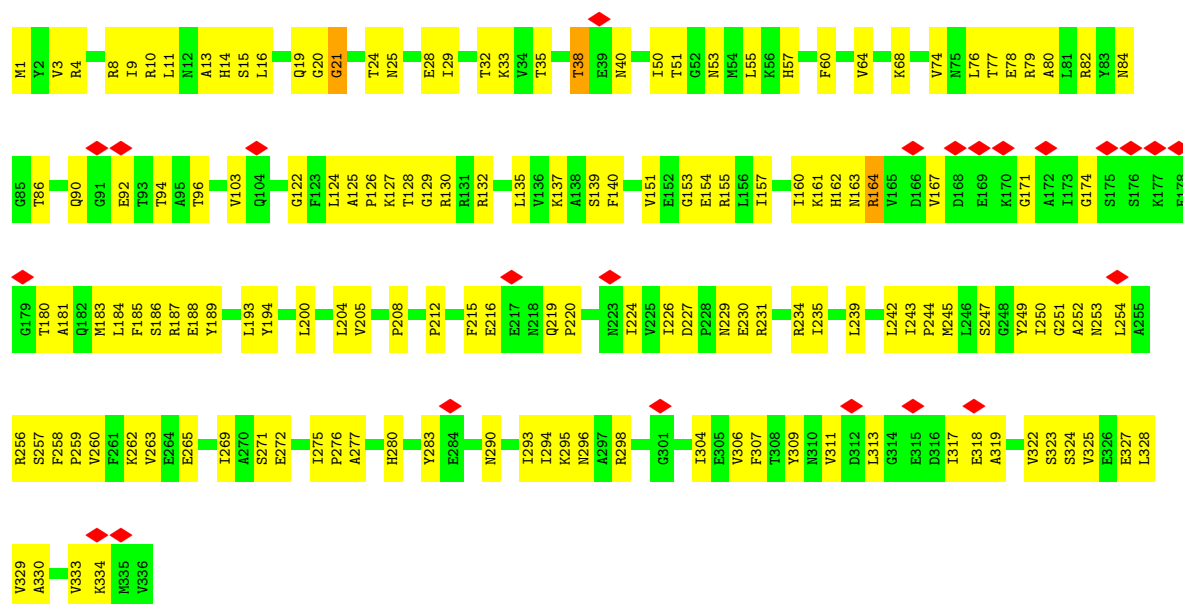




• Molecule 3: Cas7a

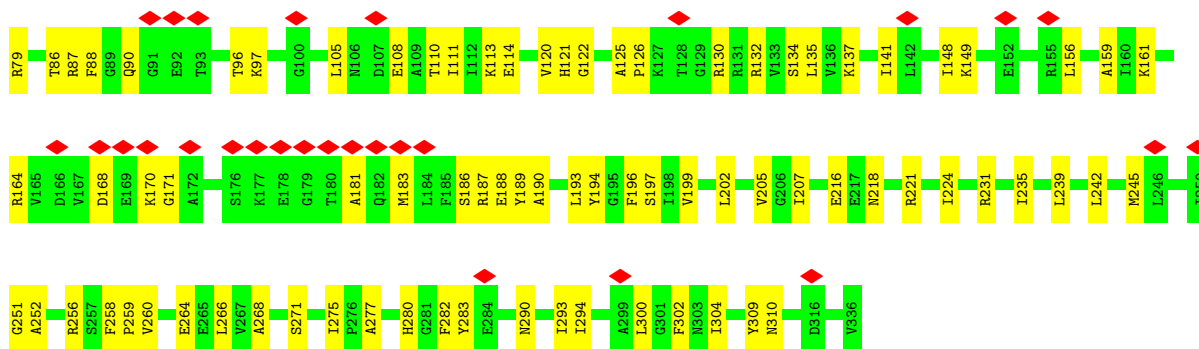


• Molecule 3: Cas7a

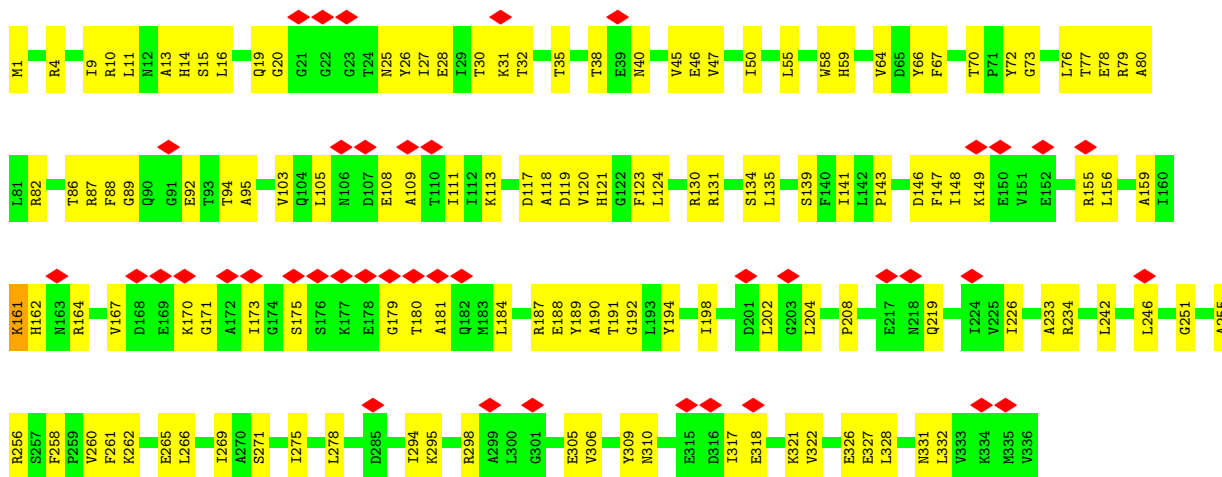


• Molecule 3: Cas7a

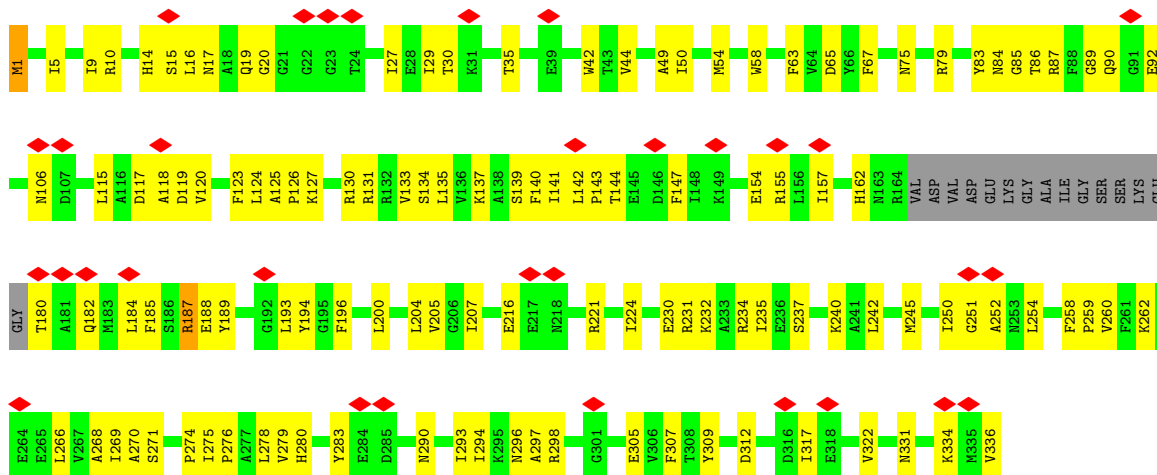




• Molecule 3: Cas7a

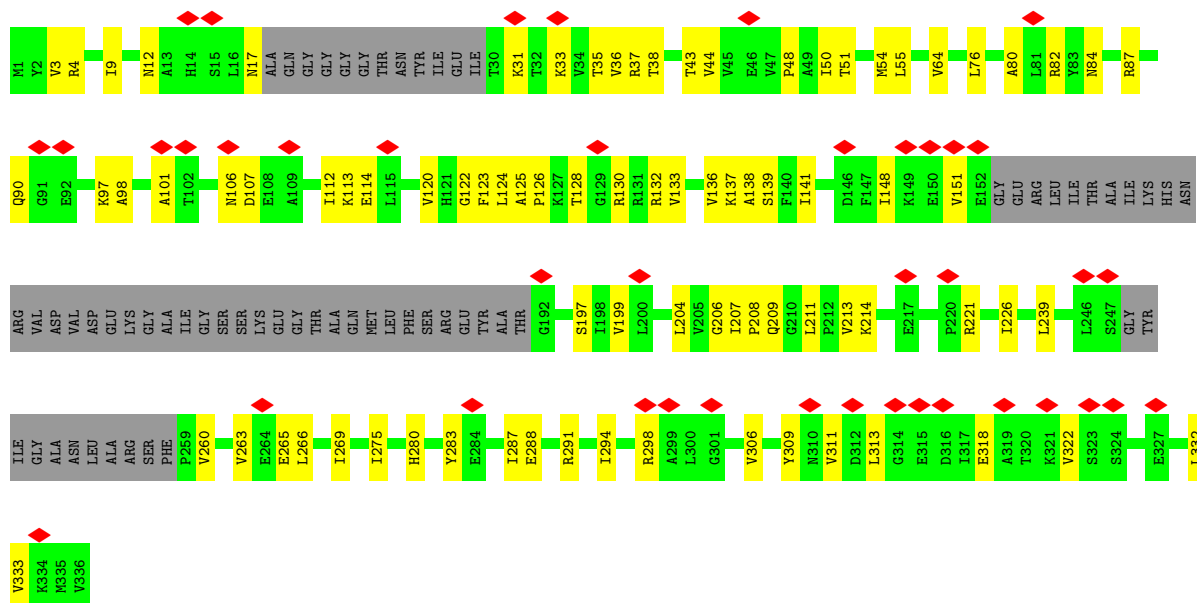


• Molecule 3: Cas7a

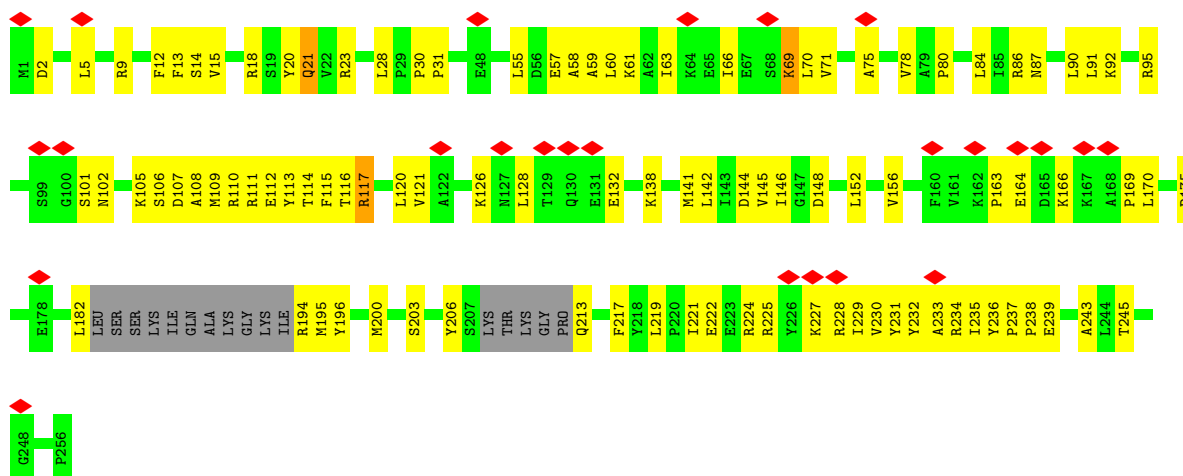


• Molecule 3: Cas7a





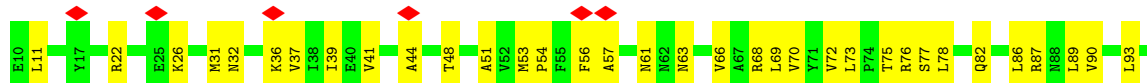
• Molecule 4: Cas5a

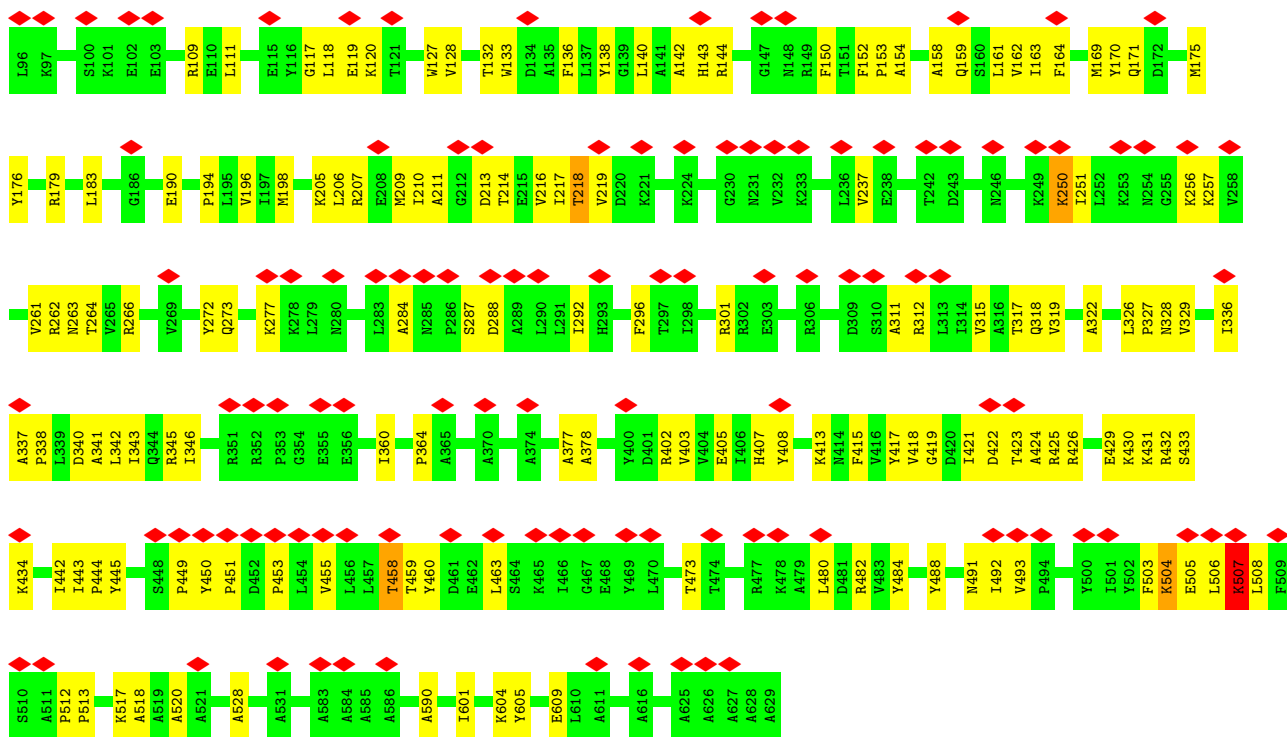


• Molecule 5: crRNA (45-MER)

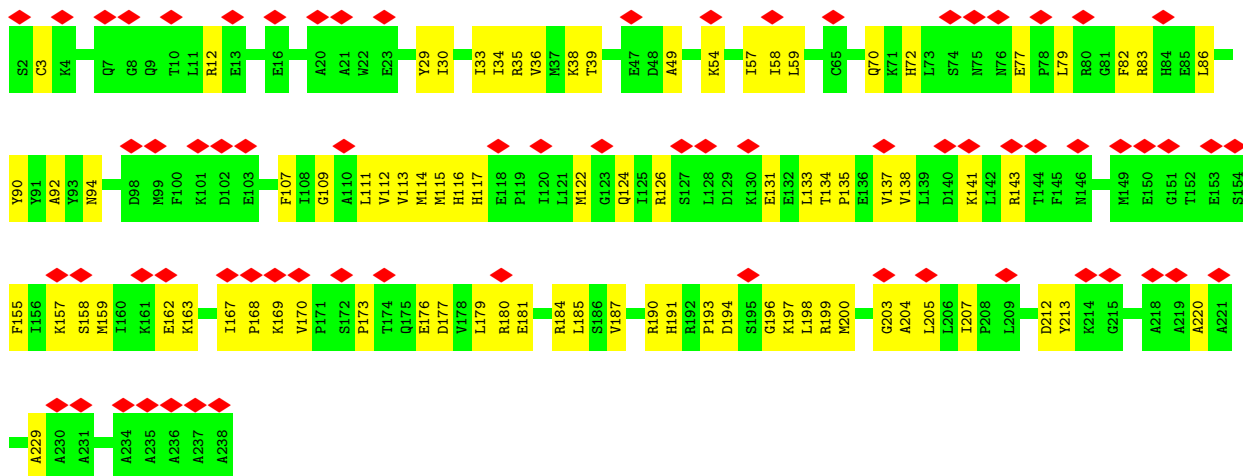


• Molecule 6: CRISPR-associated helicase Cas3

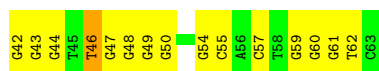
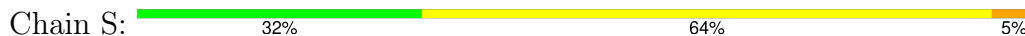




• Molecule 7: CRISPR-associated endonuclease Cas3-HD



• Molecule 8: Target strand DNA



• Molecule 9: Non-Target strand DNA



|     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|
| G17 | A18 | C19 | C20 | C21 | A22 | G23 | T24 |
|-----|-----|-----|-----|-----|-----|-----|-----|

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 13781                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS TALOS                               | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.826                                   | Depositor |
| Minimum map value                    | -0.281                                  | Depositor |
| Average map value                    | -0.001                                  | Depositor |
| Map value standard deviation         | 0.036                                   | Depositor |
| Recommended contour level            | 0.155                                   | Depositor |
| Map size (Å)                         | 372.0, 372.0, 372.0                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.24, 1.24, 1.24                        | Depositor |

## 5 Model quality [i](#)

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

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

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   | C     | 0.25         | 0/2723         | 0.49        | 0/3684         |
| 2   | D     | 0.26         | 0/876          | 0.53        | 0/1188         |
| 2   | E     | 0.26         | 0/880          | 0.52        | 0/1193         |
| 2   | F     | 0.25         | 0/876          | 0.54        | 0/1188         |
| 2   | G     | 0.25         | 0/876          | 0.51        | 0/1188         |
| 2   | H     | 0.25         | 0/876          | 0.52        | 0/1188         |
| 3   | I     | 0.27         | 0/2645         | 0.54        | 0/3583         |
| 3   | J     | 0.29         | 0/2651         | 0.56        | 1/3592 (0.0%)  |
| 3   | K     | 0.27         | 0/2644         | 0.55        | 0/3584         |
| 3   | L     | 0.27         | 0/2645         | 0.53        | 0/3585         |
| 3   | M     | 0.24         | 0/2645         | 0.51        | 0/3585         |
| 3   | N     | 0.25         | 0/2541         | 0.51        | 0/3445         |
| 3   | O     | 0.25         | 0/2173         | 0.49        | 0/2946         |
| 4   | P     | 0.25         | 0/1977         | 0.52        | 0/2673         |
| 5   | R     | 0.37         | 0/1060         | 0.77        | 1/1649 (0.1%)  |
| 6   | A     | 0.25         | 0/4379         | 0.53        | 0/5951         |
| 7   | Q     | 0.26         | 0/1854         | 0.51        | 0/2502         |
| 8   | S     | 0.60         | 1/522 (0.2%)   | 0.82        | 0/807          |
| 9   | T     | 0.34         | 0/182          | 0.81        | 0/278          |
| All | All   | 0.27         | 1/35025 (0.0%) | 0.54        | 2/47809 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 8   | S     | 46  | DT   | O3'-P | 6.04 | 1.68        | 1.61     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 5   | R     | 18  | C    | P-O3'-C3' | 5.36 | 126.14      | 119.70   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | J     | 51  | THR  | CB-CA-C | -5.02 | 98.04       | 111.60   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 2662  | 0        | 2667     | 111     | 0            |
| 2   | D     | 856   | 0        | 860      | 28      | 0            |
| 2   | E     | 860   | 0        | 863      | 28      | 0            |
| 2   | F     | 856   | 0        | 860      | 29      | 0            |
| 2   | G     | 856   | 0        | 860      | 29      | 0            |
| 2   | H     | 856   | 0        | 860      | 24      | 0            |
| 3   | I     | 2597  | 0        | 2628     | 99      | 0            |
| 3   | J     | 2603  | 0        | 2635     | 105     | 0            |
| 3   | K     | 2596  | 0        | 2621     | 127     | 0            |
| 3   | L     | 2597  | 0        | 2624     | 95      | 0            |
| 3   | M     | 2597  | 0        | 2624     | 98      | 0            |
| 3   | N     | 2494  | 0        | 2524     | 95      | 0            |
| 3   | O     | 2134  | 0        | 2168     | 58      | 0            |
| 4   | P     | 1936  | 0        | 2018     | 82      | 0            |
| 5   | R     | 949   | 0        | 481      | 37      | 0            |
| 6   | A     | 4307  | 0        | 4415     | 132     | 0            |
| 7   | Q     | 1823  | 0        | 1891     | 66      | 0            |
| 8   | S     | 464   | 0        | 247      | 53      | 0            |
| 9   | T     | 163   | 0        | 90       | 7       | 0            |
| 10  | Q     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 34208 | 0        | 33936    | 1075    | 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 16.

All (1075) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:136:LYS:NZ   | 8:S:61:DG:N7     | 1.63                     | 1.42              |
| 1:C:128:ILE:HD11 | 8:S:61:DG:OP1    | 1.44                     | 1.16              |
| 3:J:134:SER:HB2  | 5:R:12:G:OP1     | 1.55                     | 1.06              |
| 1:C:97:ASN:ND2   | 9:T:21:DC:H1'    | 1.71                     | 1.03              |
| 3:K:20:GLY:HA3   | 5:R:21:A:H8      | 1.22                     | 1.01              |
| 3:K:254:LEU:HA   | 3:L:137:LYS:HE2  | 1.41                     | 1.00              |
| 3:L:126:PRO:HB2  | 8:S:44:DG:H1'    | 1.38                     | 1.00              |
| 4:P:95:ARG:NH1   | 8:S:60:DG:P      | 2.39                     | 0.96              |
| 3:K:253:ASN:HB3  | 3:K:257:SER:HB3  | 1.52                     | 0.91              |
| 8:S:46:DT:H73    | 8:S:47:DG:H1     | 1.36                     | 0.91              |
| 3:I:22:GLY:HA2   | 8:S:57:DC:H41    | 1.33                     | 0.89              |
| 3:J:90:GLN:HE21  | 8:S:55:DC:H1'    | 1.37                     | 0.88              |
| 3:J:22:GLY:O     | 8:S:48:DG:H2'    | 1.74                     | 0.86              |
| 1:C:136:LYS:CE   | 8:S:61:DG:C8     | 2.61                     | 0.82              |
| 3:I:256:ARG:HH21 | 5:R:12:G:H3'     | 1.45                     | 0.82              |
| 4:P:95:ARG:NH1   | 8:S:60:DG:OP1    | 2.12                     | 0.82              |
| 3:I:22:GLY:HA2   | 8:S:57:DC:N4     | 1.96                     | 0.81              |
| 3:J:14:HIS:HB3   | 3:J:259:PRO:HB3  | 1.63                     | 0.81              |
| 1:C:136:LYS:CE   | 8:S:61:DG:N7     | 2.44                     | 0.80              |
| 3:O:137:LYS:HB2  | 3:O:199:VAL:HB   | 1.62                     | 0.80              |
| 4:P:95:ARG:NH1   | 8:S:60:DG:O5'    | 2.15                     | 0.79              |
| 1:C:136:LYS:HE2  | 8:S:62:DT:H73    | 1.65                     | 0.79              |
| 6:A:434:LYS:HB2  | 7:Q:124:GLN:HB3  | 1.63                     | 0.79              |
| 6:A:425:ARG:HH22 | 7:Q:198:LEU:HD12 | 1.49                     | 0.78              |
| 1:C:97:ASN:ND2   | 9:T:21:DC:C1'    | 2.47                     | 0.78              |
| 3:N:268:ALA:HB3  | 3:N:307:PHE:HB2  | 1.66                     | 0.77              |
| 6:A:449:PRO:HB2  | 6:A:453:PRO:HD3  | 1.66                     | 0.77              |
| 3:K:20:GLY:HA3   | 5:R:21:A:C8      | 2.14                     | 0.77              |
| 3:L:17:ASN:HD22  | 3:L:50:ILE:HB    | 1.49                     | 0.77              |
| 3:N:200:LEU:HD11 | 3:N:242:LEU:HD21 | 1.66                     | 0.77              |
| 3:K:25:ASN:HB3   | 3:K:185:PHE:HA   | 1.67                     | 0.77              |
| 1:C:125:THR:HG21 | 8:S:62:DT:OP1    | 1.85                     | 0.76              |
| 3:N:266:LEU:HB3  | 3:N:309:TYR:HB3  | 1.68                     | 0.76              |
| 3:O:132:ARG:HH12 | 3:O:208:PRO:HA   | 1.49                     | 0.76              |
| 3:K:14:HIS:HB3   | 3:K:259:PRO:HG3  | 1.67                     | 0.76              |
| 1:C:230:LEU:HD21 | 1:C:286:ILE:HG23 | 1.67                     | 0.75              |
| 7:Q:143:ARG:HH22 | 7:Q:179:LEU:HD11 | 1.51                     | 0.75              |
| 1:C:136:LYS:HE2  | 8:S:62:DT:C7     | 2.16                     | 0.75              |
| 3:J:14:HIS:HB2   | 3:J:16:LEU:HG    | 1.68                     | 0.75              |
| 3:K:19:GLN:HG2   | 3:K:28:GLU:HG3   | 1.69                     | 0.74              |
| 6:A:292:ILE:HD12 | 6:A:319:VAL:HB   | 1.70                     | 0.74              |
| 1:C:96:ASN:HD21  | 8:S:61:DG:H1'    | 1.51                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:25:ASN:ND2   | 8:S:47:DG:H1'    | 2.02                     | 0.74              |
| 3:K:10:ARG:NH2   | 3:L:35:THR:O     | 2.21                     | 0.73              |
| 4:P:227:LYS:HG3  | 4:P:228:ARG:HG3  | 1.68                     | 0.73              |
| 1:C:128:ILE:CD1  | 8:S:61:DG:OP1    | 2.31                     | 0.73              |
| 3:L:11:LEU:HB3   | 3:L:14:HIS:HD2   | 1.54                     | 0.72              |
| 3:J:21:GLY:H     | 3:J:24:THR:HB    | 1.53                     | 0.72              |
| 3:M:260:VAL:HG13 | 3:N:280:HIS:HB3  | 1.72                     | 0.72              |
| 3:J:243:ILE:HD11 | 3:J:329:VAL:HG21 | 1.72                     | 0.71              |
| 3:M:19:GLN:HE22  | 3:M:30:THR:HA    | 1.55                     | 0.71              |
| 3:I:35:THR:H     | 4:P:115:PHE:HE1  | 1.37                     | 0.71              |
| 3:L:122:GLY:HA2  | 3:L:132:ARG:HB3  | 1.71                     | 0.71              |
| 6:A:142:ALA:HB3  | 6:A:153:PRO:HG2  | 1.72                     | 0.71              |
| 3:M:70:THR:HG22  | 3:M:72:TYR:H     | 1.56                     | 0.71              |
| 2:D:35:ARG:HG3   | 2:D:36:THR:HG23  | 1.73                     | 0.70              |
| 1:C:128:ILE:HD11 | 8:S:61:DG:P      | 2.31                     | 0.70              |
| 6:A:87:ARG:HE    | 6:A:109:ARG:HA   | 1.56                     | 0.70              |
| 3:K:15:SER:HB3   | 3:K:253:ASN:HD22 | 1.55                     | 0.70              |
| 3:O:266:LEU:HB2  | 3:O:309:TYR:HB3  | 1.73                     | 0.70              |
| 3:K:1:MET:HA     | 3:K:272:GLU:HA   | 1.73                     | 0.70              |
| 3:L:18:ALA:HA    | 3:L:29:ILE:HA    | 1.74                     | 0.69              |
| 3:N:27:ILE:HD13  | 3:N:187:ARG:HG3  | 1.73                     | 0.69              |
| 3:J:1:MET:HA     | 3:J:272:GLU:HA   | 1.73                     | 0.69              |
| 3:N:85:GLY:O     | 3:N:87:ARG:NH1   | 2.25                     | 0.69              |
| 3:I:263:VAL:HG21 | 3:I:266:LEU:HD23 | 1.73                     | 0.69              |
| 3:J:7:GLY:HA3    | 3:J:266:LEU:HD13 | 1.73                     | 0.69              |
| 3:K:9:ILE:HG22   | 3:K:263:VAL:HA   | 1.73                     | 0.69              |
| 3:K:162:HIS:HE1  | 3:L:51:THR:HG21  | 1.58                     | 0.69              |
| 4:P:55:LEU:HD21  | 5:R:1:A:H2'      | 1.76                     | 0.68              |
| 3:I:32:THR:HB    | 4:P:87:ASN:HD21  | 1.59                     | 0.68              |
| 3:M:4:ARG:NH1    | 3:M:275:ILE:O    | 2.23                     | 0.68              |
| 3:J:134:SER:CB   | 5:R:12:G:OP1     | 2.38                     | 0.67              |
| 3:N:1:MET:HA     | 3:N:271:SER:O    | 1.92                     | 0.67              |
| 1:C:70:ILE:HG22  | 6:A:179:ARG:HH12 | 1.60                     | 0.67              |
| 3:J:202:LEU:HD12 | 3:J:235:ILE:HG12 | 1.77                     | 0.67              |
| 6:A:504:LYS:HG3  | 6:A:505:GLU:HG3  | 1.75                     | 0.67              |
| 7:Q:90:TYR:HE2   | 7:Q:173:PRO:HG3  | 1.60                     | 0.67              |
| 1:C:136:LYS:CE   | 8:S:62:DT:H73    | 2.24                     | 0.67              |
| 3:J:22:GLY:O     | 8:S:48:DG:C2'    | 2.43                     | 0.67              |
| 3:K:155:ARG:NH1  | 3:K:157:ILE:O    | 2.28                     | 0.67              |
| 4:P:70:LEU:HD21  | 4:P:75:ALA:HA    | 1.76                     | 0.67              |
| 3:J:265:GLU:HA   | 3:J:309:TYR:O    | 1.95                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:90:GLN:NE2   | 8:S:49:DG:H2'    | 2.09                     | 0.66              |
| 6:A:317:THR:OG1  | 6:A:318:GLN:OE1  | 2.12                     | 0.66              |
| 2:H:54:LEU:HD23  | 2:H:57:LYS:HZ3   | 1.58                     | 0.66              |
| 3:I:158:THR:HG21 | 3:J:32:THR:HG23  | 1.77                     | 0.66              |
| 3:I:291:ARG:NH2  | 3:I:316:ASP:OD1  | 2.28                     | 0.66              |
| 3:J:111:ILE:HD11 | 3:J:130:ARG:HH22 | 1.61                     | 0.66              |
| 3:M:131:ARG:HG3  | 5:R:29:A:H1'     | 1.78                     | 0.66              |
| 2:D:71:PRO:HD3   | 2:E:104:SER:H    | 1.60                     | 0.66              |
| 3:N:17:ASN:H     | 3:N:252:ALA:HB3  | 1.60                     | 0.66              |
| 5:R:32:G:H2'     | 5:R:34:U:H4'     | 1.77                     | 0.66              |
| 2:H:5:ILE:HD12   | 2:H:8:ILE:HD11   | 1.78                     | 0.65              |
| 3:L:65:ASP:HA    | 3:L:68:LYS:HE2   | 1.77                     | 0.65              |
| 6:A:37:VAL:HB    | 6:A:196:VAL:HG12 | 1.77                     | 0.65              |
| 4:P:14:SER:OG    | 4:P:148:ASP:OD1  | 2.14                     | 0.65              |
| 3:L:4:ARG:HG3    | 3:L:199:VAL:HG23 | 1.78                     | 0.65              |
| 3:O:298:ARG:HH12 | 3:O:318:GLU:H    | 1.43                     | 0.65              |
| 3:M:47:VAL:HG21  | 3:M:143:PRO:HG3  | 1.77                     | 0.65              |
| 3:M:95:ALA:HB3   | 3:M:103:VAL:HB   | 1.78                     | 0.65              |
| 3:M:164:ARG:NH2  | 3:M:181:ALA:O    | 2.30                     | 0.65              |
| 2:G:15:LEU:HB2   | 2:G:54:LEU:HD12  | 1.78                     | 0.65              |
| 3:J:244:PRO:HA   | 3:J:247:SER:HB3  | 1.78                     | 0.65              |
| 7:Q:181:GLU:HA   | 7:Q:184:ARG:HG2  | 1.78                     | 0.65              |
| 3:J:65:ASP:HA    | 3:J:68:LYS:HE2   | 1.78                     | 0.65              |
| 6:A:207:ARG:HD2  | 6:A:216:VAL:HG11 | 1.78                     | 0.65              |
| 7:Q:30:ILE:HA    | 7:Q:33:ILE:HG22  | 1.79                     | 0.65              |
| 3:J:271:SER:HB3  | 3:J:304:ILE:HA   | 1.79                     | 0.64              |
| 3:O:4:ARG:NH1    | 3:O:275:ILE:O    | 2.30                     | 0.64              |
| 1:C:28:ARG:HG2   | 7:Q:193:PRO:HB3  | 1.78                     | 0.64              |
| 1:C:135:GLY:HA2  | 8:S:61:DG:OP1    | 1.97                     | 0.64              |
| 2:G:68:ILE:HB    | 2:H:104:SER:HB3  | 1.79                     | 0.64              |
| 3:J:267:VAL:HG13 | 3:J:278:LEU:HD13 | 1.79                     | 0.64              |
| 3:K:157:ILE:HD12 | 3:K:188:GLU:HG3  | 1.80                     | 0.64              |
| 3:M:58:TRP:NE1   | 3:M:251:GLY:O    | 2.30                     | 0.64              |
| 1:C:304:ILE:HD12 | 1:C:307:ILE:HD12 | 1.80                     | 0.64              |
| 3:O:3:VAL:HG11   | 3:O:332:LEU:HD21 | 1.80                     | 0.64              |
| 3:M:50:ILE:HB    | 3:M:141:ILE:HB   | 1.79                     | 0.64              |
| 4:P:194:ARG:HB2  | 4:P:235:ILE:HD11 | 1.80                     | 0.64              |
| 7:Q:3:CYS:SG     | 7:Q:70:GLN:NE2   | 2.71                     | 0.64              |
| 1:C:211:TYR:CE1  | 9:T:24:DT:H4'    | 2.33                     | 0.64              |
| 3:I:5:ILE:HD11   | 3:I:266:LEU:HD13 | 1.80                     | 0.63              |
| 4:P:128:LEU:HD12 | 4:P:132:GLU:HG3  | 1.79                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:58:TRP:NE1   | 3:L:251:GLY:O    | 2.26                     | 0.63              |
| 3:O:50:ILE:HB    | 3:O:141:ILE:HB   | 1.81                     | 0.63              |
| 3:N:258:PHE:CE2  | 3:O:137:LYS:HB3  | 2.34                     | 0.63              |
| 2:E:7:ASN:HD21   | 2:E:70:SER:H     | 1.47                     | 0.63              |
| 3:L:10:ARG:NH2   | 3:M:35:THR:O     | 2.32                     | 0.63              |
| 3:N:50:ILE:HB    | 3:N:141:ILE:HB   | 1.81                     | 0.63              |
| 3:I:16:LEU:HG    | 3:I:251:GLY:HA3  | 1.81                     | 0.62              |
| 3:I:132:ARG:O    | 5:R:5:A:O2'      | 2.16                     | 0.62              |
| 3:J:104:GLN:NE2  | 3:J:106:ASN:OD1  | 2.32                     | 0.62              |
| 4:P:169:PRO:HA   | 4:P:239:GLU:HA   | 1.80                     | 0.62              |
| 1:C:184:TYR:HB3  | 1:C:245:ILE:HD11 | 1.81                     | 0.62              |
| 3:I:143:PRO:HA   | 3:I:194:TYR:HA   | 1.81                     | 0.62              |
| 1:C:126:ILE:HD12 | 1:C:127:PRO:HD2  | 1.81                     | 0.62              |
| 1:C:246:HIS:ND1  | 1:C:264:GLU:OE1  | 2.32                     | 0.62              |
| 2:D:84:LEU:HD12  | 2:D:89:ASP:HB3   | 1.81                     | 0.62              |
| 3:O:287:ILE:HD11 | 3:O:313:LEU:HA   | 1.81                     | 0.62              |
| 1:C:136:LYS:NZ   | 8:S:61:DG:C8     | 2.51                     | 0.62              |
| 3:L:8:ARG:NH2    | 3:L:283:TYR:O    | 2.32                     | 0.62              |
| 3:M:246:LEU:HA   | 3:M:261:PHE:HE2  | 1.62                     | 0.62              |
| 1:C:276:LYS:HA   | 1:C:279:ARG:HE   | 1.64                     | 0.62              |
| 3:N:154:GLU:O    | 3:O:33:LYS:NZ    | 2.33                     | 0.62              |
| 3:K:19:GLN:HG3   | 3:K:20:GLY:N     | 2.14                     | 0.62              |
| 3:L:171:GLY:O    | 3:N:130:ARG:NH2  | 2.32                     | 0.62              |
| 4:P:78:VAL:HG12  | 4:P:121:VAL:HG22 | 1.80                     | 0.62              |
| 3:J:327:GLU:O    | 3:J:331:ASN:ND2  | 2.32                     | 0.62              |
| 3:J:90:GLN:NE2   | 8:S:55:DC:H1'    | 2.14                     | 0.62              |
| 3:M:25:ASN:HB3   | 3:M:184:LEU:HB3  | 1.80                     | 0.62              |
| 3:N:131:ARG:NH2  | 5:R:34:U:O2'     | 2.33                     | 0.62              |
| 1:C:28:ARG:HA    | 7:Q:193:PRO:HG3  | 1.81                     | 0.62              |
| 3:M:38:THR:OG1   | 3:M:40:ASN:OD1   | 2.18                     | 0.62              |
| 7:Q:134:THR:HB   | 7:Q:137:VAL:HG22 | 1.82                     | 0.62              |
| 1:C:97:ASN:HD22  | 9:T:21:DC:H1'    | 1.60                     | 0.62              |
| 2:F:68:ILE:HD12  | 2:F:69:PRO:HD2   | 1.82                     | 0.62              |
| 3:M:327:GLU:O    | 3:M:331:ASN:ND2  | 2.33                     | 0.62              |
| 6:A:263:ASN:ND2  | 6:A:336:ILE:O    | 2.32                     | 0.62              |
| 1:C:135:GLY:HA2  | 8:S:61:DG:P      | 2.40                     | 0.61              |
| 2:F:49:ARG:HH21  | 2:G:102:PHE:HD2  | 1.48                     | 0.61              |
| 3:I:324:SER:OG   | 3:I:327:GLU:OE1  | 2.14                     | 0.61              |
| 1:C:108:GLU:OE1  | 1:C:112:LYS:NZ   | 2.33                     | 0.61              |
| 3:O:265:GLU:HG2  | 3:O:311:VAL:HB   | 1.81                     | 0.61              |
| 3:I:165:VAL:O    | 3:J:86:THR:OG1   | 2.19                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:255:ALA:HA   | 3:J:137:LYS:HA   | 1.82                     | 0.61              |
| 3:N:17:ASN:HD21  | 3:N:50:ILE:HG23  | 1.65                     | 0.61              |
| 6:A:143:HIS:ND1  | 6:A:429:GLU:OE2  | 2.33                     | 0.61              |
| 3:J:110:THR:HA   | 3:J:113:LYS:HG2  | 1.81                     | 0.61              |
| 3:K:161:LYS:HG2  | 3:K:186:SER:HB3  | 1.83                     | 0.61              |
| 2:H:107:ASN:OD1  | 2:H:108:CYS:N    | 2.34                     | 0.61              |
| 3:K:38:THR:HG22  | 3:K:40:ASN:H     | 1.66                     | 0.61              |
| 6:A:73:LEU:HD11  | 6:A:82:GLN:HG3   | 1.82                     | 0.61              |
| 3:J:183:MET:HA   | 8:S:46:DT:H2''   | 1.82                     | 0.61              |
| 3:K:90:GLN:OE1   | 8:S:49:DG:O3'    | 2.19                     | 0.61              |
| 3:K:249:TYR:OH   | 3:L:4:ARG:NH2    | 2.33                     | 0.61              |
| 4:P:28:LEU:HD12  | 4:P:219:LEU:HD12 | 1.82                     | 0.61              |
| 8:S:46:DT:C7     | 8:S:47:DG:H1     | 2.10                     | 0.61              |
| 1:C:96:ASN:ND2   | 8:S:61:DG:H1'    | 2.15                     | 0.61              |
| 4:P:141:MET:HG2  | 4:P:142:LEU:H    | 1.66                     | 0.61              |
| 4:P:225:ARG:HB2  | 4:P:230:VAL:HG12 | 1.83                     | 0.60              |
| 6:A:433:SER:H    | 7:Q:126:ARG:HE   | 1.49                     | 0.60              |
| 3:M:161:LYS:HE3  | 3:N:19:GLN:HB3   | 1.82                     | 0.60              |
| 3:N:35:THR:HG22  | 3:N:44:VAL:HG22  | 1.82                     | 0.60              |
| 3:L:264:GLU:O    | 3:L:310:ASN:ND2  | 2.34                     | 0.60              |
| 3:M:19:GLN:NE2   | 3:M:30:THR:HA    | 2.16                     | 0.60              |
| 7:Q:82:PHE:HB2   | 7:Q:141:LYS:HZ3  | 1.65                     | 0.60              |
| 3:N:141:ILE:HG22 | 3:N:194:TYR:HB3  | 1.83                     | 0.60              |
| 4:P:175:PRO:HA   | 4:P:217:PHE:HA   | 1.82                     | 0.60              |
| 3:J:38:THR:OG1   | 3:J:40:ASN:ND2   | 2.35                     | 0.60              |
| 3:K:160:ILE:HG23 | 3:L:30:THR:HG21  | 1.83                     | 0.60              |
| 3:L:16:LEU:HB2   | 3:L:50:ILE:HG21  | 1.83                     | 0.60              |
| 6:A:73:LEU:HD23  | 6:A:77:SER:HB3   | 1.82                     | 0.60              |
| 1:C:136:LYS:HE2  | 8:S:61:DG:C8     | 2.36                     | 0.60              |
| 2:H:7:ASN:OD1    | 2:H:8:ILE:N      | 2.35                     | 0.60              |
| 3:K:239:LEU:HB3  | 3:K:329:VAL:HB   | 1.82                     | 0.60              |
| 3:N:205:VAL:O    | 3:N:231:ARG:NH1  | 2.35                     | 0.60              |
| 2:E:35:ARG:NH1   | 3:J:154:GLU:OE1  | 2.33                     | 0.60              |
| 3:I:291:ARG:NH1  | 3:I:313:LEU:O    | 2.35                     | 0.60              |
| 3:K:307:PHE:HD2  | 3:K:328:LEU:HG   | 1.66                     | 0.60              |
| 4:P:95:ARG:CZ    | 8:S:60:DG:P      | 2.89                     | 0.60              |
| 2:D:68:ILE:HD12  | 2:D:69:PRO:HD2   | 1.82                     | 0.59              |
| 3:N:232:LYS:HE2  | 3:N:336:VAL:HG22 | 1.84                     | 0.59              |
| 6:A:257:LYS:HE3  | 6:A:311:ALA:HA   | 1.84                     | 0.59              |
| 6:A:272:TYR:HB2  | 6:A:315:VAL:HG11 | 1.83                     | 0.59              |
| 1:C:221:ARG:HH12 | 1:C:262:PHE:HA   | 1.67                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:55:LEU:HD11  | 3:M:141:ILE:HD11 | 1.85                     | 0.59              |
| 3:I:266:LEU:HG   | 3:I:309:TYR:HB3  | 1.85                     | 0.59              |
| 3:K:90:GLN:HE22  | 8:S:49:DG:H2'    | 1.67                     | 0.59              |
| 1:C:221:ARG:HD2  | 1:C:247:SER:HB2  | 1.83                     | 0.59              |
| 3:I:52:GLY:H     | 3:I:140:PHE:HD1  | 1.50                     | 0.59              |
| 3:N:144:THR:HG23 | 3:N:147:PHE:H    | 1.67                     | 0.59              |
| 3:N:298:ARG:HH22 | 3:N:317:ILE:HG12 | 1.67                     | 0.59              |
| 2:H:13:SER:HB3   | 2:H:101:ALA:HA   | 1.85                     | 0.59              |
| 3:K:151:VAL:HG23 | 3:K:153:GLY:H    | 1.67                     | 0.59              |
| 3:K:260:VAL:HA   | 3:L:280:HIS:HB3  | 1.84                     | 0.59              |
| 3:L:137:LYS:HB3  | 3:L:199:VAL:HG13 | 1.83                     | 0.59              |
| 3:N:258:PHE:HE2  | 3:O:137:LYS:HB3  | 1.68                     | 0.59              |
| 6:A:118:LEU:HD23 | 6:A:480:LEU:HA   | 1.83                     | 0.59              |
| 3:M:266:LEU:HB2  | 3:M:309:TYR:HB3  | 1.85                     | 0.59              |
| 6:A:262:ARG:H    | 6:A:317:THR:HA   | 1.65                     | 0.59              |
| 3:K:135:LEU:HD21 | 3:K:204:LEU:HB2  | 1.84                     | 0.59              |
| 3:L:11:LEU:HB3   | 3:L:14:HIS:CD2   | 2.38                     | 0.59              |
| 3:L:20:GLY:HA2   | 3:L:27:ILE:HA    | 1.85                     | 0.59              |
| 3:L:125:ALA:HB3  | 3:L:130:ARG:HB2  | 1.84                     | 0.59              |
| 1:C:22:TYR:HE1   | 1:C:159:LEU:HD13 | 1.67                     | 0.58              |
| 2:G:50:LEU:HD13  | 2:G:53:LYS:HG3   | 1.85                     | 0.58              |
| 3:I:286:TYR:O    | 3:I:290:ASN:ND2  | 2.36                     | 0.58              |
| 3:I:307:PHE:HB3  | 3:I:322:VAL:HG21 | 1.85                     | 0.58              |
| 3:K:162:HIS:HB2  | 3:K:185:PHE:CZ   | 2.38                     | 0.58              |
| 3:M:13:ALA:HB1   | 3:N:140:PHE:HD2  | 1.68                     | 0.58              |
| 3:M:119:ASP:OD2  | 3:M:234:ARG:NH1  | 2.35                     | 0.58              |
| 3:I:229:ASN:OD1  | 3:I:230:GLU:N    | 2.36                     | 0.58              |
| 3:M:67:PHE:CE2   | 3:M:73:GLY:HA2   | 2.38                     | 0.58              |
| 5:R:41:A:O2'     | 5:R:42:G:N2      | 2.34                     | 0.58              |
| 6:A:183:LEU:HD11 | 6:A:421:ILE:HD11 | 1.85                     | 0.58              |
| 7:Q:34:ILE:HD11  | 7:Q:49:ALA:HB2   | 1.86                     | 0.58              |
| 3:J:25:ASN:HD22  | 8:S:47:DG:H1'    | 1.67                     | 0.58              |
| 3:K:125:ALA:O    | 3:K:129:GLY:N    | 2.35                     | 0.58              |
| 3:K:247:SER:OG   | 3:L:277:ALA:O    | 2.22                     | 0.58              |
| 3:L:64:VAL:HG23  | 3:L:76:LEU:HD21  | 1.85                     | 0.58              |
| 3:O:9:ILE:HG22   | 3:O:263:VAL:HA   | 1.85                     | 0.58              |
| 3:K:8:ARG:NH2    | 3:K:283:TYR:O    | 2.37                     | 0.58              |
| 3:I:262:LYS:NZ   | 3:J:285:ASP:OD1  | 2.37                     | 0.58              |
| 4:P:30:PRO:HA    | 4:P:200:MET:HE1  | 1.85                     | 0.58              |
| 4:P:221:ILE:HG23 | 4:P:232:TYR:HB3  | 1.85                     | 0.58              |
| 4:P:222:GLU:O    | 4:P:233:ALA:N    | 2.36                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:311:ARG:HD3  | 3:I:155:ARG:HA   | 1.86                     | 0.58              |
| 3:N:278:LEU:HD12 | 3:N:279:VAL:H    | 1.69                     | 0.58              |
| 3:O:17:ASN:ND2   | 5:R:45:G:OP2     | 2.37                     | 0.58              |
| 4:P:92:LYS:HD2   | 4:P:106:SER:HB2  | 1.86                     | 0.58              |
| 6:A:211:ALA:HB1  | 6:A:214:THR:HB   | 1.85                     | 0.58              |
| 2:F:77:LEU:HG    | 2:F:80:LYS:HE3   | 1.86                     | 0.58              |
| 2:H:4:TRP:HH2    | 2:H:77:LEU:HB2   | 1.68                     | 0.58              |
| 3:I:45:VAL:HG11  | 3:I:148:ILE:HD12 | 1.85                     | 0.58              |
| 6:A:127:TRP:HE1  | 7:Q:229:ALA:HA   | 1.69                     | 0.57              |
| 3:L:216:GLU:OE2  | 3:L:221:ARG:NH1  | 2.37                     | 0.57              |
| 4:P:111:ARG:NE   | 4:P:113:TYR:OH   | 2.37                     | 0.57              |
| 3:J:141:ILE:HG22 | 3:J:194:TYR:HB3  | 1.86                     | 0.57              |
| 3:L:90:GLN:OE1   | 8:S:43:DG:H1'    | 2.04                     | 0.57              |
| 2:G:32:ALA:O     | 2:G:91:ARG:NH1   | 2.37                     | 0.57              |
| 3:J:38:THR:O     | 3:J:40:ASN:ND2   | 2.37                     | 0.57              |
| 3:N:207:ILE:HD11 | 3:N:224:ILE:HD13 | 1.87                     | 0.57              |
| 3:J:20:GLY:HA3   | 3:J:27:ILE:HG23  | 1.86                     | 0.57              |
| 3:J:166:ASP:HA   | 3:K:84:ASN:HD21  | 1.70                     | 0.57              |
| 3:K:229:ASN:OD1  | 3:K:230:GLU:N    | 2.38                     | 0.57              |
| 1:C:207:LEU:HD23 | 6:A:418:VAL:HG11 | 1.86                     | 0.57              |
| 2:D:48:LEU:HG    | 2:E:102:PHE:HB2  | 1.87                     | 0.57              |
| 3:I:97:LYS:NZ    | 3:I:114:GLU:OE1  | 2.38                     | 0.57              |
| 3:O:55:LEU:HD11  | 3:O:138:ALA:HB1  | 1.86                     | 0.57              |
| 6:A:76:ARG:HD3   | 6:A:319:VAL:HG22 | 1.86                     | 0.57              |
| 6:A:284:ALA:HA   | 6:A:288:ASP:HB2  | 1.87                     | 0.57              |
| 1:C:94:ASN:HA    | 1:C:129:THR:HG21 | 1.87                     | 0.57              |
| 3:K:94:THR:OG1   | 3:K:103:VAL:O    | 2.23                     | 0.57              |
| 6:A:117:GLY:O    | 6:A:144:ARG:NH2  | 2.38                     | 0.57              |
| 1:C:7:THR:HG21   | 1:C:19:ALA:HB2   | 1.86                     | 0.57              |
| 2:F:10:ARG:NE    | 2:F:14:TYR:OH    | 2.37                     | 0.57              |
| 3:L:111:ILE:HG13 | 3:L:130:ARG:HH12 | 1.68                     | 0.57              |
| 3:M:164:ARG:HD2  | 3:N:86:THR:HB    | 1.87                     | 0.57              |
| 1:C:97:ASN:HD22  | 9:T:21:DC:C1'    | 2.15                     | 0.56              |
| 2:E:21:GLU:OE1   | 2:E:61:LYS:NZ    | 2.36                     | 0.56              |
| 2:H:19:THR:OG1   | 2:H:107:ASN:ND2  | 2.28                     | 0.56              |
| 3:I:2:TYR:HD1    | 3:I:4:ARG:HH12   | 1.52                     | 0.56              |
| 3:I:44:VAL:HG22  | 4:P:229:ILE:HG21 | 1.88                     | 0.56              |
| 3:N:17:ASN:OD1   | 3:N:54:MET:HG3   | 2.06                     | 0.56              |
| 3:N:331:ASN:HA   | 3:N:334:LYS:HE2  | 1.86                     | 0.56              |
| 6:A:22:ARG:NH1   | 6:A:218:THR:O    | 2.38                     | 0.56              |
| 6:A:132:THR:O    | 6:A:136:PHE:N    | 2.37                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:54:LEU:HB3   | 2:D:66:PRO:HG3   | 1.87                     | 0.56              |
| 3:O:132:ARG:NH1  | 3:O:209:GLN:OE1  | 2.38                     | 0.56              |
| 6:A:68:ARG:HH22  | 6:A:159:GLN:HE21 | 1.53                     | 0.56              |
| 6:A:426:ARG:HE   | 7:Q:190:ARG:HD3  | 1.70                     | 0.56              |
| 3:L:97:LYS:NZ    | 3:L:114:GLU:O    | 2.38                     | 0.56              |
| 7:Q:33:ILE:HD11  | 7:Q:205:LEU:HD22 | 1.87                     | 0.56              |
| 1:C:14:PHE:HB2   | 1:C:131:MET:HG3  | 1.88                     | 0.56              |
| 3:K:164:ARG:HD3  | 3:K:181:ALA:HB1  | 1.88                     | 0.56              |
| 3:O:239:LEU:HD22 | 3:O:333:VAL:HB   | 1.87                     | 0.56              |
| 4:P:107:ASP:HB2  | 4:P:109:MET:HE1  | 1.87                     | 0.56              |
| 1:C:338:GLU:HA   | 1:C:341:ILE:HB   | 1.88                     | 0.56              |
| 3:M:26:TYR:CE2   | 3:M:28:GLU:HB3   | 2.41                     | 0.56              |
| 3:M:88:PHE:HE1   | 3:M:95:ALA:HB2   | 1.70                     | 0.56              |
| 4:P:170:LEU:HB3  | 4:P:237:PRO:HG2  | 1.86                     | 0.56              |
| 1:C:168:THR:OG1  | 1:C:184:TYR:O    | 2.22                     | 0.56              |
| 3:L:53:ASN:ND2   | 5:R:27:U:OP2     | 2.38                     | 0.56              |
| 6:A:257:LYS:NZ   | 6:A:328:ASN:O    | 2.39                     | 0.56              |
| 3:J:37:ARG:NH1   | 3:J:40:ASN:O     | 2.39                     | 0.56              |
| 4:P:80:PRO:O     | 4:P:234:ARG:NH2  | 2.39                     | 0.56              |
| 6:A:140:LEU:HA   | 6:A:154:ALA:HB2  | 1.86                     | 0.55              |
| 3:I:48:PRO:HG3   | 3:I:157:ILE:HD11 | 1.87                     | 0.55              |
| 3:I:162:HIS:HB2  | 3:I:185:PHE:CZ   | 2.41                     | 0.55              |
| 3:M:45:VAL:HG11  | 3:M:148:ILE:HG21 | 1.88                     | 0.55              |
| 6:A:403:VAL:HG22 | 6:A:407:HIS:HD1  | 1.71                     | 0.55              |
| 7:Q:82:PHE:HD1   | 7:Q:141:LYS:HB3  | 1.72                     | 0.55              |
| 1:C:331:ARG:HD2  | 2:D:105:TRP:HA   | 1.87                     | 0.55              |
| 2:G:42:GLU:HG3   | 2:H:91:ARG:HH21  | 1.72                     | 0.55              |
| 3:L:16:LEU:HD21  | 3:L:259:PRO:HG3  | 1.87                     | 0.55              |
| 3:I:207:ILE:HD11 | 3:I:224:ILE:HG12 | 1.88                     | 0.55              |
| 3:I:254:LEU:HB3  | 3:J:137:LYS:HD3  | 1.87                     | 0.55              |
| 7:Q:113:VAL:O    | 7:Q:116:HIS:NE2  | 2.39                     | 0.55              |
| 3:M:269:ILE:HD13 | 3:M:278:LEU:HD11 | 1.88                     | 0.55              |
| 3:M:294:ILE:HD13 | 3:M:306:VAL:HG21 | 1.88                     | 0.55              |
| 6:A:273:GLN:O    | 6:A:277:LYS:NZ   | 2.40                     | 0.55              |
| 3:N:14:HIS:HB3   | 3:N:259:PRO:HB3  | 1.89                     | 0.55              |
| 6:A:69:LEU:HB3   | 6:A:128:VAL:HG23 | 1.88                     | 0.55              |
| 3:L:231:ARG:O    | 3:L:235:ILE:HG12 | 2.07                     | 0.55              |
| 3:O:123:PHE:HE1  | 3:O:130:ARG:HB3  | 1.71                     | 0.55              |
| 3:K:154:GLU:O    | 3:K:155:ARG:HG3  | 2.05                     | 0.55              |
| 3:L:16:LEU:HD22  | 3:L:251:GLY:HA3  | 1.89                     | 0.55              |
| 3:L:28:GLU:OE2   | 3:L:31:LYS:NZ    | 2.36                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:23:ARG:HB2   | 4:P:111:ARG:HA   | 1.89                     | 0.55              |
| 3:N:65:ASP:OD1   | 3:N:83:TYR:OH    | 2.21                     | 0.55              |
| 1:C:123:THR:HG22 | 1:C:151:LYS:HG3  | 1.88                     | 0.54              |
| 2:F:10:ARG:NH2   | 2:F:106:ASN:OD1  | 2.40                     | 0.54              |
| 3:L:164:ARG:NH1  | 3:L:181:ALA:O    | 2.40                     | 0.54              |
| 1:C:198:LEU:HD12 | 7:Q:191:HIS:HB2  | 1.87                     | 0.54              |
| 2:G:4:TRP:CE3    | 2:G:5:ILE:HG12   | 2.43                     | 0.54              |
| 1:C:256:ASN:ND2  | 8:S:59:DG:H5'    | 2.22                     | 0.54              |
| 3:K:216:GLU:OE2  | 3:K:219:GLN:NE2  | 2.40                     | 0.54              |
| 3:L:36:VAL:O     | 3:L:42:TRP:HA    | 2.07                     | 0.54              |
| 4:P:31:PRO:HD3   | 4:P:200:MET:HE3  | 1.89                     | 0.54              |
| 6:A:68:ARG:HH22  | 6:A:159:GLN:NE2  | 2.05                     | 0.54              |
| 1:C:256:ASN:HA   | 8:S:59:DG:O4'    | 2.07                     | 0.54              |
| 2:F:73:ASP:OD1   | 2:F:74:ILE:N     | 2.40                     | 0.54              |
| 3:L:27:ILE:HG21  | 3:L:187:ARG:NH1  | 2.22                     | 0.54              |
| 3:M:159:ALA:HA   | 3:M:188:GLU:HA   | 1.90                     | 0.54              |
| 3:N:275:ILE:HD12 | 3:N:276:PRO:HD2  | 1.88                     | 0.54              |
| 3:O:125:ALA:HB3  | 3:O:130:ARG:HB2  | 1.90                     | 0.54              |
| 4:P:163:PRO:O    | 4:P:166:LYS:NZ   | 2.38                     | 0.54              |
| 6:A:11:LEU:HG    | 6:A:57:ALA:HB1   | 1.90                     | 0.54              |
| 6:A:120:LYS:HA   | 6:A:144:ARG:HD2  | 1.88                     | 0.54              |
| 2:H:4:TRP:CH2    | 2:H:77:LEU:HB2   | 2.42                     | 0.54              |
| 4:P:113:TYR:OH   | 4:P:148:ASP:OD2  | 2.20                     | 0.54              |
| 2:G:49:ARG:NH2   | 2:H:29:ASP:OD1   | 2.41                     | 0.54              |
| 3:I:50:ILE:HB    | 3:I:141:ILE:HB   | 1.89                     | 0.54              |
| 3:J:311:VAL:O    | 3:J:321:LYS:NZ   | 2.41                     | 0.54              |
| 6:A:32:ASN:HA    | 7:Q:35:ARG:HH21  | 1.72                     | 0.54              |
| 3:I:108:GLU:OE1  | 3:I:132:ARG:NH1  | 2.40                     | 0.54              |
| 3:N:5:ILE:HD11   | 3:N:266:LEU:HD11 | 1.89                     | 0.54              |
| 3:I:155:ARG:HG3  | 3:I:157:ILE:H    | 1.72                     | 0.54              |
| 3:N:133:VAL:HG23 | 5:R:35:U:H5''    | 1.90                     | 0.54              |
| 3:L:79:ARG:NH1   | 3:L:88:PHE:O     | 2.40                     | 0.54              |
| 4:P:15:VAL:HG21  | 4:P:30:PRO:HG3   | 1.89                     | 0.54              |
| 1:C:120:VAL:HG21 | 1:C:155:LEU:HB2  | 1.90                     | 0.53              |
| 3:M:20:GLY:HA2   | 3:M:27:ILE:HD12  | 1.89                     | 0.53              |
| 6:A:458:THR:OG1  | 6:A:459:THR:N    | 2.39                     | 0.53              |
| 2:G:6:ARG:HH22   | 2:G:10:ARG:HH21  | 1.57                     | 0.53              |
| 6:A:425:ARG:NH1  | 7:Q:194:ASP:O    | 2.42                     | 0.53              |
| 7:Q:83:ARG:HB3   | 7:Q:86:LEU:HD23  | 1.90                     | 0.53              |
| 8:S:54:DG:H2''   | 8:S:55:DC:C5     | 2.43                     | 0.53              |
| 3:I:167:VAL:HG22 | 3:J:84:ASN:HD22  | 1.74                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:174:GLY:HA3  | 3:K:180:THR:HG21 | 1.90                     | 0.53              |
| 6:A:433:SER:H    | 7:Q:126:ARG:NE   | 2.05                     | 0.53              |
| 3:K:269:ILE:HG22 | 3:K:306:VAL:HG22 | 1.89                     | 0.53              |
| 1:C:96:ASN:HA    | 1:C:257:GLN:HE22 | 1.72                     | 0.53              |
| 2:G:45:TYR:O     | 2:G:49:ARG:HG2   | 2.08                     | 0.53              |
| 3:N:75:ASN:HB3   | 3:N:115:LEU:HA   | 1.90                     | 0.53              |
| 3:I:1:MET:HG2    | 3:I:272:GLU:HA   | 1.91                     | 0.53              |
| 3:I:253:ASN:ND2  | 3:I:257:SER:OG   | 2.41                     | 0.53              |
| 3:J:260:VAL:HG13 | 3:K:280:HIS:HB3  | 1.91                     | 0.53              |
| 3:L:196:PHE:HZ   | 3:L:266:LEU:HD12 | 1.74                     | 0.53              |
| 3:K:19:GLN:HB3   | 3:K:28:GLU:OE2   | 2.09                     | 0.53              |
| 6:A:170:TYR:HA   | 6:A:176:TYR:HB2  | 1.91                     | 0.53              |
| 4:P:21:GLN:O     | 4:P:109:MET:HB3  | 2.09                     | 0.53              |
| 4:P:58:ALA:HA    | 4:P:61:LYS:HE3   | 1.91                     | 0.53              |
| 3:M:198:ILE:HG21 | 3:M:242:LEU:HD11 | 1.90                     | 0.53              |
| 7:Q:131:GLU:HG3  | 7:Q:133:LEU:HG   | 1.91                     | 0.53              |
| 3:I:90:GLN:HA    | 3:I:126:PRO:HD2  | 1.89                     | 0.53              |
| 3:J:270:ALA:O    | 3:J:305:GLU:HB2  | 2.08                     | 0.53              |
| 3:N:125:ALA:HB3  | 3:N:130:ARG:HB2  | 1.91                     | 0.53              |
| 4:P:84:LEU:HD13  | 4:P:116:THR:HB   | 1.90                     | 0.53              |
| 2:F:33:LYS:HA    | 2:F:91:ARG:HH22  | 1.74                     | 0.52              |
| 6:A:138:TYR:HE2  | 6:A:431:LYS:HD3  | 1.74                     | 0.52              |
| 3:N:10:ARG:NH2   | 3:O:36:VAL:O     | 2.32                     | 0.52              |
| 2:D:11:TYR:HE2   | 2:D:48:LEU:HA    | 1.73                     | 0.52              |
| 3:O:239:LEU:HD11 | 3:O:332:LEU:HG   | 1.90                     | 0.52              |
| 3:J:262:LYS:HD3  | 3:K:283:TYR:CG   | 2.44                     | 0.52              |
| 3:M:94:THR:HA    | 3:M:105:LEU:HD23 | 1.91                     | 0.52              |
| 3:M:167:VAL:HB   | 3:M:171:GLY:HA2  | 1.91                     | 0.52              |
| 3:N:10:ARG:HG2   | 3:N:193:LEU:HG   | 1.91                     | 0.52              |
| 1:C:15:ASP:HA    | 1:C:18:VAL:HG12  | 1.90                     | 0.52              |
| 3:I:25:ASN:HA    | 8:S:54:DG:H8     | 1.74                     | 0.52              |
| 3:I:148:ILE:O    | 3:I:152:GLU:N    | 2.43                     | 0.52              |
| 3:K:269:ILE:HB   | 3:K:304:ILE:HD11 | 1.91                     | 0.52              |
| 3:L:4:ARG:NH1    | 3:L:275:ILE:HG13 | 2.25                     | 0.52              |
| 3:N:180:THR:HG22 | 3:N:182:GLN:H    | 1.73                     | 0.52              |
| 3:N:269:ILE:HG12 | 3:N:294:ILE:HG21 | 1.91                     | 0.52              |
| 3:O:12:ASN:HB2   | 3:O:260:VAL:HG23 | 1.91                     | 0.52              |
| 1:C:276:LYS:HD2  | 1:C:279:ARG:HH21 | 1.75                     | 0.52              |
| 3:I:97:LYS:HD3   | 3:I:101:ALA:HB3  | 1.92                     | 0.52              |
| 3:M:173:ILE:O    | 3:M:180:THR:OG1  | 2.27                     | 0.52              |
| 6:A:326:LEU:HD12 | 6:A:327:PRO:HD2  | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:158:THR:HG21 | 3:K:32:THR:HA    | 1.92                     | 0.52              |
| 3:K:205:VAL:HB   | 3:K:234:ARG:HD2  | 1.92                     | 0.52              |
| 3:M:15:SER:HB2   | 3:M:189:TYR:HD1  | 1.75                     | 0.52              |
| 4:P:182:LEU:HB3  | 4:P:238:PRO:HD2  | 1.92                     | 0.52              |
| 3:O:269:ILE:HG22 | 3:O:306:VAL:HG22 | 1.91                     | 0.52              |
| 2:E:26:ASP:OD2   | 2:E:26:ASP:N     | 2.43                     | 0.51              |
| 2:E:50:LEU:HD12  | 2:E:53:LYS:HD3   | 1.92                     | 0.51              |
| 6:A:507:LYS:HD2  | 6:A:508:LEU:N    | 2.25                     | 0.51              |
| 2:E:32:ALA:HB1   | 2:E:95:VAL:HG12  | 1.91                     | 0.51              |
| 3:L:105:LEU:O    | 3:L:130:ARG:NH1  | 2.43                     | 0.51              |
| 3:M:143:PRO:HA   | 3:M:194:TYR:HA   | 1.91                     | 0.51              |
| 3:N:20:GLY:HA2   | 5:R:39:A:H2'     | 1.92                     | 0.51              |
| 3:O:4:ARG:HG3    | 3:O:199:VAL:HG22 | 1.93                     | 0.51              |
| 4:P:166:LYS:HG3  | 4:P:243:ALA:HB3  | 1.93                     | 0.51              |
| 6:A:317:THR:HG23 | 6:A:319:VAL:HG23 | 1.92                     | 0.51              |
| 6:A:338:PRO:O    | 6:A:340:ASP:N    | 2.41                     | 0.51              |
| 3:I:140:PHE:HD2  | 4:P:12:PHE:HD2   | 1.59                     | 0.51              |
| 3:I:324:SER:N    | 3:I:327:GLU:OE2  | 2.41                     | 0.51              |
| 3:M:64:VAL:HG11  | 3:M:80:ALA:HB1   | 1.92                     | 0.51              |
| 3:O:124:LEU:HG   | 3:O:126:PRO:HD3  | 1.92                     | 0.51              |
| 6:A:264:THR:HG22 | 6:A:266:ARG:H    | 1.75                     | 0.51              |
| 3:O:309:TYR:HD1  | 3:O:322:VAL:HG23 | 1.75                     | 0.51              |
| 1:C:226:LEU:HD12 | 1:C:304:ILE:HD13 | 1.93                     | 0.51              |
| 3:J:51:THR:HG22  | 3:J:53:ASN:H     | 1.75                     | 0.51              |
| 3:J:167:VAL:HG13 | 3:K:82:ARG:HH12  | 1.76                     | 0.51              |
| 3:K:16:LEU:HD22  | 3:K:251:GLY:HA3  | 1.93                     | 0.51              |
| 3:O:31:LYS:HA    | 3:O:48:PRO:HA    | 1.92                     | 0.51              |
| 3:J:81:LEU:HB3   | 3:K:212:PRO:HG3  | 1.92                     | 0.51              |
| 3:J:158:THR:HG21 | 3:K:33:LYS:H     | 1.75                     | 0.51              |
| 8:S:54:DG:H2''   | 8:S:55:DC:H5     | 1.75                     | 0.51              |
| 1:C:24:VAL:HB    | 1:C:167:TYR:HE2  | 1.75                     | 0.51              |
| 1:C:241:LYS:O    | 4:P:225:ARG:NH2  | 2.40                     | 0.51              |
| 3:I:231:ARG:O    | 3:I:235:ILE:HG12 | 2.10                     | 0.51              |
| 3:J:87:ARG:NH2   | 3:J:121:HIS:O    | 2.44                     | 0.51              |
| 3:J:143:PRO:HA   | 3:J:194:TYR:HA   | 1.93                     | 0.51              |
| 3:K:227:ASP:OD1  | 3:K:227:ASP:N    | 2.43                     | 0.51              |
| 1:C:306:ALA:HB2  | 1:C:314:GLY:HA3  | 1.93                     | 0.51              |
| 2:F:7:ASN:HD21   | 2:F:73:ASP:HB3   | 1.74                     | 0.51              |
| 3:K:57:HIS:HB2   | 5:R:20:A:H5'     | 1.92                     | 0.51              |
| 3:M:146:ASP:OD1  | 3:M:147:PHE:N    | 2.44                     | 0.51              |
| 6:A:251:ILE:HB   | 6:A:256:LYS:HB2  | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:A:343:ILE:HD12 | 6:A:346:ILE:HD11 | 1.93                     | 0.51              |
| 6:A:491:ASN:O    | 6:A:493:VAL:N    | 2.44                     | 0.51              |
| 1:C:58:LEU:HD11  | 1:C:159:LEU:HD23 | 1.94                     | 0.50              |
| 3:M:109:ALA:HA   | 3:M:208:PRO:HB3  | 1.92                     | 0.50              |
| 3:M:141:ILE:HG22 | 3:M:194:TYR:HB3  | 1.93                     | 0.50              |
| 6:A:445:TYR:HH   | 6:A:460:TYR:HH   | 1.58                     | 0.50              |
| 7:Q:159:MET:O    | 7:Q:163:LYS:NZ   | 2.43                     | 0.50              |
| 1:C:338:GLU:O    | 1:C:342:CYS:N    | 2.41                     | 0.50              |
| 3:I:35:THR:HG22  | 3:I:44:VAL:HG12  | 1.93                     | 0.50              |
| 3:J:322:VAL:HG11 | 3:J:328:LEU:HD12 | 1.93                     | 0.50              |
| 3:L:79:ARG:HD3   | 3:L:86:THR:HB    | 1.94                     | 0.50              |
| 3:N:270:ALA:HB3  | 3:N:305:GLU:HG2  | 1.93                     | 0.50              |
| 6:A:463:LEU:HD23 | 6:A:473:THR:HB   | 1.93                     | 0.50              |
| 7:Q:155:PHE:O    | 7:Q:158:SER:OG   | 2.23                     | 0.50              |
| 3:I:32:THR:HG21  | 3:I:49:ALA:HB3   | 1.92                     | 0.50              |
| 3:J:134:SER:HB2  | 5:R:12:G:P       | 2.51                     | 0.50              |
| 3:M:16:LEU:HD22  | 3:M:251:GLY:HA3  | 1.94                     | 0.50              |
| 3:M:162:HIS:HB2  | 5:R:39:A:P       | 2.52                     | 0.50              |
| 2:F:31:ILE:HD11  | 2:F:44:VAL:N     | 2.27                     | 0.50              |
| 3:J:247:SER:OG   | 3:K:277:ALA:N    | 2.32                     | 0.50              |
| 7:Q:135:PRO:HA   | 7:Q:138:VAL:HG12 | 1.92                     | 0.50              |
| 3:K:317:ILE:HG22 | 3:K:319:ALA:H    | 1.77                     | 0.50              |
| 6:A:56:PHE:CE2   | 6:A:89:LEU:HB3   | 2.47                     | 0.50              |
| 1:C:23:VAL:HA    | 1:C:26:LEU:HG    | 1.93                     | 0.50              |
| 1:C:136:LYS:HE2  | 8:S:62:DT:H71    | 1.92                     | 0.50              |
| 3:M:32:THR:N     | 3:M:46:GLU:OE2   | 2.45                     | 0.50              |
| 3:I:5:ILE:HD12   | 3:I:268:ALA:HB2  | 1.94                     | 0.50              |
| 3:I:239:LEU:HG   | 3:I:329:VAL:HG13 | 1.94                     | 0.50              |
| 3:K:254:LEU:O    | 3:L:137:LYS:HD2  | 2.12                     | 0.50              |
| 6:A:237:VAL:HG21 | 6:A:360:ILE:HD12 | 1.93                     | 0.50              |
| 3:M:15:SER:O     | 3:M:187:ARG:NH2  | 2.45                     | 0.49              |
| 3:M:121:HIS:O    | 3:M:134:SER:OG   | 2.30                     | 0.49              |
| 6:A:119:GLU:HB3  | 6:A:480:LEU:HD21 | 1.94                     | 0.49              |
| 2:D:44:VAL:HG13  | 2:E:99:LEU:HD21  | 1.94                     | 0.49              |
| 2:D:71:PRO:HA    | 2:D:74:ILE:HG12  | 1.93                     | 0.49              |
| 3:L:205:VAL:O    | 3:L:231:ARG:NE   | 2.46                     | 0.49              |
| 6:A:66:VAL:HG21  | 6:A:161:LEU:HB2  | 1.93                     | 0.49              |
| 6:A:171:GLN:HE21 | 6:A:175:MET:HB3  | 1.77                     | 0.49              |
| 2:F:46:LYS:HE2   | 2:F:46:LYS:HA    | 1.94                     | 0.49              |
| 2:G:39:GLU:OE1   | 3:M:155:ARG:NH2  | 2.42                     | 0.49              |
| 3:K:132:ARG:HH12 | 3:K:208:PRO:HA   | 1.77                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:162:HIS:O    | 3:N:184:LEU:HA   | 2.12                     | 0.49              |
| 1:C:180:TRP:NE1  | 1:C:251:GLU:OE2  | 2.41                     | 0.49              |
| 2:E:33:LYS:HD2   | 2:E:33:LYS:O     | 2.13                     | 0.49              |
| 3:I:137:LYS:HG2  | 4:P:145:VAL:HG21 | 1.95                     | 0.49              |
| 3:L:309:TYR:O    | 3:L:310:ASN:ND2  | 2.45                     | 0.49              |
| 3:M:262:LYS:HB2  | 3:N:283:TYR:CE1  | 2.47                     | 0.49              |
| 6:A:170:TYR:HB3  | 6:A:338:PRO:HG3  | 1.94                     | 0.49              |
| 3:I:15:SER:HB3   | 3:I:253:ASN:HD22 | 1.77                     | 0.49              |
| 3:J:4:ARG:HH11   | 3:J:199:VAL:HB   | 1.77                     | 0.49              |
| 3:K:322:VAL:HG23 | 3:K:327:GLU:HG3  | 1.94                     | 0.49              |
| 3:O:82:ARG:HG3   | 3:O:84:ASN:HB2   | 1.93                     | 0.49              |
| 7:Q:177:ASP:OD1  | 7:Q:177:ASP:N    | 2.45                     | 0.49              |
| 1:C:22:TYR:CE1   | 1:C:159:LEU:HD13 | 2.46                     | 0.49              |
| 3:M:321:LYS:NZ   | 3:M:322:VAL:O    | 2.43                     | 0.49              |
| 6:A:77:SER:OG    | 6:A:322:ALA:O    | 2.20                     | 0.49              |
| 7:Q:35:ARG:HA    | 7:Q:38:LYS:HE2   | 1.93                     | 0.49              |
| 1:C:277:LEU:HA   | 1:C:336:ALA:HB1  | 1.94                     | 0.49              |
| 2:G:38:GLU:HG3   | 2:H:92:LYS:HG2   | 1.93                     | 0.49              |
| 3:I:254:LEU:HD13 | 3:I:258:PHE:HA   | 1.94                     | 0.49              |
| 3:J:15:SER:HB3   | 3:J:253:ASN:HD22 | 1.76                     | 0.49              |
| 3:N:1:MET:SD     | 3:N:1:MET:N      | 2.85                     | 0.49              |
| 3:N:115:LEU:HD13 | 3:N:117:ASP:HB3  | 1.94                     | 0.49              |
| 2:D:10:ARG:HH12  | 2:D:69:PRO:HD3   | 1.76                     | 0.49              |
| 3:M:108:GLU:HA   | 3:M:111:ILE:HB   | 1.93                     | 0.49              |
| 3:O:87:ARG:NH2   | 3:O:122:GLY:O    | 2.41                     | 0.49              |
| 6:A:22:ARG:HH21  | 6:A:41:VAL:HB    | 1.78                     | 0.49              |
| 1:C:217:PHE:HB2  | 1:C:293:LEU:HG   | 1.94                     | 0.49              |
| 1:C:269:LYS:HD3  | 4:P:228:ARG:HB3  | 1.95                     | 0.49              |
| 2:G:75:GLU:HA    | 2:G:78:GLU:HB2   | 1.94                     | 0.49              |
| 2:H:35:ARG:HH12  | 2:H:91:ARG:NH1   | 2.11                     | 0.49              |
| 3:I:300:LEU:HB3  | 4:P:138:LYS:HE3  | 1.94                     | 0.49              |
| 3:K:330:ALA:HB1  | 3:K:334:LYS:NZ   | 2.28                     | 0.49              |
| 3:L:45:VAL:HG11  | 3:L:148:ILE:HG21 | 1.95                     | 0.49              |
| 3:O:106:ASN:OD1  | 3:O:107:ASP:N    | 2.45                     | 0.49              |
| 6:A:75:THR:OG1   | 6:A:175:MET:HG2  | 2.13                     | 0.49              |
| 6:A:601:ILE:HG23 | 6:A:609:GLU:HA   | 1.95                     | 0.49              |
| 3:K:295:LYS:NZ   | 3:K:296:ASN:OD1  | 2.41                     | 0.49              |
| 1:C:39:HIS:HB2   | 1:C:42:SER:HB3   | 1.93                     | 0.48              |
| 1:C:40:GLY:HA3   | 4:P:196:TYR:CE1  | 2.48                     | 0.48              |
| 2:G:10:ARG:HH22  | 2:G:67:ARG:HE    | 1.60                     | 0.48              |
| 2:G:38:GLU:HG2   | 2:H:91:ARG:HB3   | 1.93                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:256:ARG:NH2  | 5:R:12:G:H8      | 2.11                     | 0.48              |
| 3:M:295:LYS:HB2  | 3:M:317:ILE:HD11 | 1.95                     | 0.48              |
| 6:A:338:PRO:O    | 6:A:402:ARG:NH2  | 2.44                     | 0.48              |
| 3:J:166:ASP:HB3  | 3:J:182:GLN:HB2  | 1.95                     | 0.48              |
| 3:O:90:GLN:HG2   | 3:O:126:PRO:HG2  | 1.95                     | 0.48              |
| 4:P:66:ILE:HG23  | 4:P:69:LYS:HE3   | 1.95                     | 0.48              |
| 4:P:224:ARG:HH12 | 4:P:236:TYR:HE1  | 1.60                     | 0.48              |
| 5:R:1:A:O2'      | 5:R:2:U:OP2      | 2.22                     | 0.48              |
| 7:Q:194:ASP:OD1  | 7:Q:194:ASP:N    | 2.44                     | 0.48              |
| 3:M:38:THR:H     | 3:M:149:LYS:HE2  | 1.79                     | 0.48              |
| 6:A:44:ALA:O     | 6:A:48:THR:OG1   | 2.24                     | 0.48              |
| 1:C:55:ARG:NH2   | 1:C:118:ARG:O    | 2.47                     | 0.48              |
| 2:G:41:LEU:HD21  | 2:G:81:VAL:HG21  | 1.95                     | 0.48              |
| 3:J:128:THR:HG21 | 3:J:130:ARG:HE   | 1.77                     | 0.48              |
| 3:M:89:GLY:N     | 3:M:92:GLU:OE2   | 2.41                     | 0.48              |
| 6:A:86:LEU:HD13  | 6:A:128:VAL:HG22 | 1.94                     | 0.48              |
| 2:D:52:PRO:HG2   | 3:K:24:THR:HG22  | 1.94                     | 0.48              |
| 3:I:132:ARG:HH12 | 3:I:209:GLN:H    | 1.61                     | 0.48              |
| 1:C:238:PHE:CG   | 1:C:271:MET:HG3  | 2.48                     | 0.48              |
| 3:J:4:ARG:NH1    | 3:J:201:ASP:OD1  | 2.47                     | 0.48              |
| 3:K:74:VAL:HG21  | 3:L:218:ASN:HB3  | 1.96                     | 0.48              |
| 3:O:113:LYS:HB3  | 3:O:226:ILE:HG22 | 1.96                     | 0.48              |
| 4:P:235:ILE:HG23 | 4:P:237:PRO:HD3  | 1.96                     | 0.48              |
| 2:H:27:VAL:HG12  | 2:H:46:LYS:HG3   | 1.94                     | 0.48              |
| 1:C:39:HIS:HD2   | 1:C:44:LEU:H     | 1.62                     | 0.48              |
| 1:C:269:LYS:NZ   | 1:C:308:MET:O    | 2.41                     | 0.48              |
| 3:O:51:THR:HG23  | 3:O:54:MET:HG2   | 1.94                     | 0.48              |
| 7:Q:29:TYR:O     | 7:Q:33:ILE:N     | 2.46                     | 0.48              |
| 3:J:254:LEU:HB3  | 3:J:258:PHE:HD1  | 1.79                     | 0.48              |
| 3:K:243:ILE:HG23 | 3:K:325:VAL:HG23 | 1.96                     | 0.48              |
| 3:L:197:SER:HB3  | 3:L:280:HIS:HA   | 1.95                     | 0.48              |
| 3:L:271:SER:HB3  | 3:L:304:ILE:HG22 | 1.95                     | 0.48              |
| 3:N:260:VAL:HG13 | 3:O:280:HIS:HB3  | 1.96                     | 0.48              |
| 2:D:26:ASP:N     | 2:D:26:ASP:OD2   | 2.45                     | 0.48              |
| 3:K:15:SER:OG    | 3:K:187:ARG:NE   | 2.34                     | 0.48              |
| 3:O:139:SER:OG   | 3:O:197:SER:O    | 2.27                     | 0.48              |
| 3:N:269:ILE:HD13 | 3:N:278:LEU:HD22 | 1.95                     | 0.47              |
| 3:O:35:THR:HG22  | 3:O:44:VAL:HG12  | 1.96                     | 0.47              |
| 3:O:288:GLU:HA   | 3:O:291:ARG:HG2  | 1.95                     | 0.47              |
| 1:C:96:ASN:HB3   | 1:C:99:TYR:HD2   | 1.79                     | 0.47              |
| 1:C:233:GLU:OE1  | 7:Q:134:THR:HG23 | 2.13                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:16:LEU:HD13  | 3:N:251:GLY:HA3  | 1.97                     | 0.47              |
| 1:C:308:MET:SD   | 1:C:308:MET:N    | 2.87                     | 0.47              |
| 2:F:40:LEU:HD22  | 2:F:94:ALA:HB2   | 1.95                     | 0.47              |
| 3:I:239:LEU:HD21 | 3:I:332:LEU:HB3  | 1.95                     | 0.47              |
| 3:L:5:ILE:HD11   | 3:L:266:LEU:HD11 | 1.96                     | 0.47              |
| 4:P:90:LEU:HD11  | 4:P:108:ALA:HB1  | 1.97                     | 0.47              |
| 4:P:166:LYS:HE2  | 4:P:245:THR:HG22 | 1.96                     | 0.47              |
| 8:S:42:DG:H2'    | 8:S:43:DG:C8     | 2.49                     | 0.47              |
| 3:K:8:ARG:HD3    | 3:K:193:LEU:HD21 | 1.96                     | 0.47              |
| 3:K:161:LYS:HB3  | 3:K:184:LEU:HD11 | 1.96                     | 0.47              |
| 3:K:324:SER:HB2  | 3:L:293:ILE:HD13 | 1.96                     | 0.47              |
| 6:A:444:PRO:HD2  | 6:A:484:TYR:H    | 1.79                     | 0.47              |
| 7:Q:90:TYR:CE2   | 7:Q:173:PRO:HG3  | 2.44                     | 0.47              |
| 2:D:11:TYR:CE2   | 2:D:48:LEU:HA    | 2.50                     | 0.47              |
| 3:K:3:VAL:HB     | 3:K:200:LEU:HB2  | 1.95                     | 0.47              |
| 1:C:38:PRO:HA    | 1:C:43:TYR:HD1   | 1.78                     | 0.47              |
| 3:I:2:TYR:HB2    | 3:I:271:SER:O    | 2.14                     | 0.47              |
| 3:I:162:HIS:HB2  | 3:I:185:PHE:CE1  | 2.50                     | 0.47              |
| 3:I:277:ALA:N    | 4:P:144:ASP:OD1  | 2.45                     | 0.47              |
| 3:I:291:ARG:CZ   | 3:I:314:GLY:HA3  | 2.45                     | 0.47              |
| 3:J:221:ARG:HH21 | 3:J:222:PRO:HG2  | 1.80                     | 0.47              |
| 3:M:14:HIS:N     | 3:M:190:ALA:O    | 2.43                     | 0.47              |
| 3:M:327:GLU:HB3  | 3:N:296:ASN:HB3  | 1.95                     | 0.47              |
| 3:N:162:HIS:CE1  | 3:O:51:THR:HG21  | 2.49                     | 0.47              |
| 4:P:60:LEU:HD21  | 4:P:206:TYR:HB2  | 1.97                     | 0.47              |
| 7:Q:167:ILE:HD12 | 7:Q:168:PRO:HD2  | 1.95                     | 0.47              |
| 3:J:225:VAL:HG13 | 3:J:226:ILE:HG23 | 1.97                     | 0.47              |
| 3:J:247:SER:HG   | 3:K:277:ALA:H    | 1.60                     | 0.47              |
| 3:N:131:ARG:HH21 | 5:R:35:U:H5'     | 1.80                     | 0.47              |
| 3:N:293:ILE:HG23 | 3:N:294:ILE:HG23 | 1.97                     | 0.47              |
| 9:T:22:DA:H4'    | 9:T:23:DG:C5     | 2.50                     | 0.47              |
| 3:I:13:ALA:H     | 3:I:191:THR:HG22 | 1.79                     | 0.47              |
| 3:K:29:ILE:N     | 3:K:188:GLU:OE2  | 2.47                     | 0.47              |
| 3:L:14:HIS:HB2   | 3:L:16:LEU:HG    | 1.96                     | 0.47              |
| 3:L:300:LEU:HD23 | 3:L:302:PHE:HE2  | 1.80                     | 0.47              |
| 5:R:42:G:O2'     | 5:R:43:U:O4'     | 2.33                     | 0.47              |
| 6:A:403:VAL:HG22 | 6:A:407:HIS:ND1  | 2.30                     | 0.47              |
| 2:D:56:LYS:HG3   | 2:D:57:LYS:N     | 2.28                     | 0.47              |
| 2:G:17:ASP:OD2   | 2:G:107:ASN:ND2  | 2.44                     | 0.47              |
| 2:H:4:TRP:CZ3    | 2:H:8:ILE:HD13   | 2.50                     | 0.47              |
| 3:K:60:PHE:HZ    | 3:K:80:ALA:HA    | 1.79                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:12:ASN:HB2   | 3:L:260:VAL:HB   | 1.97                     | 0.47              |
| 3:M:326:GLU:HG3  | 3:N:297:ALA:HA   | 1.96                     | 0.47              |
| 3:N:79:ARG:HB3   | 3:N:84:ASN:HB3   | 1.97                     | 0.47              |
| 6:A:194:PRO:HG3  | 7:Q:35:ARG:HH22  | 1.79                     | 0.47              |
| 1:C:206:HIS:H    | 6:A:434:LYS:NZ   | 2.13                     | 0.46              |
| 2:D:10:ARG:NH1   | 2:D:11:TYR:HB2   | 2.30                     | 0.46              |
| 3:I:174:GLY:HA3  | 3:I:178:GLU:HB2  | 1.96                     | 0.46              |
| 3:K:258:PHE:HB2  | 3:L:137:LYS:HZ2  | 1.80                     | 0.46              |
| 3:N:307:PHE:HB3  | 3:N:322:VAL:HG11 | 1.97                     | 0.46              |
| 6:A:450:TYR:HB3  | 6:A:451:PRO:HD3  | 1.97                     | 0.46              |
| 2:F:20:PHE:O     | 2:F:22:GLU:N     | 2.46                     | 0.46              |
| 2:F:31:ILE:HD11  | 2:F:44:VAL:H     | 1.79                     | 0.46              |
| 2:G:84:LEU:HD11  | 2:G:89:ASP:HB3   | 1.97                     | 0.46              |
| 3:J:50:ILE:HB    | 3:J:141:ILE:HB   | 1.96                     | 0.46              |
| 3:K:11:LEU:HB3   | 3:K:14:HIS:HD2   | 1.80                     | 0.46              |
| 3:K:215:PHE:HE1  | 3:K:220:PRO:HA   | 1.80                     | 0.46              |
| 3:L:258:PHE:HB3  | 3:M:139:SER:HA   | 1.97                     | 0.46              |
| 3:M:262:LYS:HD2  | 3:N:283:TYR:CG   | 2.49                     | 0.46              |
| 3:N:216:GLU:OE2  | 3:N:221:ARG:NH2  | 2.47                     | 0.46              |
| 3:I:243:ILE:HG22 | 3:J:276:PRO:HB3  | 1.97                     | 0.46              |
| 3:N:185:PHE:O    | 3:N:187:ARG:NH1  | 2.48                     | 0.46              |
| 8:S:42:DG:H2''   | 8:S:43:DG:O5'    | 2.16                     | 0.46              |
| 1:C:61:ALA:O     | 1:C:64:SER:OG    | 2.26                     | 0.46              |
| 1:C:261:SER:HA   | 4:P:110:ARG:HE   | 1.79                     | 0.46              |
| 3:J:12:ASN:OD1   | 3:J:260:VAL:HB   | 2.15                     | 0.46              |
| 3:K:77:THR:HG22  | 3:K:79:ARG:H     | 1.80                     | 0.46              |
| 3:L:64:VAL:O     | 3:L:68:LYS:HG3   | 2.16                     | 0.46              |
| 3:M:113:LYS:HG3  | 3:M:226:ILE:HG22 | 1.97                     | 0.46              |
| 6:A:133:TRP:HD1  | 6:A:133:TRP:O    | 1.98                     | 0.46              |
| 6:A:250:LYS:HD2  | 6:A:251:ILE:HG23 | 1.98                     | 0.46              |
| 3:I:16:LEU:HD23  | 3:I:50:ILE:HG21  | 1.97                     | 0.46              |
| 3:K:14:HIS:HB2   | 3:K:16:LEU:HG    | 1.97                     | 0.46              |
| 3:M:204:LEU:HD23 | 3:M:204:LEU:O    | 2.15                     | 0.46              |
| 3:M:310:ASN:H    | 3:M:321:LYS:HE2  | 1.81                     | 0.46              |
| 4:P:231:TYR:HE1  | 4:P:233:ALA:HB2  | 1.81                     | 0.46              |
| 6:A:161:LEU:HD13 | 6:A:194:PRO:HG2  | 1.97                     | 0.46              |
| 6:A:292:ILE:HD11 | 6:A:317:THR:H    | 1.80                     | 0.46              |
| 6:A:503:PHE:O    | 6:A:504:LYS:HG2  | 2.16                     | 0.46              |
| 1:C:20:TYR:HE1   | 1:C:197:ILE:HG22 | 1.81                     | 0.46              |
| 2:E:50:LEU:HD12  | 2:E:53:LYS:HB2   | 1.98                     | 0.46              |
| 3:I:87:ARG:NH2   | 3:I:117:ASP:O    | 2.49                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:122:GLY:HA3  | 3:K:132:ARG:O    | 2.16                     | 0.46              |
| 3:K:311:VAL:HG12 | 3:K:313:LEU:H    | 1.81                     | 0.46              |
| 3:K:330:ALA:O    | 3:K:333:VAL:HG12 | 2.16                     | 0.46              |
| 3:N:89:GLY:N     | 3:N:92:GLU:OE2   | 2.48                     | 0.46              |
| 3:O:133:VAL:HA   | 5:R:41:A:H5''    | 1.96                     | 0.46              |
| 9:T:19:DC:H2'    | 9:T:20:DC:C6     | 2.51                     | 0.46              |
| 2:F:10:ARG:HG2   | 2:F:67:ARG:HD2   | 1.97                     | 0.46              |
| 2:G:11:TYR:CD1   | 2:G:69:PRO:HD3   | 2.51                     | 0.46              |
| 3:K:271:SER:HB3  | 3:K:275:ILE:HG21 | 1.97                     | 0.46              |
| 3:L:110:THR:HA   | 3:L:113:LYS:HB3  | 1.98                     | 0.46              |
| 3:L:14:HIS:CE1   | 3:L:190:ALA:HB3  | 2.50                     | 0.46              |
| 3:M:298:ARG:HH21 | 3:M:306:VAL:HG12 | 1.81                     | 0.46              |
| 4:P:2:ASP:OD1    | 4:P:2:ASP:N      | 2.46                     | 0.46              |
| 4:P:234:ARG:HG3  | 4:P:236:TYR:H    | 1.81                     | 0.46              |
| 7:Q:184:ARG:HA   | 7:Q:187:VAL:HG12 | 1.98                     | 0.46              |
| 2:F:52:PRO:HG2   | 2:G:25:TYR:OH    | 2.15                     | 0.46              |
| 7:Q:212:ASP:N    | 7:Q:212:ASP:OD1  | 2.49                     | 0.46              |
| 2:D:80:LYS:HE2   | 2:D:84:LEU:HG    | 1.98                     | 0.46              |
| 2:F:50:LEU:HA    | 2:F:53:LYS:HD3   | 1.97                     | 0.46              |
| 3:L:56:LYS:NZ    | 3:L:134:SER:OG   | 2.49                     | 0.46              |
| 3:M:156:LEU:HD22 | 3:M:191:THR:HG23 | 1.98                     | 0.46              |
| 3:M:305:GLU:HG2  | 3:M:305:GLU:O    | 2.16                     | 0.46              |
| 6:A:415:PHE:CZ   | 6:A:417:TYR:HB3  | 2.51                     | 0.46              |
| 2:E:42:GLU:O     | 2:E:46:LYS:HG2   | 2.16                     | 0.45              |
| 2:E:80:LYS:HA    | 2:E:83:GLN:HE22  | 1.79                     | 0.45              |
| 2:F:92:LYS:HA    | 2:F:95:VAL:HG12  | 1.98                     | 0.45              |
| 3:M:120:VAL:HG13 | 3:M:121:HIS:CD2  | 2.51                     | 0.45              |
| 1:C:174:ALA:HA   | 1:C:179:THR:HA   | 1.97                     | 0.45              |
| 3:I:58:TRP:NE1   | 3:I:251:GLY:O    | 2.35                     | 0.45              |
| 3:I:139:SER:HB3  | 4:P:152:LEU:HD12 | 1.97                     | 0.45              |
| 3:K:14:HIS:HE1   | 3:K:50:ILE:HD11  | 1.82                     | 0.45              |
| 3:L:17:ASN:ND2   | 3:L:51:THR:H     | 2.14                     | 0.45              |
| 3:L:17:ASN:ND2   | 3:L:51:THR:HG22  | 2.31                     | 0.45              |
| 3:M:59:HIS:HE1   | 3:M:242:LEU:HD22 | 1.81                     | 0.45              |
| 3:M:255:ALA:HA   | 3:N:137:LYS:HA   | 1.98                     | 0.45              |
| 6:A:445:TYR:OH   | 6:A:460:TYR:OH   | 2.32                     | 0.45              |
| 2:F:9:GLY:HA2    | 2:F:12:LEU:HB2   | 1.98                     | 0.45              |
| 3:J:22:GLY:HA2   | 8:S:49:DG:N7     | 2.32                     | 0.45              |
| 3:K:76:LEU:HG    | 3:K:77:THR:H     | 1.81                     | 0.45              |
| 3:K:257:SER:C    | 3:L:137:LYS:HZ1  | 2.20                     | 0.45              |
| 3:L:87:ARG:HE    | 3:L:121:HIS:HB3  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:252:ALA:HB1  | 5:R:28:A:H5''    | 1.99                     | 0.45              |
| 6:A:72:VAL:HB    | 6:A:164:PHE:HA   | 1.98                     | 0.45              |
| 6:A:287:SER:HB3  | 6:A:312:ARG:HG3  | 1.97                     | 0.45              |
| 2:D:5:ILE:HD13   | 2:D:8:ILE:HD11   | 1.99                     | 0.45              |
| 2:F:37:GLN:HB2   | 2:F:90:LEU:HD11  | 1.99                     | 0.45              |
| 3:K:323:SER:N    | 3:K:327:GLU:OE2  | 2.43                     | 0.45              |
| 3:L:202:LEU:HD23 | 3:L:235:ILE:HG23 | 1.98                     | 0.45              |
| 3:M:117:ASP:OD1  | 3:M:118:ALA:N    | 2.48                     | 0.45              |
| 3:M:258:PHE:HD2  | 3:N:139:SER:HB2  | 1.81                     | 0.45              |
| 6:A:39:ILE:O     | 6:A:198:MET:HA   | 2.16                     | 0.45              |
| 6:A:118:LEU:HG   | 6:A:119:GLU:H    | 1.80                     | 0.45              |
| 8:S:59:DG:H2'    | 8:S:60:DG:C8     | 2.51                     | 0.45              |
| 2:H:29:ASP:HB2   | 3:N:155:ARG:HH12 | 1.81                     | 0.45              |
| 3:J:311:VAL:HG22 | 3:J:313:LEU:H    | 1.82                     | 0.45              |
| 3:M:66:TYR:HE1   | 3:N:274:PRO:HB2  | 1.82                     | 0.45              |
| 3:O:211:LEU:HD21 | 3:O:214:LYS:HA   | 1.98                     | 0.45              |
| 6:A:430:LYS:O    | 7:Q:126:ARG:NH2  | 2.48                     | 0.45              |
| 3:O:128:THR:HG23 | 3:O:130:ARG:HD3  | 1.97                     | 0.45              |
| 4:P:203:SER:O    | 4:P:213:GLN:NE2  | 2.50                     | 0.45              |
| 6:A:53:MET:N     | 6:A:54:PRO:HD2   | 2.31                     | 0.45              |
| 6:A:61:ASN:OD1   | 6:A:63:ASN:ND2   | 2.46                     | 0.45              |
| 6:A:424:ALA:HA   | 7:Q:199:ARG:CZ   | 2.46                     | 0.45              |
| 7:Q:34:ILE:O     | 7:Q:38:LYS:HG3   | 2.15                     | 0.45              |
| 2:D:88:LYS:HD3   | 2:D:88:LYS:HA    | 1.71                     | 0.45              |
| 3:I:283:TYR:HE1  | 4:P:117:ARG:HG2  | 1.82                     | 0.45              |
| 3:J:164:ARG:HG3  | 3:J:182:GLN:HG2  | 1.99                     | 0.45              |
| 3:L:156:LEU:HD23 | 3:L:156:LEU:H    | 1.81                     | 0.45              |
| 3:L:170:LYS:O    | 3:N:130:ARG:NH2  | 2.49                     | 0.45              |
| 3:M:322:VAL:HB   | 3:M:327:GLU:OE2  | 2.17                     | 0.45              |
| 3:O:112:ILE:HG21 | 3:O:206:GLY:HA2  | 1.99                     | 0.45              |
| 1:C:166:TYR:HB3  | 1:C:201:LYS:HE3  | 1.98                     | 0.45              |
| 1:C:229:LEU:HD21 | 1:C:271:MET:HE1  | 1.98                     | 0.45              |
| 3:I:55:LEU:HD23  | 3:I:138:ALA:HB1  | 1.99                     | 0.45              |
| 3:K:231:ARG:NH1  | 3:K:235:ILE:HD11 | 2.32                     | 0.45              |
| 3:N:58:TRP:CD1   | 3:N:250:ILE:HD12 | 2.52                     | 0.45              |
| 6:A:150:PHE:HB2  | 7:Q:117:HIS:O    | 2.17                     | 0.45              |
| 6:A:158:ALA:HB1  | 7:Q:36:VAL:HG21  | 1.98                     | 0.45              |
| 6:A:405:GLU:HA   | 6:A:408:TYR:HE1  | 1.82                     | 0.45              |
| 2:F:54:LEU:HD13  | 2:F:57:LYS:HD3   | 1.99                     | 0.45              |
| 3:J:120:VAL:HG13 | 3:J:121:HIS:ND1  | 2.32                     | 0.45              |
| 6:A:56:PHE:HE2   | 6:A:89:LEU:HD12  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:A:78:LEU:HA    | 6:A:301:ARG:HH22 | 1.82                     | 0.45              |
| 3:K:55:LEU:HD13  | 3:K:250:ILE:HD12 | 1.99                     | 0.45              |
| 3:M:87:ARG:HH22  | 3:M:121:HIS:HB3  | 1.81                     | 0.45              |
| 3:N:135:LEU:HD11 | 3:N:204:LEU:HB2  | 1.99                     | 0.45              |
| 7:Q:213:TYR:OH   | 7:Q:220:ALA:N    | 2.50                     | 0.45              |
| 3:J:154:GLU:O    | 3:J:156:LEU:N    | 2.50                     | 0.44              |
| 3:L:18:ALA:HB2   | 3:L:29:ILE:HG22  | 1.98                     | 0.44              |
| 3:O:76:LEU:O     | 3:O:98:ALA:N     | 2.49                     | 0.44              |
| 4:P:86:ARG:HA    | 4:P:86:ARG:HD3   | 1.66                     | 0.44              |
| 6:A:425:ARG:NE   | 7:Q:190:ARG:O    | 2.50                     | 0.44              |
| 1:C:131:MET:SD   | 1:C:133:SER:HB2  | 2.57                     | 0.44              |
| 2:G:34:ALA:HA    | 2:G:39:GLU:OE2   | 2.18                     | 0.44              |
| 3:I:79:ARG:HB3   | 3:I:84:ASN:HB3   | 1.99                     | 0.44              |
| 3:I:258:PHE:HB3  | 3:J:139:SER:HA   | 1.99                     | 0.44              |
| 3:N:118:ALA:HB1  | 3:N:123:PHE:HD2  | 1.82                     | 0.44              |
| 4:P:145:VAL:HG13 | 5:R:2:U:O4       | 2.16                     | 0.44              |
| 6:A:326:LEU:HD23 | 6:A:329:VAL:HG22 | 2.00                     | 0.44              |
| 7:Q:12:ARG:HD3   | 7:Q:155:PHE:HZ   | 1.82                     | 0.44              |
| 2:F:33:LYS:HA    | 2:F:91:ARG:NH2   | 2.32                     | 0.44              |
| 3:K:200:LEU:HD11 | 3:K:242:LEU:HD21 | 1.99                     | 0.44              |
| 3:L:37:ARG:H     | 3:L:149:LYS:HE2  | 1.82                     | 0.44              |
| 3:L:183:MET:SD   | 3:L:183:MET:N    | 2.90                     | 0.44              |
| 5:R:12:G:H1      | 8:S:55:DC:H42    | 1.65                     | 0.44              |
| 1:C:206:HIS:ND1  | 6:A:422:ASP:OD2  | 2.50                     | 0.44              |
| 3:I:25:ASN:HA    | 8:S:54:DG:C8     | 2.51                     | 0.44              |
| 3:I:316:ASP:OD1  | 3:I:317:ILE:N    | 2.51                     | 0.44              |
| 3:J:107:ASP:HB3  | 3:J:110:THR:HG22 | 2.00                     | 0.44              |
| 3:K:122:GLY:CA   | 3:K:132:ARG:O    | 2.65                     | 0.44              |
| 3:K:224:ILE:HG22 | 3:K:226:ILE:H    | 1.83                     | 0.44              |
| 3:N:30:THR:OG1   | 3:N:49:ALA:O     | 2.35                     | 0.44              |
| 6:A:120:LYS:HA   | 6:A:144:ARG:HH11 | 1.82                     | 0.44              |
| 2:G:37:GLN:HG3   | 2:H:92:LYS:HD3   | 2.00                     | 0.44              |
| 3:K:90:GLN:OE1   | 8:S:50:DG:P      | 2.75                     | 0.44              |
| 3:K:128:THR:HG23 | 3:K:130:ARG:HG2  | 2.00                     | 0.44              |
| 3:K:269:ILE:HD11 | 3:K:276:PRO:O    | 2.18                     | 0.44              |
| 3:M:67:PHE:HD2   | 3:M:76:LEU:HD11  | 1.82                     | 0.44              |
| 3:M:219:GLN:O    | 3:M:219:GLN:HG2  | 2.17                     | 0.44              |
| 7:Q:111:LEU:O    | 7:Q:115:MET:HG2  | 2.16                     | 0.44              |
| 3:I:107:ASP:HA   | 3:I:130:ARG:HD3  | 1.99                     | 0.44              |
| 3:I:135:LEU:HD21 | 3:I:204:LEU:HB3  | 1.98                     | 0.44              |
| 3:J:110:THR:HA   | 3:J:113:LYS:HE3  | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:11:LEU:HB3   | 3:K:14:HIS:CD2   | 2.53                     | 0.44              |
| 6:A:26:LYS:HE2   | 6:A:217:ILE:HB   | 2.00                     | 0.44              |
| 1:C:39:HIS:CD2   | 1:C:44:LEU:H     | 2.36                     | 0.44              |
| 1:C:40:GLY:HA3   | 4:P:196:TYR:HE1  | 1.83                     | 0.44              |
| 3:I:87:ARG:HH12  | 3:I:121:HIS:HB2  | 1.82                     | 0.44              |
| 3:J:8:ARG:NH2    | 3:J:144:THR:HG23 | 2.32                     | 0.44              |
| 3:J:13:ALA:HB1   | 3:K:140:PHE:CD2  | 2.53                     | 0.44              |
| 3:K:14:HIS:NE2   | 3:K:194:TYR:HE2  | 2.16                     | 0.44              |
| 1:C:279:ARG:HA   | 7:Q:137:VAL:HG12 | 2.00                     | 0.44              |
| 2:E:10:ARG:HG2   | 2:E:67:ARG:HE    | 1.83                     | 0.44              |
| 2:F:54:LEU:HB3   | 2:F:66:PRO:HG3   | 2.00                     | 0.44              |
| 3:I:32:THR:OG1   | 3:I:47:VAL:O     | 2.21                     | 0.44              |
| 3:K:167:VAL:HG13 | 3:K:171:GLY:HA2  | 2.00                     | 0.44              |
| 3:M:260:VAL:HG12 | 3:N:283:TYR:OH   | 2.18                     | 0.44              |
| 1:C:190:GLU:HG2  | 1:C:191:GLU:OE1  | 2.18                     | 0.44              |
| 3:J:175:SER:O    | 3:J:178:GLU:HB3  | 2.17                     | 0.44              |
| 3:N:10:ARG:HH12  | 3:O:37:ARG:HA    | 1.83                     | 0.44              |
| 3:N:143:PRO:HA   | 3:N:194:TYR:HA   | 2.00                     | 0.44              |
| 3:N:242:LEU:HD13 | 3:N:245:MET:SD   | 2.58                     | 0.44              |
| 4:P:71:VAL:HG12  | 4:P:126:LYS:HB3  | 2.00                     | 0.44              |
| 6:A:51:ALA:HB3   | 6:A:163:ILE:HD13 | 2.00                     | 0.44              |
| 6:A:90:VAL:HG11  | 6:A:111:LEU:HD11 | 1.98                     | 0.44              |
| 6:A:206:LEU:O    | 6:A:210:ILE:HG12 | 2.18                     | 0.44              |
| 1:C:296:ALA:HB2  | 1:C:322:GLY:HA2  | 2.00                     | 0.43              |
| 3:I:283:TYR:CE1  | 4:P:117:ARG:HG2  | 2.53                     | 0.43              |
| 3:J:213:VAL:HG12 | 3:J:222:PRO:HA   | 1.98                     | 0.43              |
| 3:K:20:GLY:O     | 3:K:21:GLY:C     | 2.56                     | 0.43              |
| 3:L:164:ARG:HB2  | 5:R:31:U:H1'     | 2.00                     | 0.43              |
| 3:M:260:VAL:HG21 | 3:N:142:LEU:HD12 | 2.00                     | 0.43              |
| 3:N:9:ILE:HG12   | 3:N:196:PHE:CE1  | 2.53                     | 0.43              |
| 3:N:90:GLN:HA    | 3:N:127:LYS:HZ2  | 1.83                     | 0.43              |
| 3:L:15:SER:HB2   | 3:L:189:TYR:CD2  | 2.53                     | 0.43              |
| 3:L:141:ILE:HG22 | 3:L:194:TYR:HB3  | 2.00                     | 0.43              |
| 4:P:101:SER:HB2  | 4:P:105:LYS:HD2  | 1.99                     | 0.43              |
| 6:A:206:LEU:HA   | 6:A:209:MET:HG3  | 2.00                     | 0.43              |
| 6:A:419:GLY:O    | 6:A:423:THR:OG1  | 2.36                     | 0.43              |
| 2:E:7:ASN:ND2    | 2:E:73:ASP:OD2   | 2.30                     | 0.43              |
| 3:I:214:LYS:HB3  | 3:I:216:GLU:OE1  | 2.18                     | 0.43              |
| 3:J:254:LEU:HB2  | 3:K:137:LYS:HD2  | 2.00                     | 0.43              |
| 3:L:242:LEU:HA   | 3:L:245:MET:HE2  | 2.01                     | 0.43              |
| 3:O:148:ILE:HA   | 3:O:151:VAL:HG12 | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:A:444:PRO:HG2  | 6:A:484:TYR:HB2  | 2.00                     | 0.43              |
| 7:Q:196:GLY:O    | 7:Q:200:MET:HG2  | 2.18                     | 0.43              |
| 2:E:103:ALA:HB3  | 2:E:105:TRP:CD1  | 2.53                     | 0.43              |
| 2:H:77:LEU:HA    | 2:H:80:LYS:HE2   | 2.00                     | 0.43              |
| 3:J:202:LEU:HG   | 3:J:235:ILE:HG23 | 2.01                     | 0.43              |
| 3:J:216:GLU:HG2  | 3:J:217:GLU:OE1  | 2.18                     | 0.43              |
| 3:K:64:VAL:O     | 3:K:68:LYS:HG3   | 2.19                     | 0.43              |
| 3:K:92:GLU:O     | 3:K:127:LYS:HE3  | 2.18                     | 0.43              |
| 3:L:3:VAL:C      | 3:L:4:ARG:HD2    | 2.38                     | 0.43              |
| 3:L:14:HIS:NE2   | 3:L:194:TYR:HE1  | 2.16                     | 0.43              |
| 3:M:328:LEU:O    | 3:M:332:LEU:HG   | 2.17                     | 0.43              |
| 3:N:262:LYS:HD3  | 3:O:283:TYR:HD2  | 1.83                     | 0.43              |
| 3:O:64:VAL:HG21  | 3:O:80:ALA:HB1   | 2.01                     | 0.43              |
| 6:A:506:LEU:HD23 | 6:A:507:LYS:N    | 2.32                     | 0.43              |
| 1:C:256:ASN:HA   | 8:S:59:DG:C1'    | 2.48                     | 0.43              |
| 1:C:288:PHE:HE1  | 1:C:329:SER:HA   | 1.83                     | 0.43              |
| 2:F:54:LEU:HA    | 2:F:57:LYS:HG2   | 2.00                     | 0.43              |
| 2:G:3:GLY:O      | 2:G:5:ILE:N      | 2.52                     | 0.43              |
| 3:J:243:ILE:HD12 | 3:J:243:ILE:H    | 1.82                     | 0.43              |
| 3:K:290:ASN:HA   | 3:K:293:ILE:HG22 | 2.00                     | 0.43              |
| 3:M:108:GLU:HA   | 3:M:111:ILE:HD12 | 2.01                     | 0.43              |
| 4:P:5:LEU:HD11   | 4:P:120:LEU:HB3  | 2.00                     | 0.43              |
| 6:A:338:PRO:HB3  | 6:A:378:ALA:HB1  | 1.99                     | 0.43              |
| 1:C:20:TYR:HE2   | 1:C:167:TYR:HB3  | 1.84                     | 0.43              |
| 1:C:169:PRO:HA   | 1:C:204:LYS:HD2  | 2.01                     | 0.43              |
| 1:C:212:GLU:HB3  | 1:C:213:SER:H    | 1.72                     | 0.43              |
| 3:I:247:SER:HB3  | 3:J:277:ALA:HB3  | 2.01                     | 0.43              |
| 3:J:184:LEU:HG   | 5:R:21:A:C2      | 2.54                     | 0.43              |
| 3:J:191:THR:OG1  | 3:K:35:THR:HG23  | 2.19                     | 0.43              |
| 6:A:408:TYR:OH   | 6:A:590:ALA:O    | 2.31                     | 0.43              |
| 3:J:128:THR:CG2  | 3:J:130:ARG:HE   | 2.32                     | 0.43              |
| 3:L:5:ILE:HD12   | 3:L:268:ALA:HB2  | 2.01                     | 0.43              |
| 3:L:159:ALA:HA   | 3:L:188:GLU:HA   | 2.00                     | 0.43              |
| 3:L:256:ARG:HH21 | 5:R:30:C:H3'     | 1.84                     | 0.43              |
| 3:M:10:ARG:HH21  | 3:N:42:TRP:HH2   | 1.66                     | 0.43              |
| 3:M:123:PHE:HE1  | 3:M:130:ARG:HB3  | 1.84                     | 0.43              |
| 7:Q:157:LYS:HE3  | 7:Q:170:VAL:HG13 | 1.99                     | 0.43              |
| 1:C:97:ASN:HA    | 1:C:100:TRP:CD2  | 2.54                     | 0.43              |
| 3:K:157:ILE:HG23 | 3:K:188:GLU:HB2  | 1.99                     | 0.43              |
| 3:L:33:LYS:HD3   | 3:L:44:VAL:HG21  | 2.00                     | 0.43              |
| 3:M:9:ILE:HD12   | 3:M:11:LEU:HB2   | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:A:169:MET:O    | 6:A:171:GLN:NE2  | 2.49                     | 0.43              |
| 1:C:39:HIS:ND1   | 4:P:195:MET:SD   | 2.91                     | 0.43              |
| 1:C:227:TYR:HB2  | 1:C:293:LEU:HD21 | 2.00                     | 0.43              |
| 3:J:258:PHE:HB3  | 3:K:139:SER:HA   | 2.00                     | 0.43              |
| 3:N:232:LYS:HA   | 3:N:235:ILE:HG12 | 2.01                     | 0.43              |
| 6:A:70:VAL:HB    | 6:A:162:VAL:HG12 | 2.01                     | 0.43              |
| 6:A:445:TYR:O    | 6:A:520:ALA:N    | 2.51                     | 0.43              |
| 3:I:123:PHE:H    | 3:I:132:ARG:HB3  | 1.84                     | 0.43              |
| 3:J:38:THR:H     | 3:J:149:LYS:HE2  | 1.83                     | 0.43              |
| 3:K:309:TYR:O    | 3:K:311:VAL:N    | 2.52                     | 0.43              |
| 3:L:5:ILE:HG13   | 3:L:196:PHE:HE2  | 1.83                     | 0.43              |
| 3:M:265:GLU:HG3  | 3:M:310:ASN:HB2  | 2.01                     | 0.43              |
| 3:N:29:ILE:N     | 3:N:188:GLU:OE2  | 2.52                     | 0.43              |
| 3:O:97:LYS:NZ    | 3:O:114:GLU:O    | 2.52                     | 0.43              |
| 3:O:97:LYS:HD3   | 3:O:101:ALA:HB3  | 2.01                     | 0.43              |
| 4:P:146:ILE:HA   | 5:R:2:U:H3       | 1.84                     | 0.43              |
| 3:I:5:ILE:CD1    | 3:I:268:ALA:HB2  | 2.49                     | 0.42              |
| 3:K:78:GLU:HG2   | 3:K:96:THR:HB    | 2.00                     | 0.42              |
| 3:K:290:ASN:O    | 3:K:294:ILE:HG12 | 2.19                     | 0.42              |
| 3:M:261:PHE:O    | 3:N:279:VAL:HG23 | 2.19                     | 0.42              |
| 6:A:296:PHE:CD2  | 6:A:528:ALA:HA   | 2.53                     | 0.42              |
| 2:E:38:GLU:HG3   | 2:F:92:LYS:HB3   | 2.01                     | 0.42              |
| 2:F:45:TYR:O     | 2:F:49:ARG:HG2   | 2.18                     | 0.42              |
| 2:H:93:LEU:O     | 2:H:97:LEU:HG    | 2.20                     | 0.42              |
| 3:K:16:LEU:HD22  | 3:K:252:ALA:H    | 1.84                     | 0.42              |
| 3:L:239:LEU:HD23 | 3:L:239:LEU:HA   | 1.90                     | 0.42              |
| 3:M:70:THR:HG21  | 3:M:233:ALA:HB1  | 2.01                     | 0.42              |
| 3:N:119:ASP:OD1  | 3:N:120:VAL:N    | 2.52                     | 0.42              |
| 3:O:204:LEU:HA   | 3:O:207:ILE:HD12 | 1.99                     | 0.42              |
| 6:A:152:PHE:HE2  | 6:A:154:ALA:HB3  | 1.84                     | 0.42              |
| 2:D:68:ILE:O     | 2:E:104:SER:OG   | 2.36                     | 0.42              |
| 2:E:17:ASP:OD2   | 2:E:107:ASN:ND2  | 2.47                     | 0.42              |
| 3:J:164:ARG:NH1  | 3:K:86:THR:OG1   | 2.52                     | 0.42              |
| 3:K:258:PHE:HB2  | 3:L:137:LYS:NZ   | 2.33                     | 0.42              |
| 6:A:26:LYS:HG2   | 6:A:217:ILE:HG21 | 2.01                     | 0.42              |
| 6:A:261:VAL:HG11 | 6:A:345:ARG:HE   | 1.84                     | 0.42              |
| 3:L:282:PHE:HD2  | 3:L:283:TYR:CZ   | 2.37                     | 0.42              |
| 3:M:135:LEU:HD23 | 3:M:202:LEU:HA   | 2.01                     | 0.42              |
| 4:P:13:PHE:HB2   | 4:P:114:THR:H    | 1.84                     | 0.42              |
| 2:D:27:VAL:HG21  | 2:D:47:ALA:HB2   | 2.01                     | 0.42              |
| 3:J:258:PHE:HD2  | 3:K:139:SER:HB3  | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:13:ALA:C     | 3:K:189:TYR:HB3  | 2.40                     | 0.42              |
| 3:L:120:VAL:O    | 3:L:135:LEU:N    | 2.53                     | 0.42              |
| 3:N:16:LEU:HB3   | 3:N:252:ALA:H    | 1.83                     | 0.42              |
| 2:D:14:TYR:OH    | 2:D:67:ARG:NH1   | 2.53                     | 0.42              |
| 2:F:7:ASN:HB2    | 2:F:67:ARG:HH12  | 1.84                     | 0.42              |
| 3:I:54:MET:HG3   | 3:I:251:GLY:HA2  | 2.02                     | 0.42              |
| 3:I:292:SER:O    | 3:I:295:LYS:HG2  | 2.20                     | 0.42              |
| 3:J:37:ARG:H     | 3:J:149:LYS:HE2  | 1.85                     | 0.42              |
| 3:J:104:GLN:HE22 | 3:J:106:ASN:HB2  | 1.85                     | 0.42              |
| 3:K:51:THR:HG23  | 3:K:53:ASN:H     | 1.84                     | 0.42              |
| 3:M:31:LYS:HE3   | 3:M:46:GLU:HG3   | 2.02                     | 0.42              |
| 3:M:298:ARG:HH12 | 3:M:318:GLU:H    | 1.67                     | 0.42              |
| 4:P:91:LEU:HD12  | 4:P:91:LEU:HA    | 1.87                     | 0.42              |
| 7:Q:72:HIS:HA    | 7:Q:77:GLU:HB2   | 2.01                     | 0.42              |
| 3:K:163:ASN:ND2  | 5:R:27:U:O2'     | 2.53                     | 0.42              |
| 3:L:105:LEU:H    | 3:L:105:LEU:HD23 | 1.85                     | 0.42              |
| 3:L:108:GLU:HA   | 3:L:111:ILE:HB   | 2.01                     | 0.42              |
| 6:A:426:ARG:HH21 | 7:Q:122:MET:HB2  | 1.85                     | 0.42              |
| 7:Q:107:PHE:HE1  | 7:Q:185:LEU:HA   | 1.84                     | 0.42              |
| 2:D:75:GLU:HG3   | 2:E:6:ARG:HH21   | 1.85                     | 0.42              |
| 3:I:53:ASN:HB2   | 4:P:91:LEU:HD11  | 2.01                     | 0.42              |
| 3:I:279:VAL:HG11 | 3:I:286:TYR:HB2  | 2.00                     | 0.42              |
| 3:I:290:ASN:HA   | 3:I:293:ILE:HG22 | 2.01                     | 0.42              |
| 3:J:247:SER:O    | 3:K:277:ALA:HB3  | 2.20                     | 0.42              |
| 3:M:256:ARG:NH1  | 5:R:36:G:H5''    | 2.35                     | 0.42              |
| 3:N:290:ASN:O    | 3:N:294:ILE:HG12 | 2.20                     | 0.42              |
| 6:A:273:GLN:N    | 6:A:273:GLN:OE1  | 2.53                     | 0.42              |
| 6:A:604:LYS:HG3  | 6:A:605:TYR:H    | 1.84                     | 0.42              |
| 1:C:21:GLY:O     | 1:C:24:VAL:HG12  | 2.20                     | 0.42              |
| 2:G:15:LEU:HD23  | 2:G:15:LEU:H     | 1.84                     | 0.42              |
| 3:I:13:ALA:HB2   | 3:J:32:THR:HG21  | 2.01                     | 0.42              |
| 3:J:33:LYS:HB2   | 3:J:33:LYS:HE2   | 1.87                     | 0.42              |
| 3:M:124:LEU:HD13 | 5:R:30:C:C2      | 2.55                     | 0.42              |
| 3:O:31:LYS:HE2   | 3:O:31:LYS:HB2   | 1.88                     | 0.42              |
| 3:O:38:THR:HG21  | 3:O:43:THR:H     | 1.84                     | 0.42              |
| 3:O:120:VAL:HG22 | 3:O:136:VAL:HG13 | 2.01                     | 0.42              |
| 6:A:90:VAL:O     | 6:A:93:LEU:HG    | 2.19                     | 0.42              |
| 2:H:76:ALA:O     | 2:H:79:GLU:HG3   | 2.19                     | 0.42              |
| 3:K:4:ARG:HG3    | 3:K:276:PRO:O    | 2.20                     | 0.42              |
| 3:L:168:ASP:O    | 3:M:82:ARG:NH2   | 2.53                     | 0.42              |
| 3:M:79:ARG:HD3   | 3:M:86:THR:HG23  | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:124:LEU:HG   | 3:N:126:PRO:HD3  | 2.01                     | 0.42              |
| 3:N:230:GLU:OE2  | 3:N:234:ARG:NH2  | 2.53                     | 0.42              |
| 3:N:254:LEU:HB3  | 3:N:258:PHE:CE1  | 2.55                     | 0.42              |
| 3:N:312:ASP:OD2  | 3:N:312:ASP:N    | 2.49                     | 0.42              |
| 6:A:442:ILE:HD11 | 6:A:488:TYR:HB2  | 2.02                     | 0.42              |
| 3:I:187:ARG:HD3  | 3:I:188:GLU:N    | 2.35                     | 0.41              |
| 3:J:147:PHE:CZ   | 3:K:35:THR:HG22  | 2.55                     | 0.41              |
| 3:K:14:HIS:CE1   | 3:K:50:ILE:HD11  | 2.55                     | 0.41              |
| 3:L:207:ILE:HD11 | 3:L:224:ILE:HG13 | 2.02                     | 0.41              |
| 3:M:78:GLU:OE1   | 3:M:82:ARG:NH1   | 2.53                     | 0.41              |
| 4:P:229:ILE:HG13 | 4:P:231:TYR:HD2  | 1.85                     | 0.41              |
| 1:C:149:PRO:HB2  | 4:P:18:ARG:NH2   | 2.36                     | 0.41              |
| 2:E:29:ASP:O     | 2:E:33:LYS:HG3   | 2.20                     | 0.41              |
| 2:G:42:GLU:HG3   | 2:H:91:ARG:NH2   | 2.35                     | 0.41              |
| 2:H:11:TYR:HE2   | 2:H:48:LEU:HA    | 1.84                     | 0.41              |
| 3:I:19:GLN:HG2   | 3:I:28:GLU:O     | 2.19                     | 0.41              |
| 3:I:162:HIS:CE1  | 3:J:51:THR:HG21  | 2.55                     | 0.41              |
| 3:L:161:LYS:HA   | 3:L:186:SER:HA   | 2.02                     | 0.41              |
| 3:M:9:ILE:HD12   | 3:M:261:PHE:HE1  | 1.85                     | 0.41              |
| 3:N:237:SER:HA   | 3:N:240:LYS:HG2  | 2.02                     | 0.41              |
| 4:P:59:ALA:O     | 4:P:63:ILE:HG12  | 2.20                     | 0.41              |
| 1:C:179:THR:OG1  | 1:C:252:ARG:NH2  | 2.50                     | 0.41              |
| 2:E:10:ARG:HG2   | 2:E:67:ARG:NE    | 2.35                     | 0.41              |
| 3:I:50:ILE:O     | 3:I:141:ILE:N    | 2.48                     | 0.41              |
| 3:J:258:PHE:CD2  | 3:K:139:SER:HB3  | 2.55                     | 0.41              |
| 3:K:53:ASN:HD21  | 5:R:19:C:H2'     | 1.85                     | 0.41              |
| 6:A:257:LYS:HD2  | 6:A:326:LEU:HD21 | 2.01                     | 0.41              |
| 6:A:337:ALA:HB3  | 6:A:342:LEU:HB2  | 2.02                     | 0.41              |
| 7:Q:92:ALA:HB3   | 7:Q:113:VAL:HG11 | 2.01                     | 0.41              |
| 7:Q:203:GLY:O    | 7:Q:207:ILE:HG12 | 2.19                     | 0.41              |
| 1:C:55:ARG:HH21  | 1:C:114:LEU:HA   | 1.85                     | 0.41              |
| 1:C:85:SER:OG    | 1:C:86:ASP:N     | 2.53                     | 0.41              |
| 2:E:84:LEU:HD22  | 2:E:93:LEU:HD21  | 2.01                     | 0.41              |
| 3:J:162:HIS:HB2  | 3:J:185:PHE:CE2  | 2.55                     | 0.41              |
| 3:K:125:ALA:HB3  | 3:K:130:ARG:HB2  | 2.02                     | 0.41              |
| 3:K:244:PRO:HA   | 3:K:247:SER:HB3  | 2.01                     | 0.41              |
| 3:L:78:GLU:HB3   | 3:L:96:THR:HG23  | 2.03                     | 0.41              |
| 3:N:106:ASN:HA   | 3:N:130:ARG:HH11 | 1.84                     | 0.41              |
| 6:A:218:THR:OG1  | 6:A:219:VAL:N    | 2.51                     | 0.41              |
| 6:A:377:ALA:HB2  | 6:A:405:GLU:HB3  | 2.02                     | 0.41              |
| 7:Q:79:LEU:O     | 7:Q:141:LYS:NZ   | 2.53                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:137:LYS:HB2  | 3:J:199:VAL:CG2  | 2.50                     | 0.41              |
| 3:M:1:MET:N      | 3:M:271:SER:O    | 2.53                     | 0.41              |
| 3:N:134:SER:N    | 5:R:36:G:OP1     | 2.40                     | 0.41              |
| 3:N:157:ILE:HG23 | 3:N:188:GLU:HB2  | 2.02                     | 0.41              |
| 3:O:76:LEU:HB2   | 3:O:98:ALA:HB2   | 2.03                     | 0.41              |
| 4:P:86:ARG:NE    | 4:P:114:THR:OG1  | 2.53                     | 0.41              |
| 6:A:36:LYS:NZ    | 6:A:213:ASP:OD1  | 2.33                     | 0.41              |
| 6:A:445:TYR:CZ   | 6:A:482:ARG:HD3  | 2.56                     | 0.41              |
| 7:Q:58:ILE:HG23  | 7:Q:59:LEU:HD12  | 2.02                     | 0.41              |
| 7:Q:114:MET:SD   | 7:Q:115:MET:HE2  | 2.60                     | 0.41              |
| 2:D:52:PRO:CG    | 3:K:24:THR:HG22  | 2.51                     | 0.41              |
| 2:F:103:ALA:HB3  | 2:F:105:TRP:NE1  | 2.36                     | 0.41              |
| 3:I:131:ARG:HG3  | 4:P:55:LEU:HD23  | 2.03                     | 0.41              |
| 3:J:104:GLN:HE22 | 3:J:106:ASN:CB   | 2.34                     | 0.41              |
| 3:L:10:ARG:HG2   | 3:L:193:LEU:HG   | 2.02                     | 0.41              |
| 3:L:290:ASN:O    | 3:L:294:ILE:HG12 | 2.20                     | 0.41              |
| 3:M:87:ARG:NH2   | 3:M:121:HIS:HB3  | 2.35                     | 0.41              |
| 3:N:298:ARG:HH12 | 3:N:317:ILE:HG23 | 1.85                     | 0.41              |
| 3:O:213:VAL:HG13 | 3:O:221:ARG:O    | 2.20                     | 0.41              |
| 4:P:57:GLU:O     | 4:P:61:LYS:HG2   | 2.21                     | 0.41              |
| 6:A:190:GLU:O    | 7:Q:39:THR:OG1   | 2.38                     | 0.41              |
| 6:A:512:PRO:HA   | 6:A:513:PRO:HD3  | 1.88                     | 0.41              |
| 1:C:221:ARG:NH2  | 1:C:261:SER:OG   | 2.54                     | 0.41              |
| 1:C:288:PHE:CE1  | 1:C:329:SER:HA   | 2.56                     | 0.41              |
| 2:D:45:TYR:OH    | 2:E:28:VAL:HG22  | 2.21                     | 0.41              |
| 2:E:40:LEU:O     | 2:E:44:VAL:HG23  | 2.20                     | 0.41              |
| 2:H:77:LEU:HA    | 2:H:80:LYS:HG2   | 2.02                     | 0.41              |
| 3:L:6:SER:HA     | 3:L:196:PHE:O    | 2.21                     | 0.41              |
| 3:M:175:SER:O    | 3:M:179:GLY:N    | 2.50                     | 0.41              |
| 1:C:126:ILE:HD11 | 1:C:130:LEU:HB2  | 2.03                     | 0.41              |
| 1:C:135:GLY:HA3  | 4:P:20:TYR:CD2   | 2.56                     | 0.41              |
| 1:C:276:LYS:HD2  | 1:C:279:ARG:NH2  | 2.35                     | 0.41              |
| 2:G:57:LYS:HE3   | 2:G:61:LYS:HE3   | 2.02                     | 0.41              |
| 3:J:79:ARG:HA    | 3:J:82:ARG:HD3   | 2.03                     | 0.41              |
| 3:K:245:MET:HA   | 3:K:250:ILE:HD11 | 2.03                     | 0.41              |
| 3:K:298:ARG:HH12 | 3:K:318:GLU:H    | 1.67                     | 0.41              |
| 3:O:298:ARG:NH1  | 3:O:318:GLU:H    | 2.15                     | 0.41              |
| 1:C:24:VAL:HB    | 1:C:167:TYR:CE2  | 2.56                     | 0.41              |
| 2:D:68:ILE:HG23  | 2:E:104:SER:OG   | 2.21                     | 0.41              |
| 2:E:86:ASN:HA    | 2:E:87:PRO:HD3   | 1.95                     | 0.41              |
| 2:F:68:ILE:HG23  | 2:G:104:SER:HB3  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:256:ARG:NH2  | 5:R:12:G:H3'     | 2.23                     | 0.41              |
| 3:M:191:THR:OG1  | 3:M:192:GLY:N    | 2.54                     | 0.41              |
| 3:N:278:LEU:HD11 | 3:N:290:ASN:OD1  | 2.21                     | 0.41              |
| 4:P:28:LEU:HB3   | 4:P:78:VAL:HG21  | 2.03                     | 0.41              |
| 4:P:141:MET:HG2  | 4:P:142:LEU:N    | 2.32                     | 0.41              |
| 6:A:152:PHE:CE2  | 6:A:154:ALA:HB3  | 2.56                     | 0.41              |
| 6:A:338:PRO:HD2  | 6:A:341:ALA:HB3  | 2.03                     | 0.41              |
| 7:Q:94:ASN:O     | 7:Q:169:LYS:NZ   | 2.54                     | 0.41              |
| 7:Q:159:MET:HA   | 7:Q:162:GLU:HG2  | 2.03                     | 0.41              |
| 1:C:136:LYS:HE3  | 8:S:61:DG:C8     | 2.54                     | 0.41              |
| 1:C:195:ILE:O    | 7:Q:187:VAL:HG21 | 2.21                     | 0.41              |
| 3:I:12:ASN:HA    | 3:I:191:THR:HA   | 2.03                     | 0.41              |
| 3:I:312:ASP:N    | 3:I:312:ASP:OD1  | 2.52                     | 0.41              |
| 3:J:14:HIS:HB3   | 3:J:259:PRO:CB   | 2.43                     | 0.41              |
| 3:J:187:ARG:HH11 | 3:J:187:ARG:HA   | 1.85                     | 0.41              |
| 3:J:327:GLU:HG2  | 3:J:331:ASN:HD21 | 1.86                     | 0.41              |
| 3:M:77:THR:HG22  | 3:M:79:ARG:H     | 1.86                     | 0.41              |
| 3:N:63:PHE:O     | 3:N:67:PHE:HB2   | 2.21                     | 0.41              |
| 4:P:86:ARG:HD2   | 4:P:112:GLU:OE1  | 2.21                     | 0.41              |
| 7:Q:109:GLY:HA2  | 7:Q:112:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:301:LEU:HA   | 1:C:304:ILE:HG22 | 2.03                     | 0.40              |
| 2:D:11:TYR:HA    | 2:D:14:TYR:CD2   | 2.56                     | 0.40              |
| 2:E:50:LEU:HG    | 2:E:54:LEU:HG    | 2.03                     | 0.40              |
| 2:F:38:GLU:HG2   | 2:G:88:LYS:O     | 2.21                     | 0.40              |
| 2:G:10:ARG:HH12  | 2:G:67:ARG:HB3   | 1.86                     | 0.40              |
| 3:J:163:ASN:HB3  | 3:J:184:LEU:HD23 | 2.03                     | 0.40              |
| 6:A:158:ALA:HB3  | 7:Q:204:ALA:HB2  | 2.02                     | 0.40              |
| 7:Q:194:ASP:OD2  | 7:Q:197:LYS:HE3  | 2.21                     | 0.40              |
| 1:C:257:GLN:O    | 8:S:60:DG:H5'    | 2.20                     | 0.40              |
| 3:I:14:HIS:HB2   | 3:I:16:LEU:HD13  | 2.03                     | 0.40              |
| 3:K:79:ARG:HG2   | 3:K:82:ARG:HH21  | 1.86                     | 0.40              |
| 3:M:170:LYS:O    | 3:O:130:ARG:NH2  | 2.55                     | 0.40              |
| 4:P:108:ALA:HB2  | 5:R:9:A:O4'      | 2.21                     | 0.40              |
| 3:I:25:ASN:HB2   | 8:S:54:DG:H5''   | 2.03                     | 0.40              |
| 3:I:278:LEU:HB3  | 3:I:290:ASN:OD1  | 2.22                     | 0.40              |
| 3:K:124:LEU:HG   | 3:K:126:PRO:HD3  | 2.03                     | 0.40              |
| 6:A:443:ILE:O    | 6:A:443:ILE:HG13 | 2.21                     | 0.40              |
| 7:Q:176:GLU:HA   | 7:Q:179:LEU:HD12 | 2.02                     | 0.40              |
| 3:K:8:ARG:HD2    | 3:K:265:GLU:OE2  | 2.22                     | 0.40              |
| 3:K:271:SER:HB2  | 3:K:304:ILE:HA   | 2.04                     | 0.40              |
| 3:O:291:ARG:HA   | 3:O:294:ILE:HG22 | 2.03                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:164:GLU:HG2  | 4:P:166:LYS:HZ2  | 1.85                     | 0.40              |
| 6:A:342:LEU:HD12 | 6:A:345:ARG:NH1  | 2.36                     | 0.40              |
| 7:Q:54:LYS:HA    | 7:Q:57:ILE:HG22  | 2.03                     | 0.40              |
| 1:C:316:TYR:OH   | 2:D:29:ASP:OD1   | 2.39                     | 0.40              |
| 3:I:14:HIS:CE1   | 3:I:190:ALA:HB3  | 2.55                     | 0.40              |
| 3:J:8:ARG:HG3    | 3:J:8:ARG:HH11   | 1.86                     | 0.40              |
| 3:N:15:SER:HB3   | 3:N:189:TYR:CD1  | 2.57                     | 0.40              |
| 4:P:9:ARG:HH21   | 4:P:156:VAL:HG11 | 1.87                     | 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   | C     | 329/341 (96%) | 306 (93%) | 23 (7%)  | 0        | 100         | 100 |
| 2   | D     | 105/108 (97%) | 92 (88%)  | 13 (12%) | 0        | 100         | 100 |
| 2   | E     | 106/108 (98%) | 100 (94%) | 5 (5%)   | 1 (1%)   | 14          | 48  |
| 2   | F     | 105/108 (97%) | 90 (86%)  | 15 (14%) | 0        | 100         | 100 |
| 2   | G     | 105/108 (97%) | 96 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 2   | H     | 105/108 (97%) | 101 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 3   | I     | 333/336 (99%) | 310 (93%) | 22 (7%)  | 1 (0%)   | 37          | 70  |
| 3   | J     | 334/336 (99%) | 303 (91%) | 31 (9%)  | 0        | 100         | 100 |
| 3   | K     | 334/336 (99%) | 305 (91%) | 27 (8%)  | 2 (1%)   | 22          | 57  |
| 3   | L     | 334/336 (99%) | 302 (90%) | 32 (10%) | 0        | 100         | 100 |
| 3   | M     | 334/336 (99%) | 307 (92%) | 27 (8%)  | 0        | 100         | 100 |
| 3   | N     | 317/336 (94%) | 300 (95%) | 17 (5%)  | 0        | 100         | 100 |
| 3   | O     | 266/336 (79%) | 251 (94%) | 15 (6%)  | 0        | 100         | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | P     | 234/256 (91%)   | 214 (92%)  | 18 (8%)  | 2 (1%)   | 14          | 48  |
| 6   | A     | 568/572 (99%)   | 476 (84%)  | 82 (14%) | 10 (2%)  | 7           | 35  |
| 7   | Q     | 235/237 (99%)   | 213 (91%)  | 22 (9%)  | 0        | 100         | 100 |
| All | All   | 4144/4298 (96%) | 3766 (91%) | 362 (9%) | 16 (0%)  | 32          | 65  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | P     | 102 | ASN  |
| 6   | A     | 455 | VAL  |
| 2   | E     | 19  | THR  |
| 6   | A     | 507 | LYS  |
| 3   | K     | 21  | GLY  |
| 3   | K     | 38  | THR  |
| 4   | P     | 21  | GLN  |
| 6   | A     | 218 | THR  |
| 6   | A     | 458 | THR  |
| 6   | A     | 31  | MET  |
| 6   | A     | 504 | LYS  |
| 6   | A     | 517 | LYS  |
| 6   | A     | 518 | ALA  |
| 6   | A     | 492 | ILE  |
| 3   | I     | 23  | GLY  |
| 6   | A     | 364 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | C     | 282/292 (97%) | 282 (100%) | 0        | 100         | 100 |
| 2   | D     | 91/91 (100%)  | 87 (96%)   | 4 (4%)   | 24          | 48  |
| 2   | E     | 91/91 (100%)  | 88 (97%)   | 3 (3%)   | 33          | 56  |
| 2   | F     | 91/91 (100%)  | 90 (99%)   | 1 (1%)   | 70          | 79  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 2   | G     | 91/91 (100%)    | 89 (98%)   | 2 (2%)   | 47          | 65  |
| 2   | H     | 91/91 (100%)    | 91 (100%)  | 0        | 100         | 100 |
| 3   | I     | 275/277 (99%)   | 273 (99%)  | 2 (1%)   | 81          | 86  |
| 3   | J     | 276/277 (100%)  | 273 (99%)  | 3 (1%)   | 70          | 79  |
| 3   | K     | 274/277 (99%)   | 270 (98%)  | 4 (2%)   | 60          | 74  |
| 3   | L     | 275/277 (99%)   | 275 (100%) | 0        | 100         | 100 |
| 3   | M     | 275/277 (99%)   | 274 (100%) | 1 (0%)   | 89          | 91  |
| 3   | N     | 264/277 (95%)   | 262 (99%)  | 2 (1%)   | 79          | 84  |
| 3   | O     | 230/277 (83%)   | 230 (100%) | 0        | 100         | 100 |
| 4   | P     | 211/224 (94%)   | 209 (99%)  | 2 (1%)   | 75          | 83  |
| 6   | A     | 422/427 (99%)   | 417 (99%)  | 5 (1%)   | 67          | 78  |
| 7   | Q     | 191/191 (100%)  | 190 (100%) | 1 (0%)   | 86          | 90  |
| All | All   | 3430/3528 (97%) | 3400 (99%) | 30 (1%)  | 74          | 83  |

All (30) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 10  | ARG  |
| 2   | D     | 52  | PRO  |
| 2   | D     | 56  | LYS  |
| 2   | D     | 67  | ARG  |
| 2   | E     | 33  | LYS  |
| 2   | E     | 56  | LYS  |
| 2   | E     | 92  | LYS  |
| 2   | F     | 80  | LYS  |
| 2   | G     | 56  | LYS  |
| 2   | G     | 91  | ARG  |
| 3   | I     | 53  | ASN  |
| 3   | I     | 183 | MET  |
| 3   | J     | 53  | ASN  |
| 3   | J     | 173 | ILE  |
| 3   | J     | 184 | LEU  |
| 3   | K     | 164 | ARG  |
| 3   | K     | 183 | MET  |
| 3   | K     | 256 | ARG  |
| 3   | K     | 262 | LYS  |
| 3   | M     | 161 | LYS  |
| 3   | N     | 1   | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 187 | ARG  |
| 4   | P     | 69  | LYS  |
| 4   | P     | 117 | ARG  |
| 6   | A     | 205 | LYS  |
| 6   | A     | 250 | LYS  |
| 6   | A     | 413 | LYS  |
| 6   | A     | 432 | ARG  |
| 6   | A     | 507 | LYS  |
| 7   | Q     | 180 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 94  | ASN  |
| 1   | C     | 97  | ASN  |
| 1   | C     | 257 | GLN  |
| 3   | J     | 40  | ASN  |
| 3   | J     | 53  | ASN  |
| 3   | J     | 84  | ASN  |
| 3   | J     | 90  | GLN  |
| 3   | J     | 104 | GLN  |
| 3   | J     | 106 | ASN  |
| 3   | J     | 182 | GLN  |
| 3   | K     | 25  | ASN  |
| 3   | L     | 17  | ASN  |
| 3   | M     | 17  | ASN  |
| 3   | M     | 59  | HIS  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed     | Backbone Outliers | Pucker Outliers |
|-----|-------|--------------|-------------------|-----------------|
| 5   | R     | 45/45 (100%) | 17 (37%)          | 7 (15%)         |

All (17) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | R     | 2   | U    |
| 5   | R     | 9   | A    |
| 5   | R     | 11  | U    |
| 5   | R     | 14  | U    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | R     | 15  | U    |
| 5   | R     | 16  | C    |
| 5   | R     | 19  | C    |
| 5   | R     | 20  | A    |
| 5   | R     | 21  | A    |
| 5   | R     | 22  | A    |
| 5   | R     | 26  | U    |
| 5   | R     | 33  | G    |
| 5   | R     | 39  | A    |
| 5   | R     | 40  | C    |
| 5   | R     | 42  | G    |
| 5   | R     | 43  | U    |
| 5   | R     | 44  | U    |

All (7) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | R     | 1   | A    |
| 5   | R     | 13  | C    |
| 5   | R     | 14  | U    |
| 5   | R     | 15  | U    |
| 5   | R     | 18  | C    |
| 5   | R     | 19  | C    |
| 5   | R     | 21  | A    |

## 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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 6   | A     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 531:ALA   | C      | 580:ALA   | N      | 37.08        |

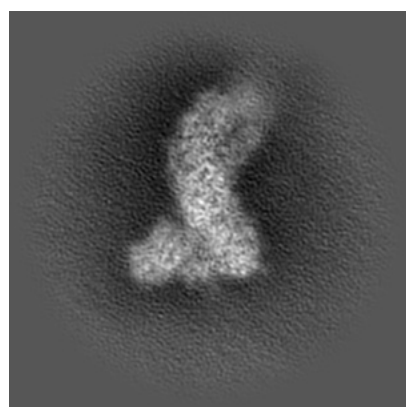
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26083. These allow visual inspection of the internal detail of the map and identification of artifacts.

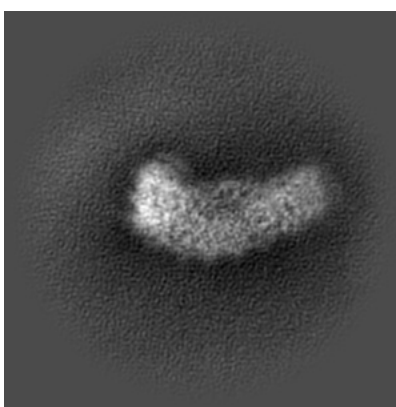
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

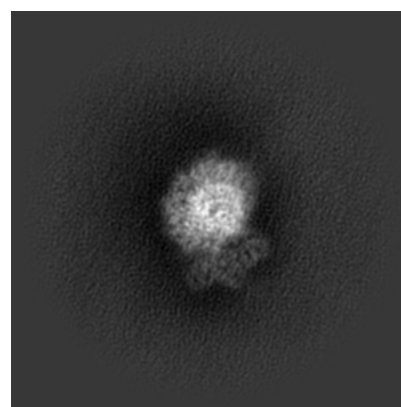
#### 6.1.1 Primary map



X



Y

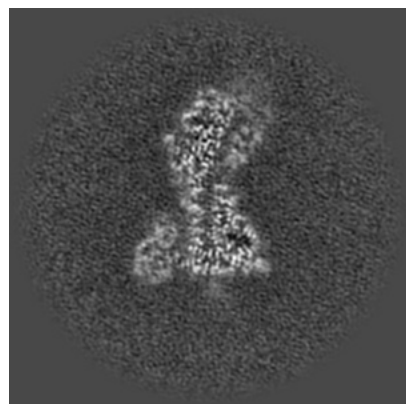


Z

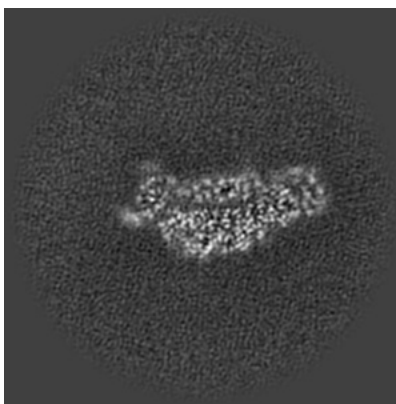
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

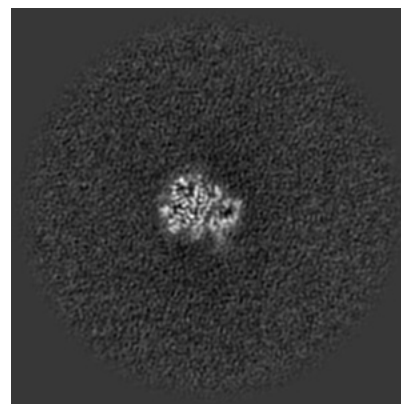
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

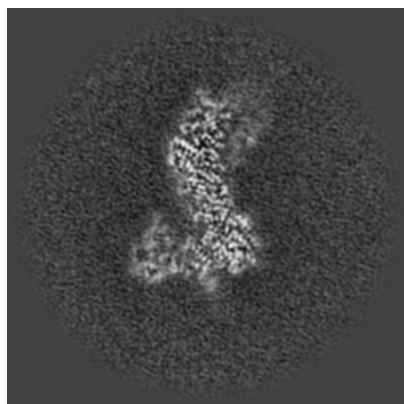


Z Index: 150

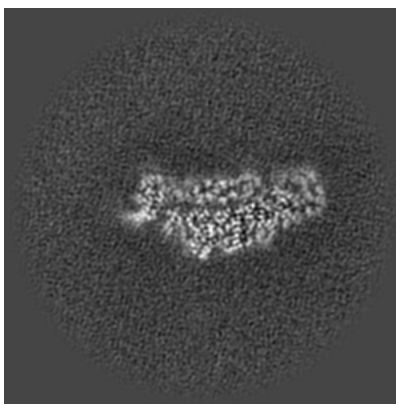
The images above show central slices of the map in three orthogonal directions.

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

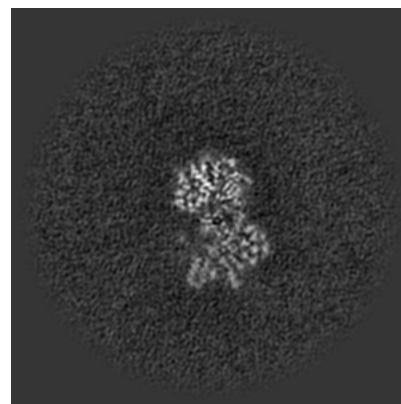
### 6.3.1 Primary map



X Index: 146



Y Index: 148

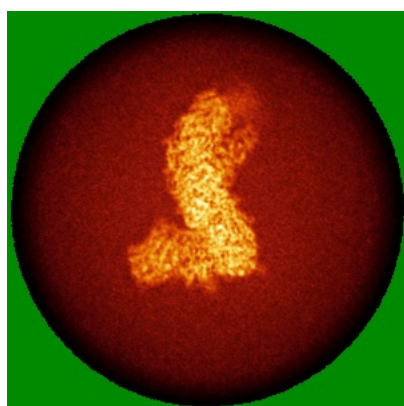


Z Index: 121

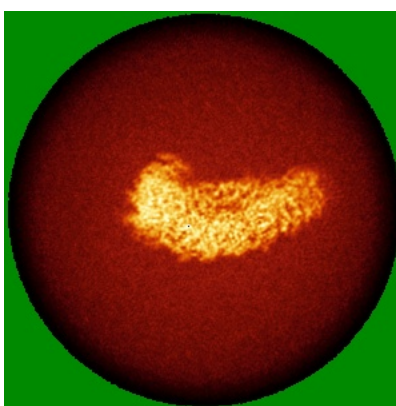
The images above show the largest variance slices of the map in three orthogonal directions.

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

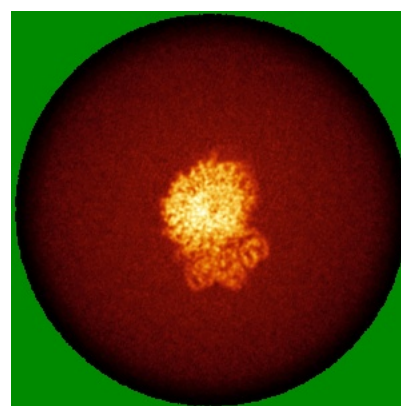
### 6.4.1 Primary map



X



Y

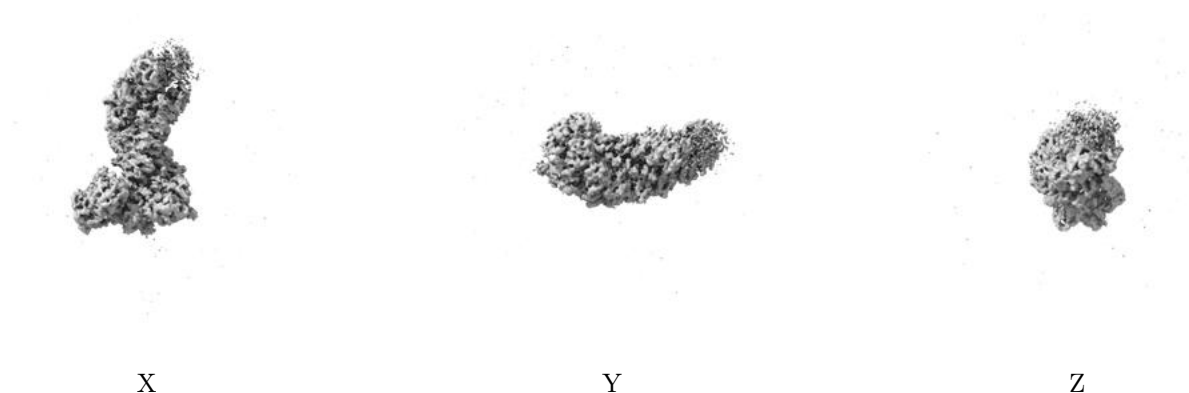


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

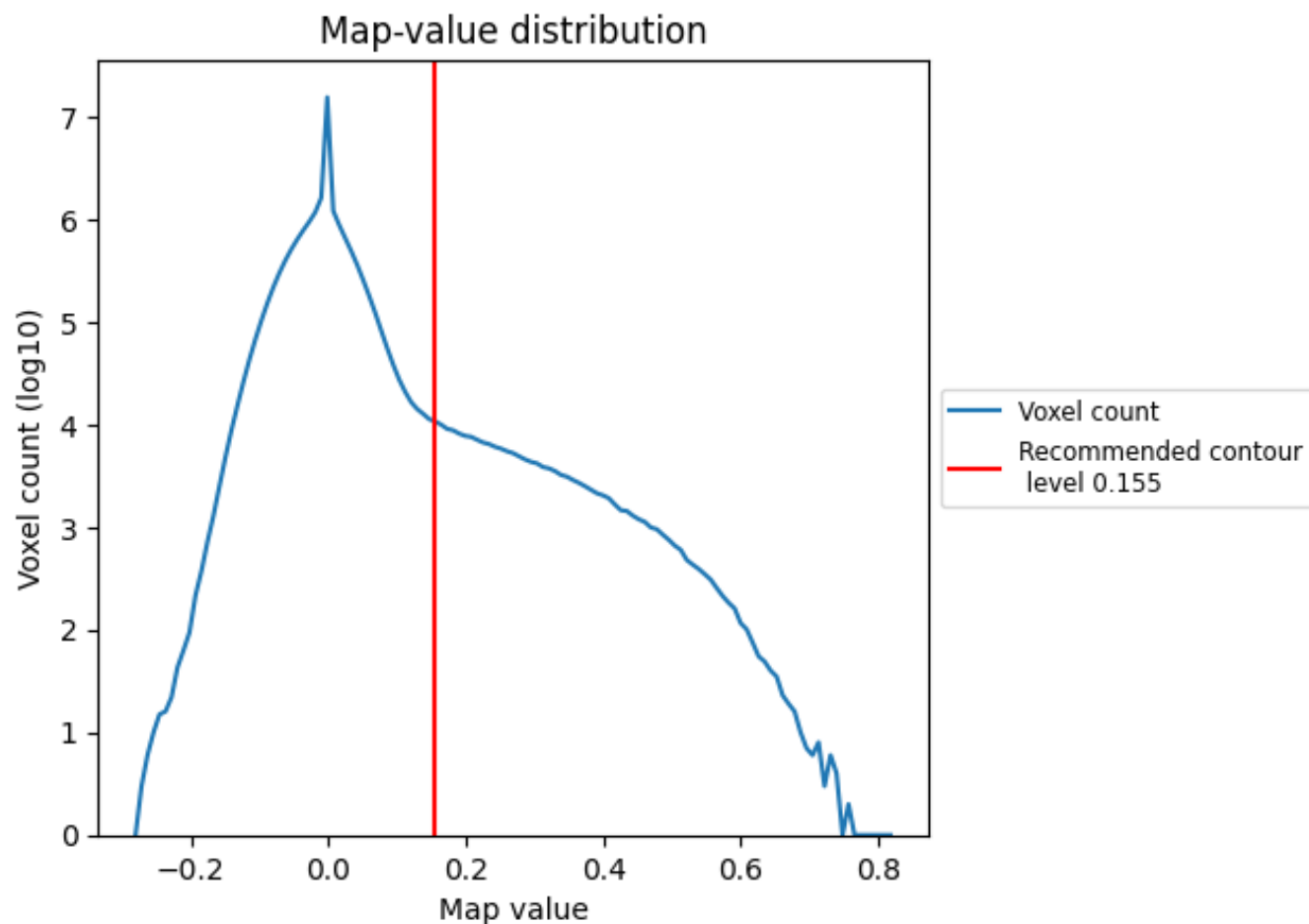
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

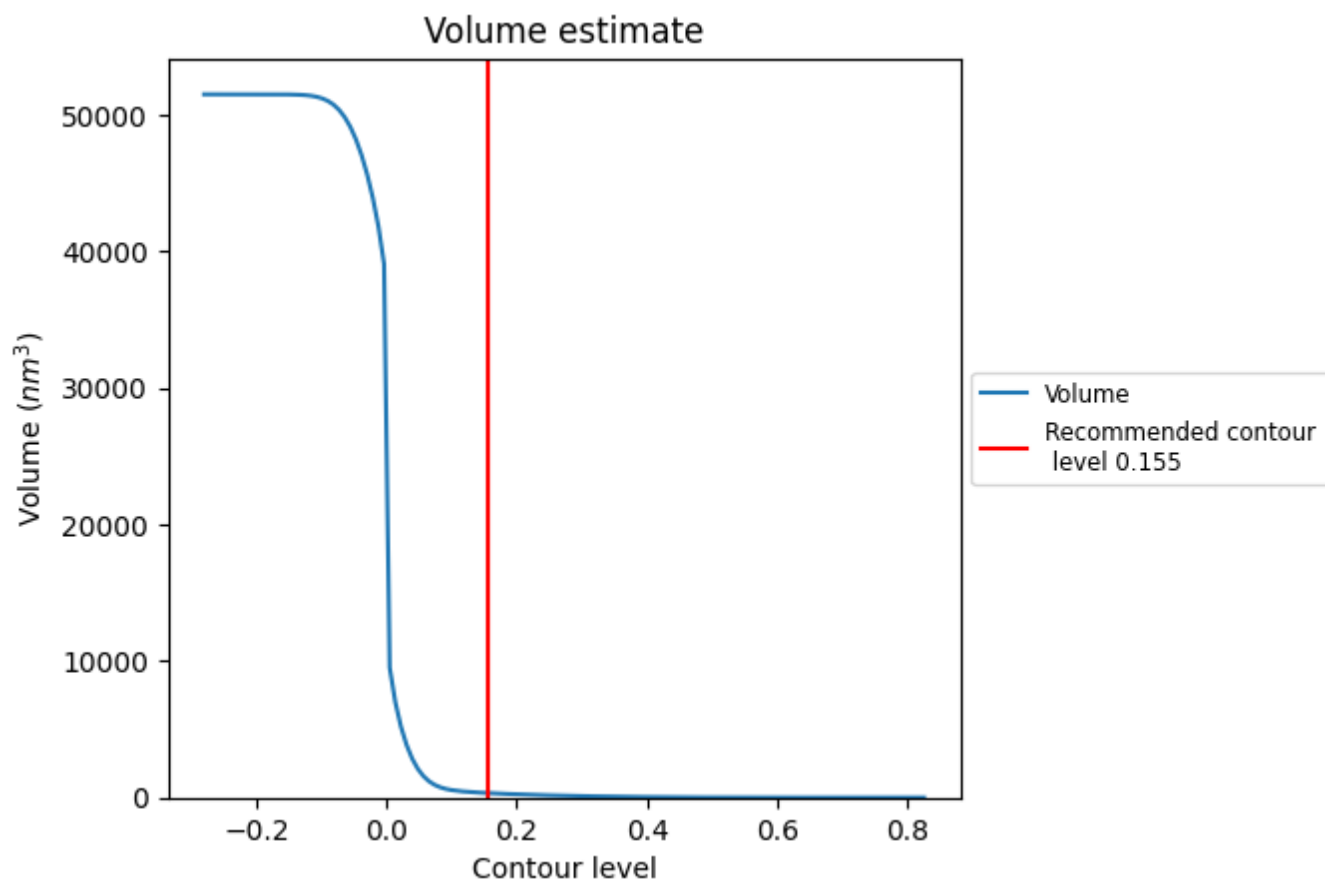
This section contains the results of statistical analysis of the map.

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



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

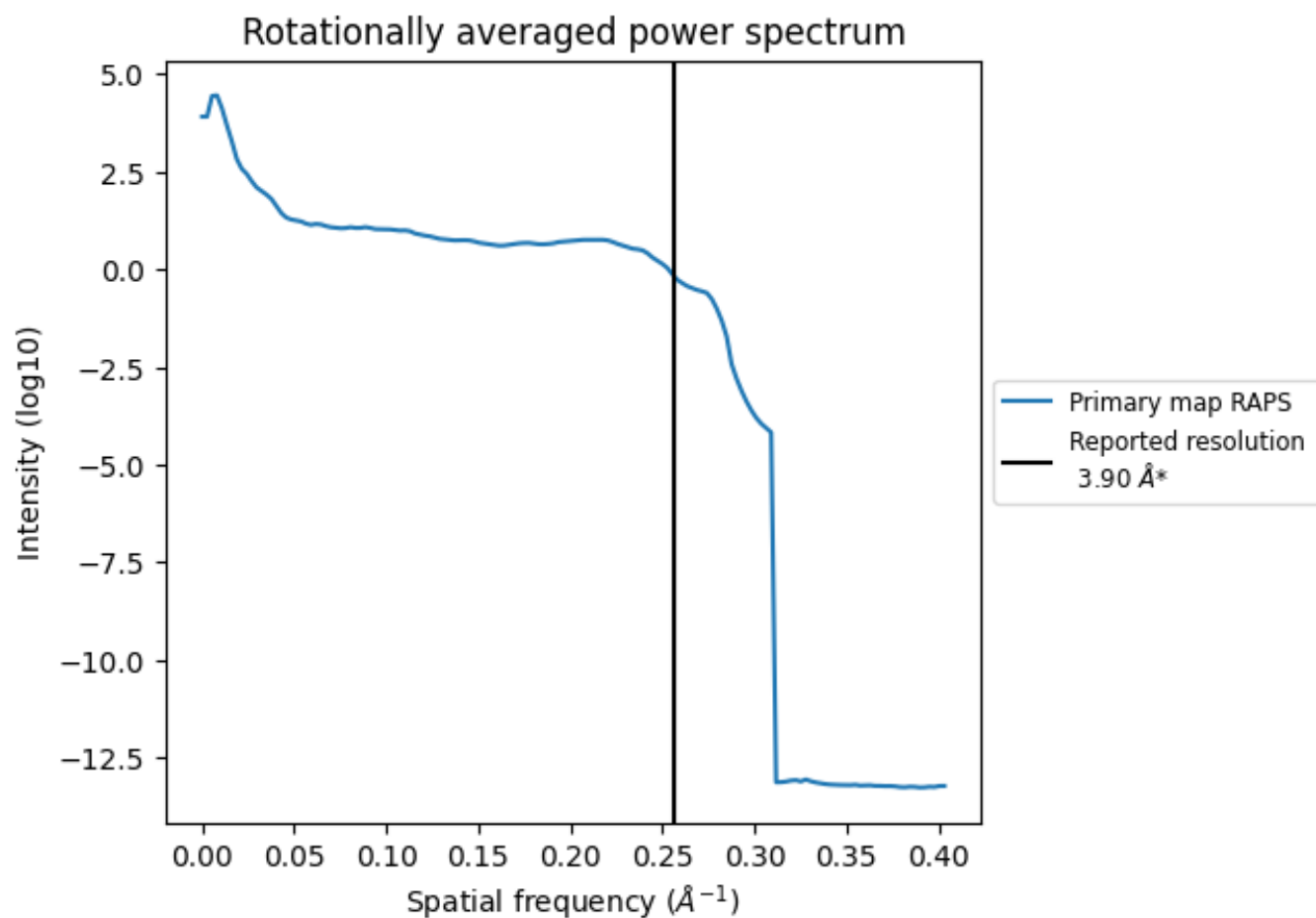
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm<sup>3</sup>; this corresponds to an approximate mass of 298 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 0.256 Å<sup>-1</sup>

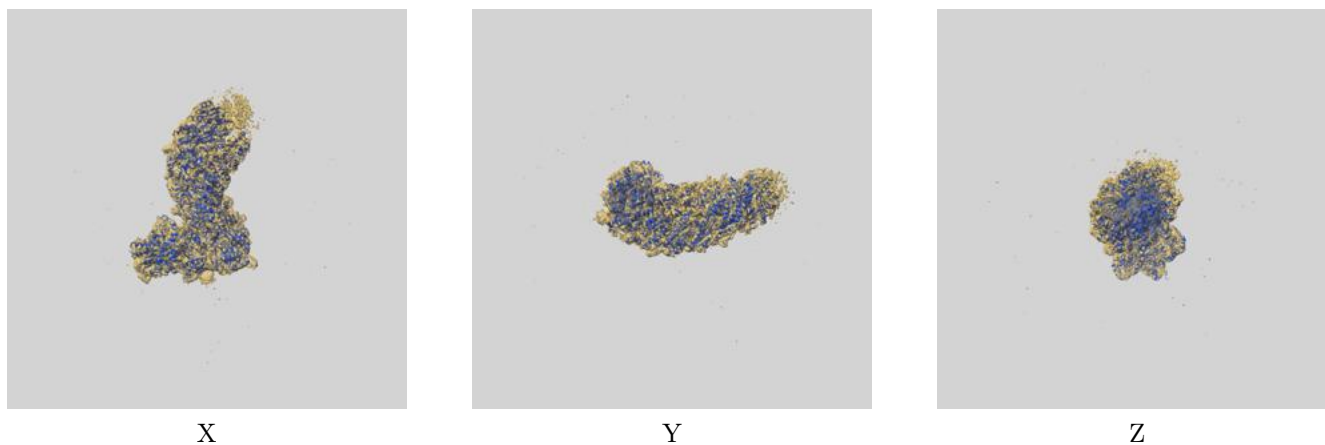
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-26083 and PDB model 7TR9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



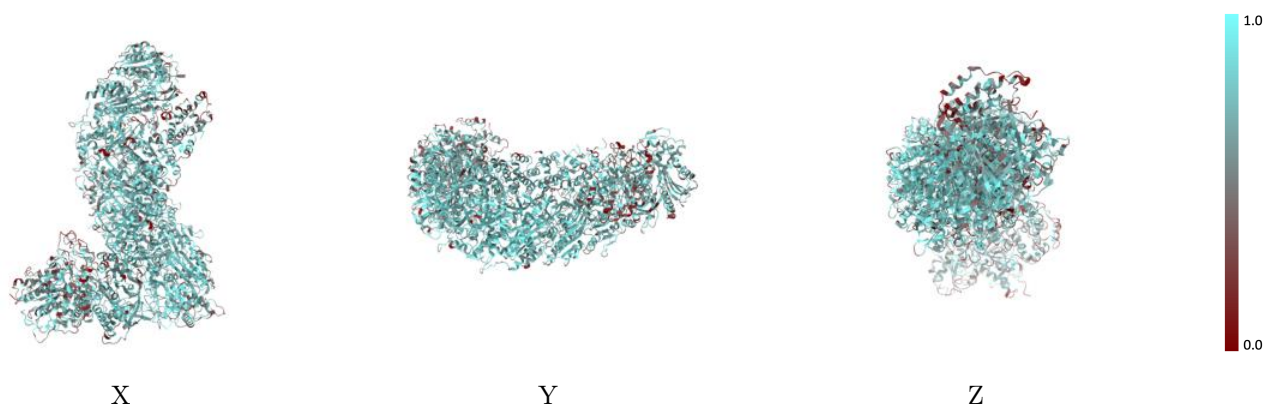
The images above show the 3D surface view of the map at the recommended contour level 0.155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



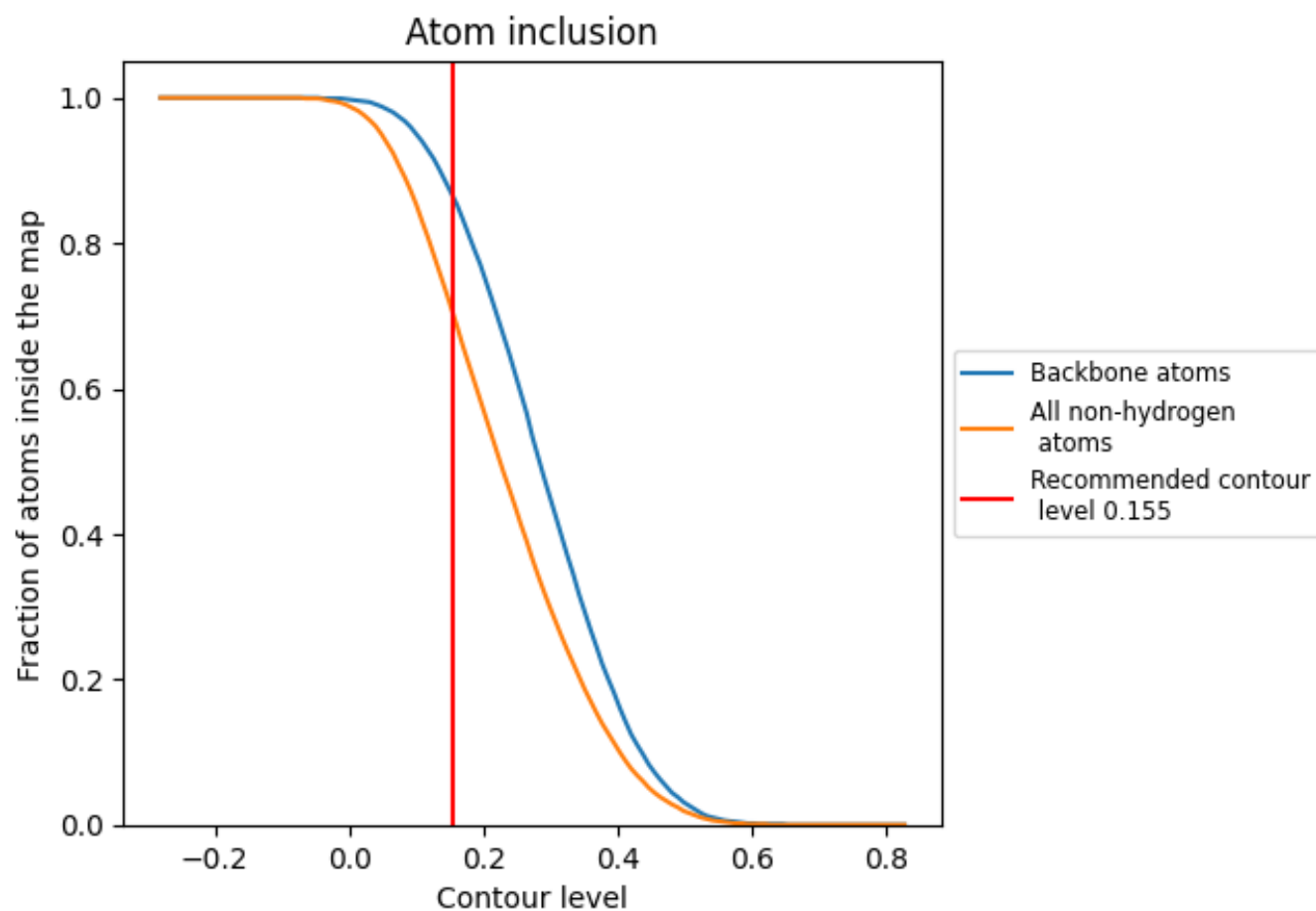
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.155).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 70% 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 (0.155) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7010   |  0.2250   |
| A     |  0.6120   |  0.1930   |
| C     |  0.7080   |  0.2490   |
| D     |  0.7390   |  0.2220   |
| E     |  0.7580   |  0.2600   |
| F     |  0.6880   |  0.2090   |
| G     |  0.6120   |  0.1840   |
| H     |  0.4490   |  0.1520   |
| I     |  0.7480   |  0.2400   |
| J     |  0.7950   |  0.2730   |
| K     |  0.7820   |  0.2490   |
| L     |  0.7480   |  0.2460   |
| M     |  0.7050   |  0.2320   |
| N     |  0.6990   |  0.2320   |
| O     |  0.6550  |  0.1940  |
| P     |  0.7080 |  0.1950 |
| Q     |  0.5790 |  0.1890 |
| R     |  0.8710 |  0.2850 |
| S     |  0.7500 |  0.2030 |
| T     |  0.7670 |  0.2260 |

