



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:48 PM UTC

PDB ID : 6ZFB / pdb\_00006zfb  
EMDB ID : EMD-11105  
Title : Structure of the B. subtilis RNA POLYMERASE in complex with HelD (dimer)  
Authors : Pei, H.-P.; Hilal, T.; Huang, Y.-H.; Said, N.; Loll, B.; Wahl, M.C.  
Deposited on : 2020-06-17  
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>.

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

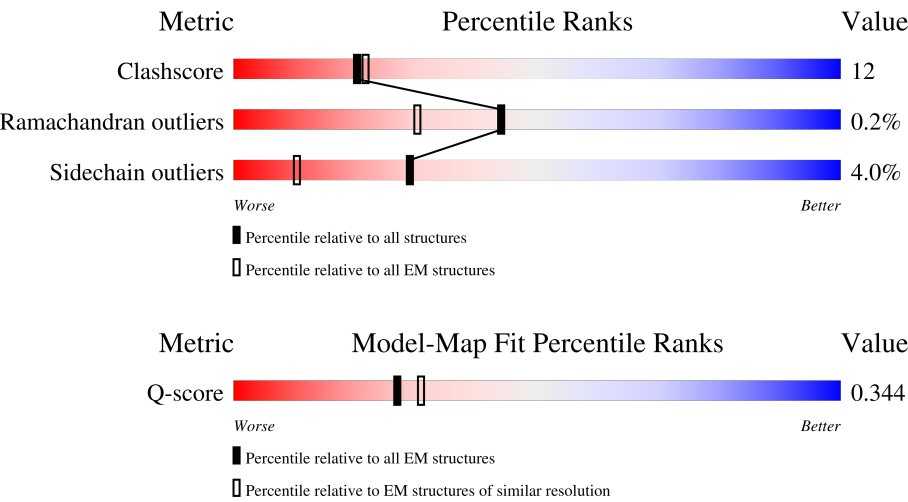
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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.



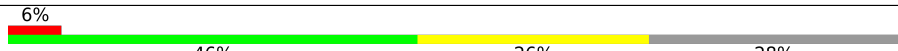
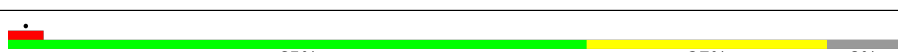
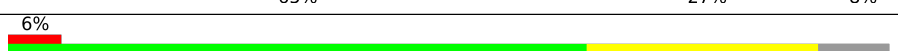
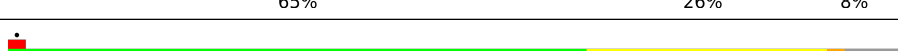
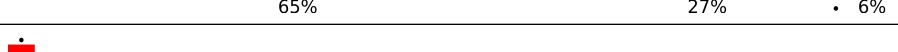
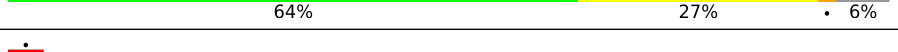
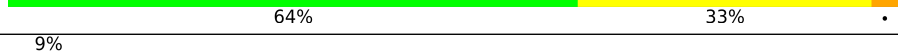
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 8989 ( 3.35 - 4.35 )                                     |

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   | D     | 139    |                  |
| 1   | d     | 139    |                  |
| 2   | E     | 69     |                  |
| 2   | e     | 69     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3   | U     | 314    |  |
| 3   | V     | 314    |  |
| 3   | u     | 314    |  |
| 3   | v     | 314    |  |
| 4   | X     | 1193   |  |
| 4   | x     | 1193   |  |
| 5   | Y     | 1199   |  |
| 5   | y     | 1199   |  |
| 6   | H     | 774    |  |
| 6   | h     | 774    |  |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 57505 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 DNA-directed RNA polymerase subunit delta.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | D     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 998   | 630 | 169 | 197 | 2 |         |       |
| 1   | d     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 998   | 630 | 169 | 197 | 2 |         |       |

- Molecule 2 is a protein called RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 2   | E     | 69       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 580   | 373 | 92 | 114 | 1 |         |       |
| 2   | e     | 69       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 580   | 373 | 92 | 114 | 1 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|--|---------|-------|
| 3   | U     | 231      | Total | C    | N   | O   |  | 0       | 0     |
|     |       |          | 1774  | 1116 | 300 | 358 |  |         |       |
| 3   | V     | 227      | Total | C    | N   | O   |  | 0       | 0     |
|     |       |          | 1745  | 1099 | 293 | 353 |  |         |       |
| 3   | u     | 231      | Total | C    | N   | O   |  | 0       | 0     |
|     |       |          | 1774  | 1116 | 300 | 358 |  |         |       |
| 3   | v     | 227      | Total | C    | N   | O   |  | 0       | 0     |
|     |       |          | 1745  | 1099 | 293 | 353 |  |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | X     | 1093     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8485  | 5323 | 1486 | 1643 | 33 |         |       |
| 4   | x     | 1092     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8478  | 5318 | 1485 | 1642 | 33 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 5   | Y     | 1127     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8867  | 5594 | 1571 | 1661 | 41 |         |       |
| 5   | y     | 1127     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8867  | 5594 | 1571 | 1661 | 41 |         |       |

- Molecule 6 is a protein called DNA helicase.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 6   | H     | 771      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6306  | 4005 | 1086 | 1184 | 31 |         |       |
| 6   | h     | 771      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6306  | 4005 | 1086 | 1184 | 31 |         |       |

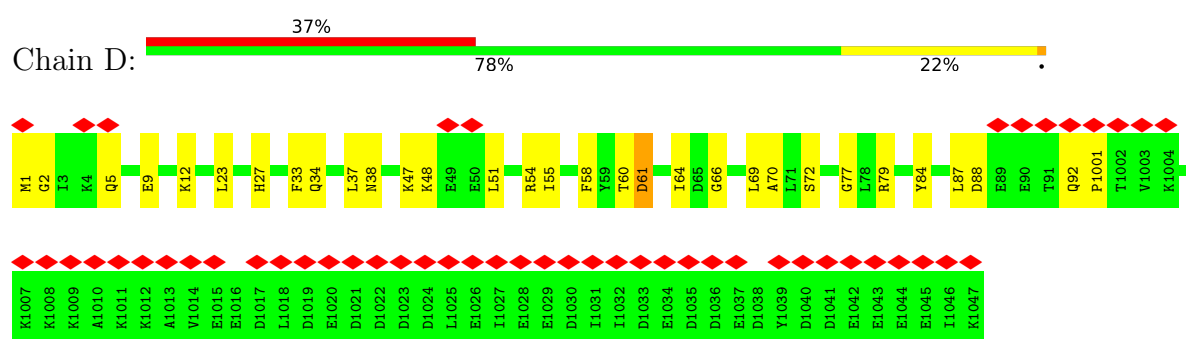
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 7   | Y     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 7   | y     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

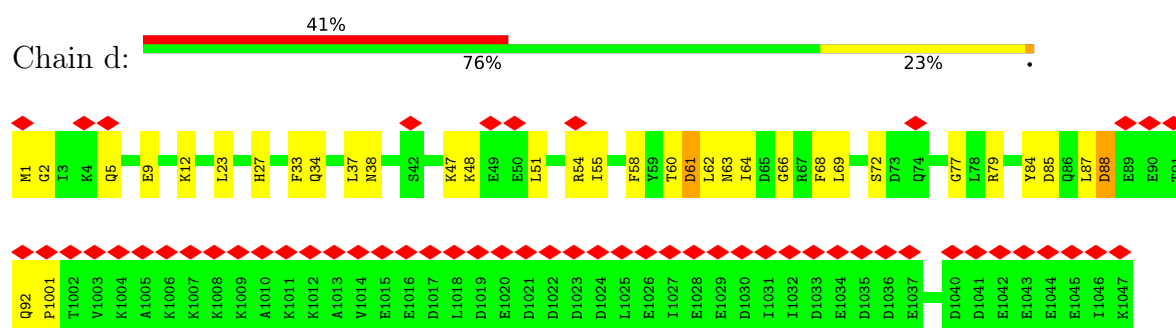
### 3 Residue-property plots

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

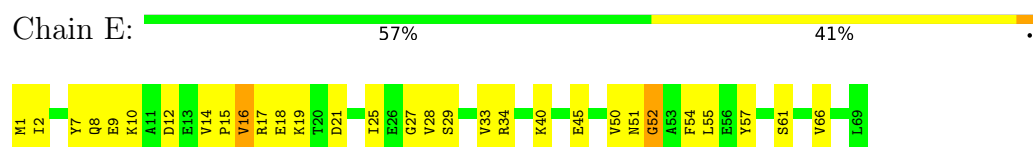
- Molecule 1: DNA-directed RNA polymerase subunit delta



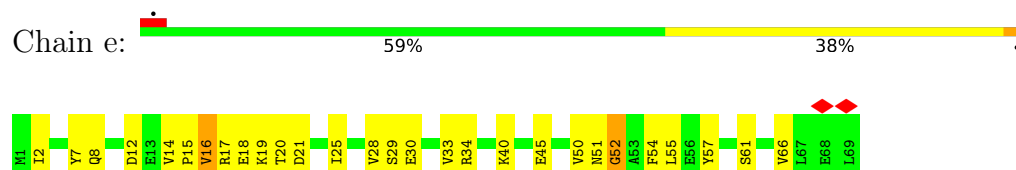
- Molecule 1: DNA-directed RNA polymerase subunit delta



- Molecule 2: RNA polymerase subunit omega



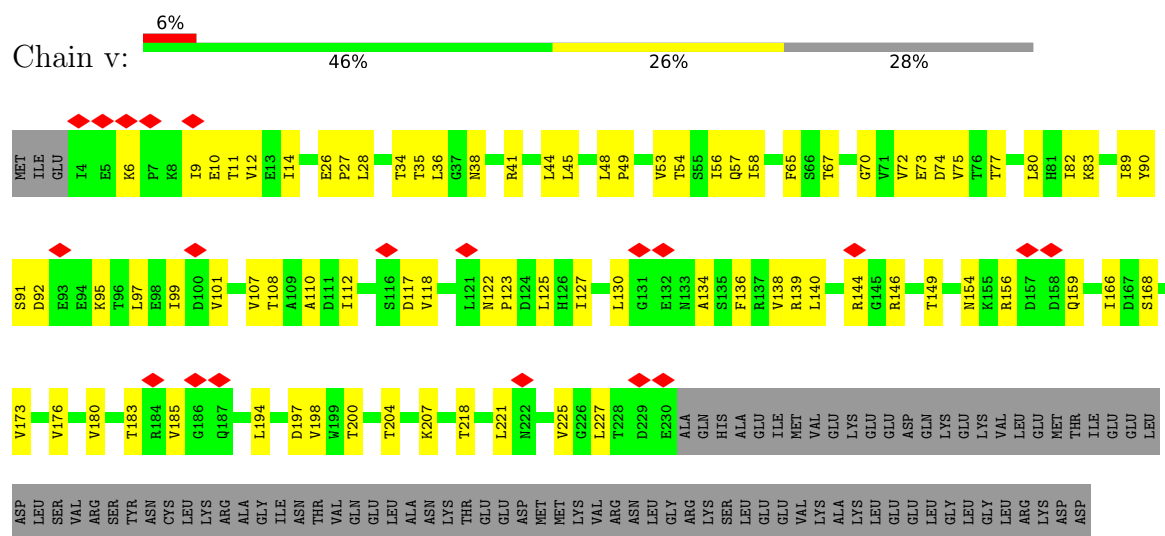
- Molecule 2: RNA polymerase subunit omega



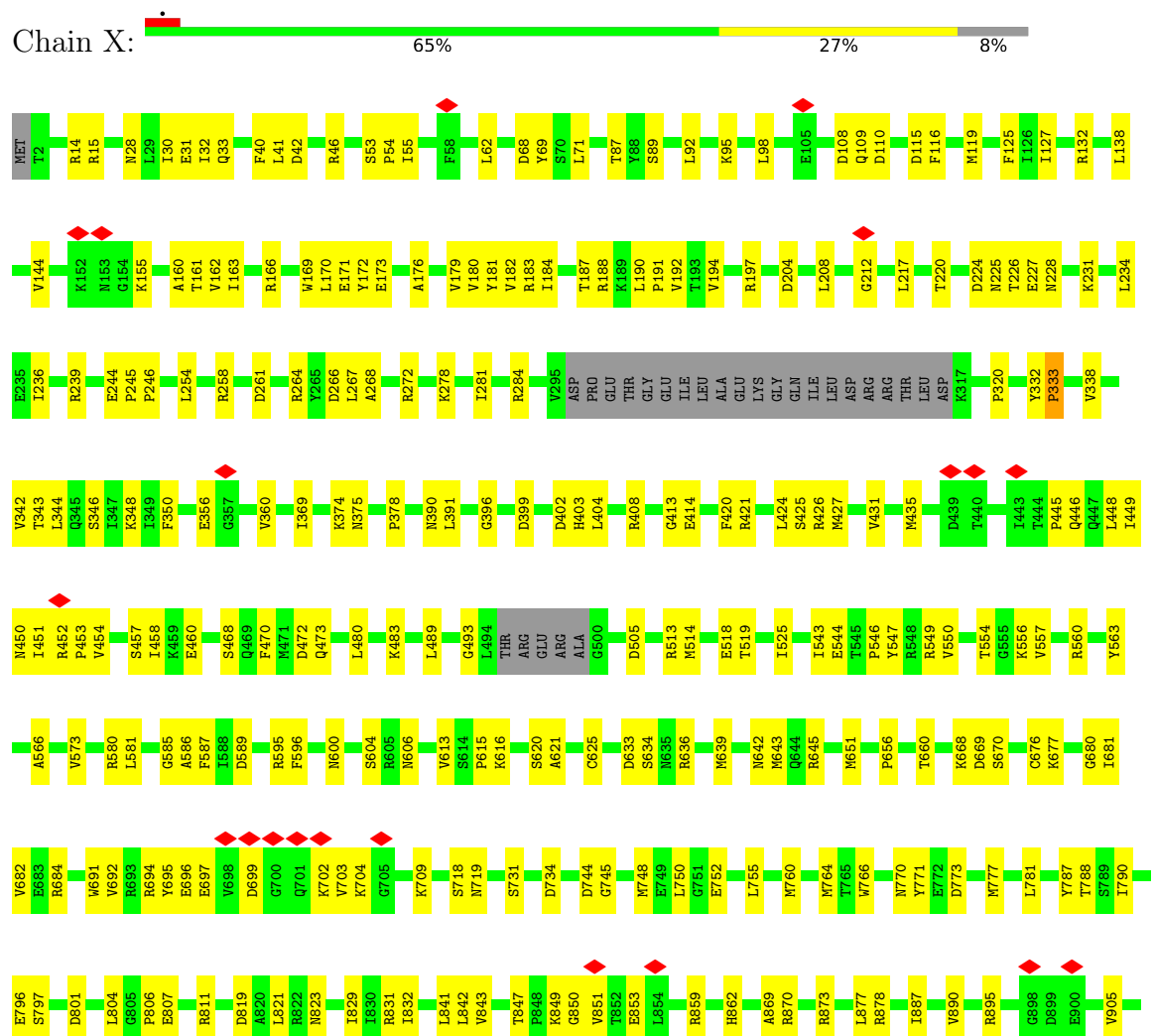
Chain U: 

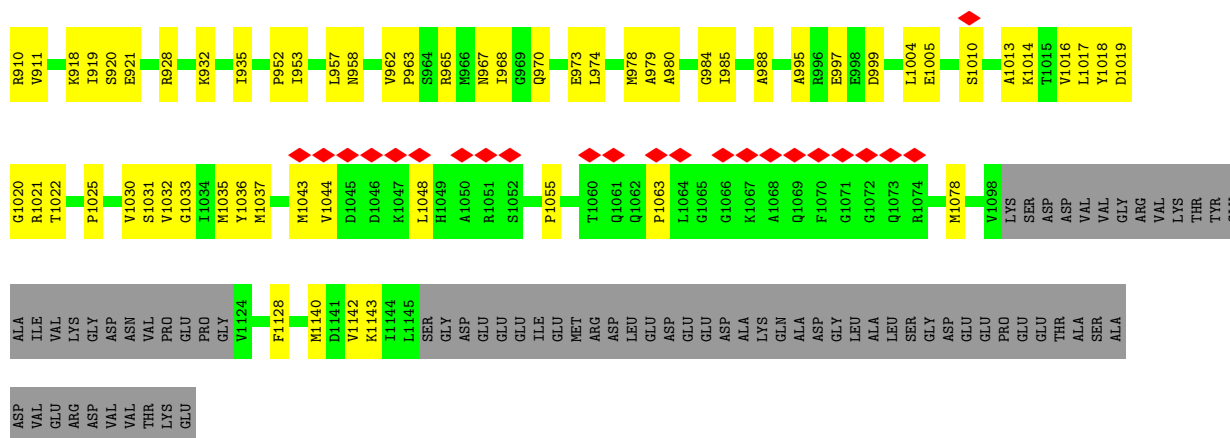


• Molecule 3: DNA-directed RNA polymerase subunit alpha

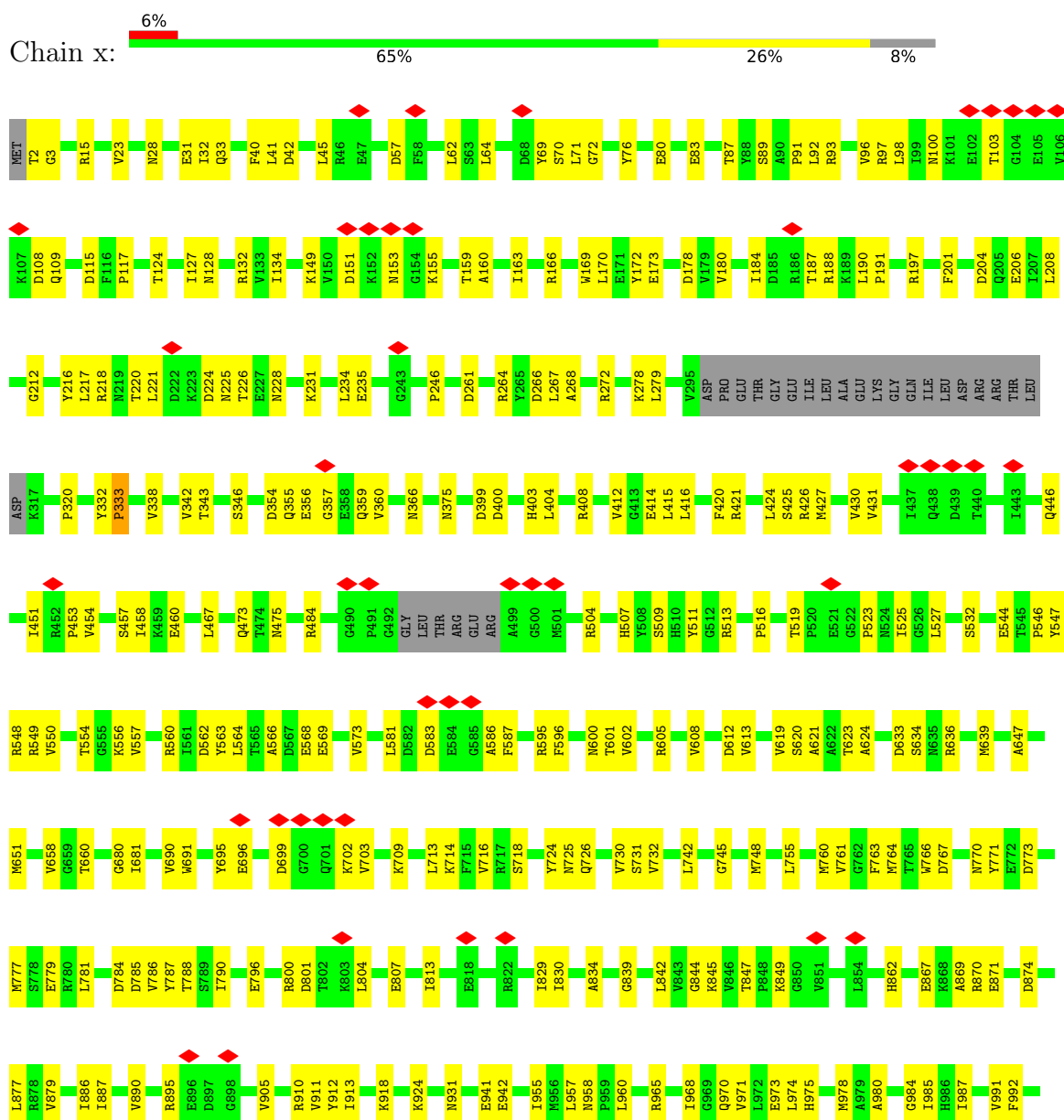


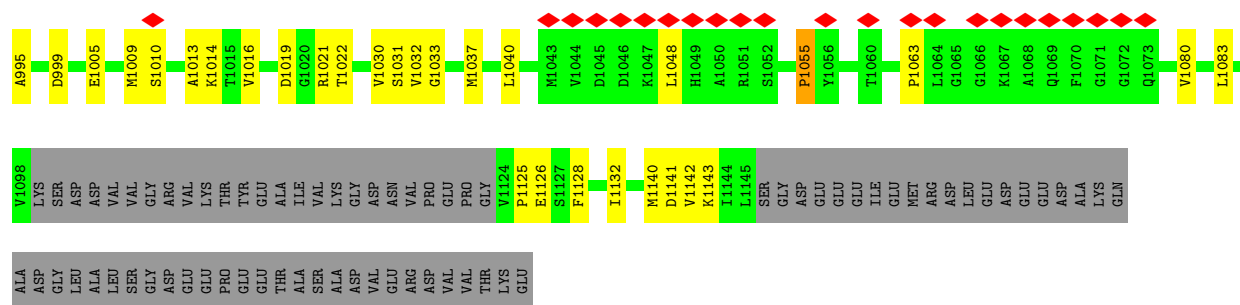
• Molecule 4: DNA-directed RNA polymerase subunit beta





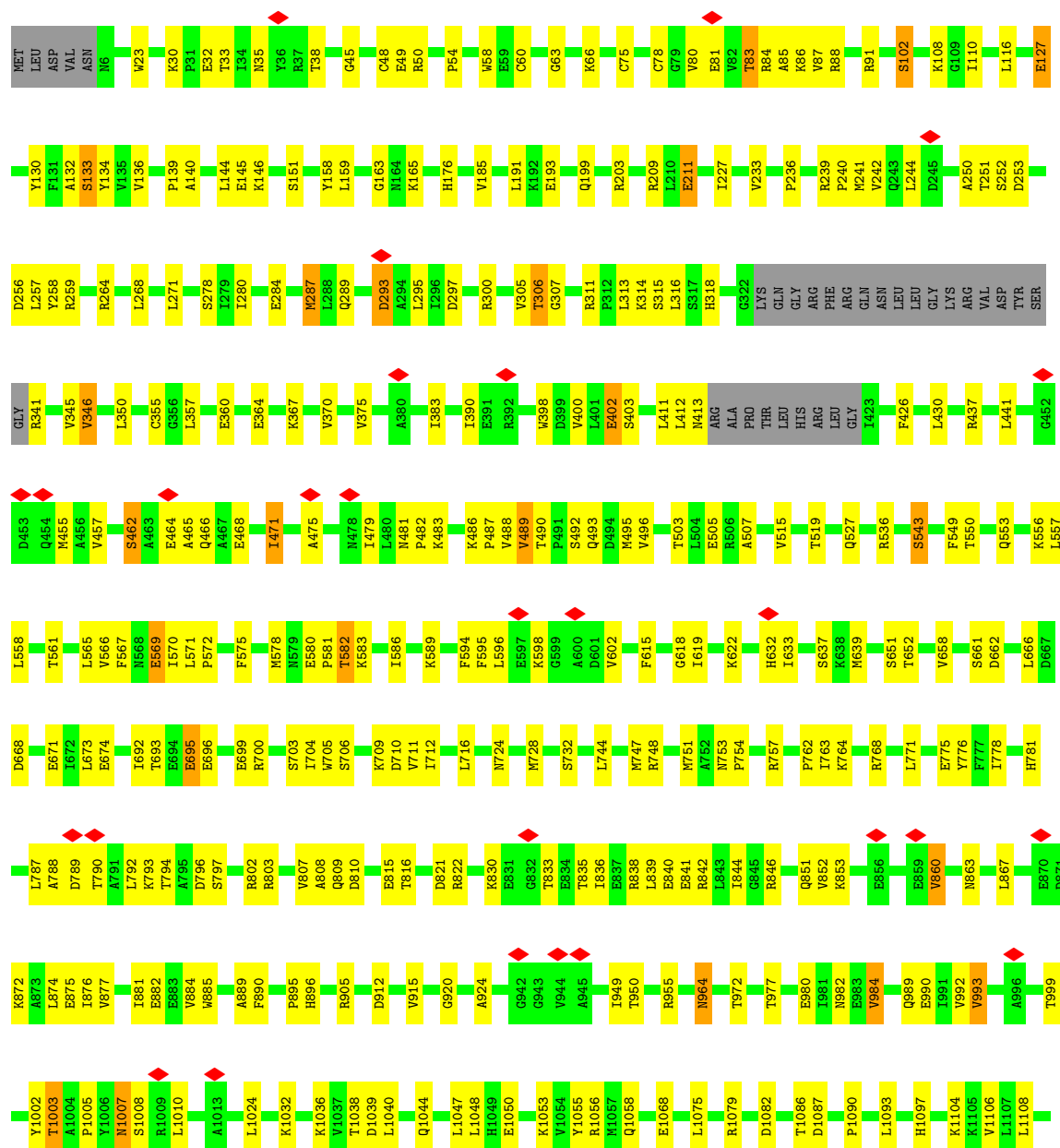
• Molecule 4: DNA-directed RNA polymerase subunit beta



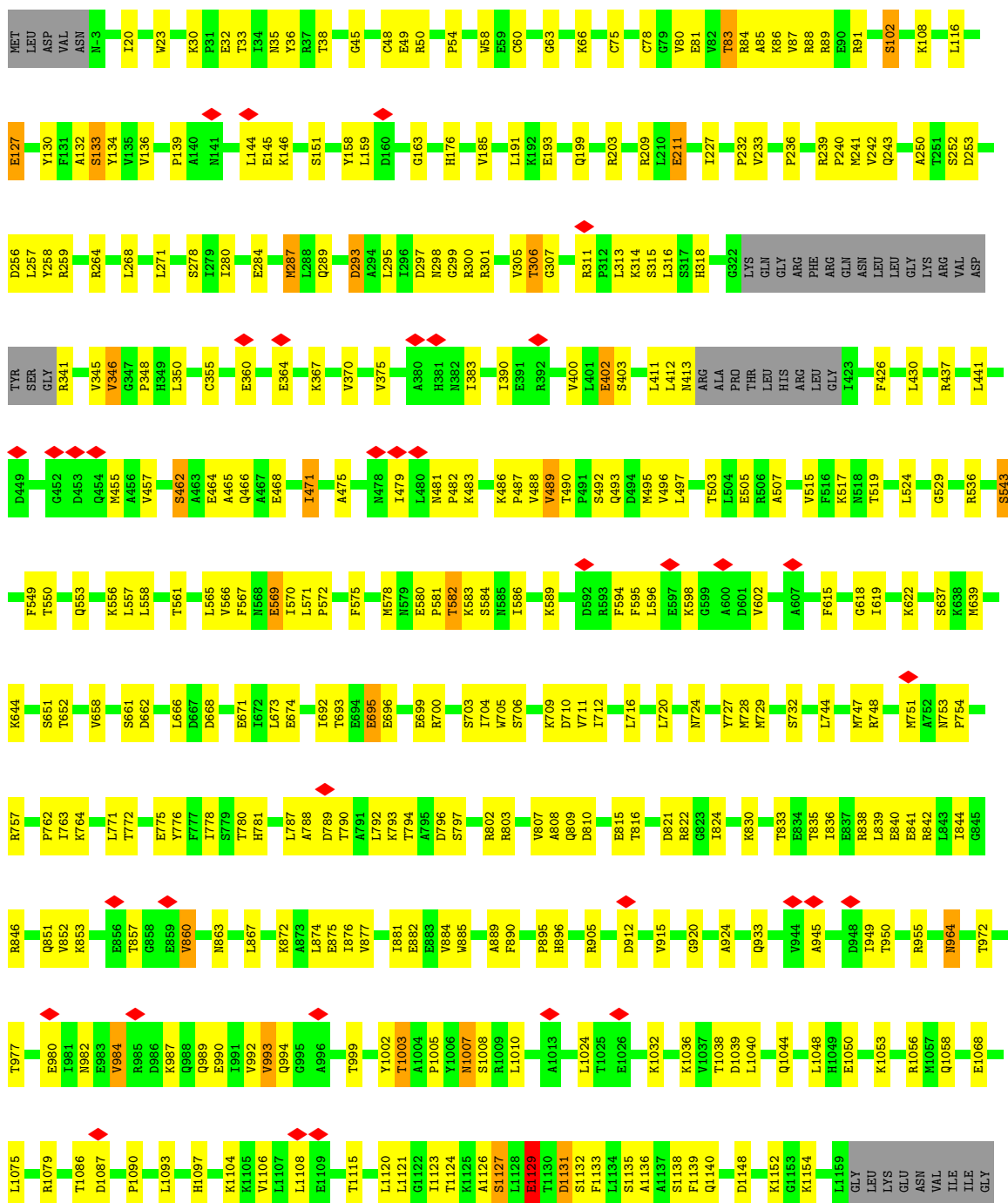


• Molecule 5: DNA-directed RNA polymerase subunit beta'

Chain Y: 65% 27% 6%



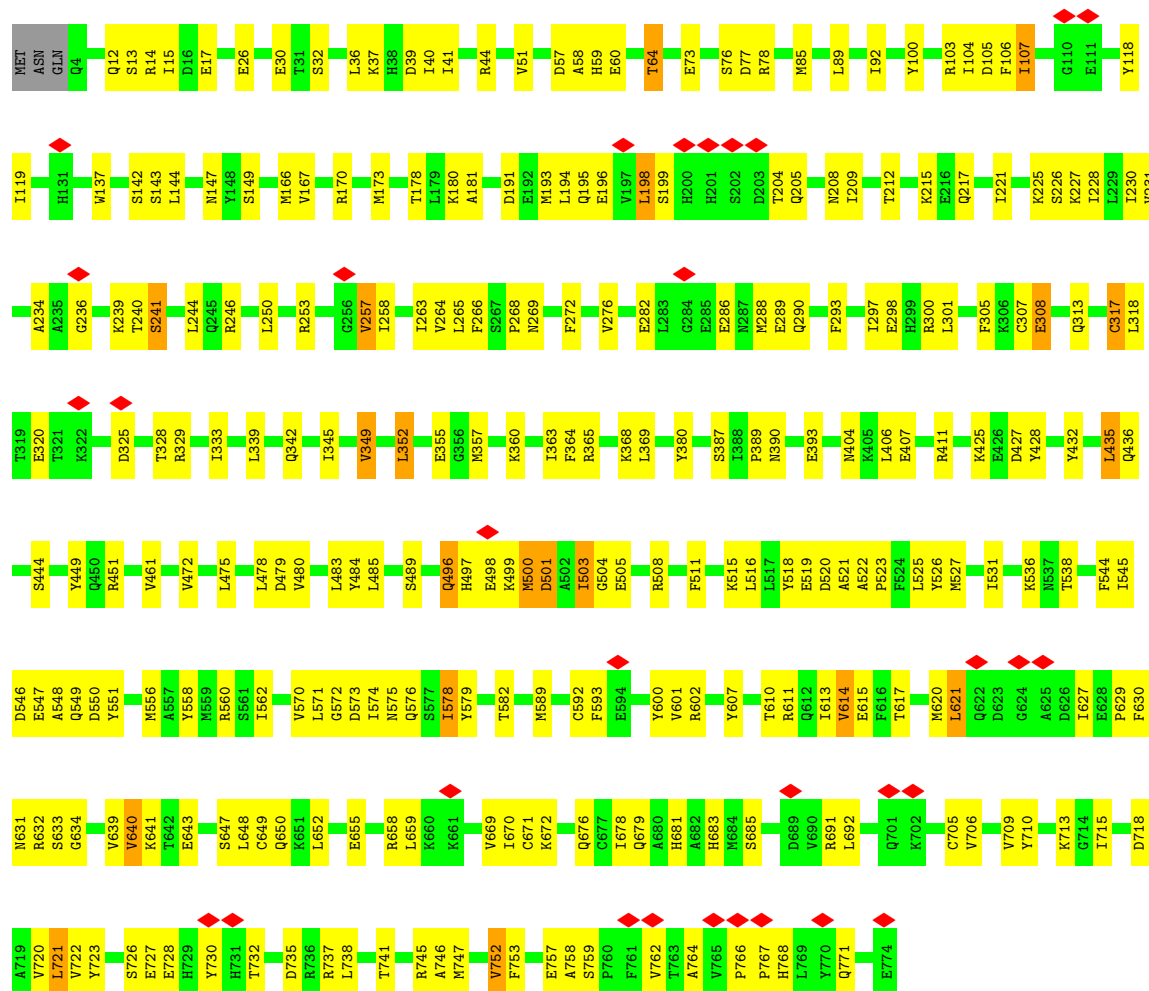
- Molecule 5: DNA-directed RNA polymerase subunit beta'



LYS  
LEU  
VAL  
PRO  
ALA  
GLY  
THR  
GLY  
MET  
MET  
LYS  
TYR  
ARG  
LYS  
VAL  
LYS  
PRO  
VAL  
SER  
ASN  
VAL  
GLN  
PRO  
THR  
ASP  
ASP  
MET  
VAL  
PRO  
VAL  
GLU

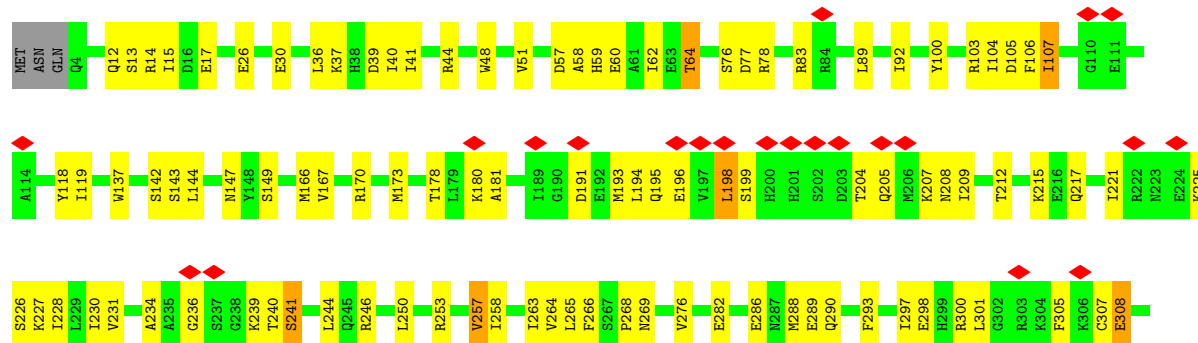
• Molecule 6: DNA helicase

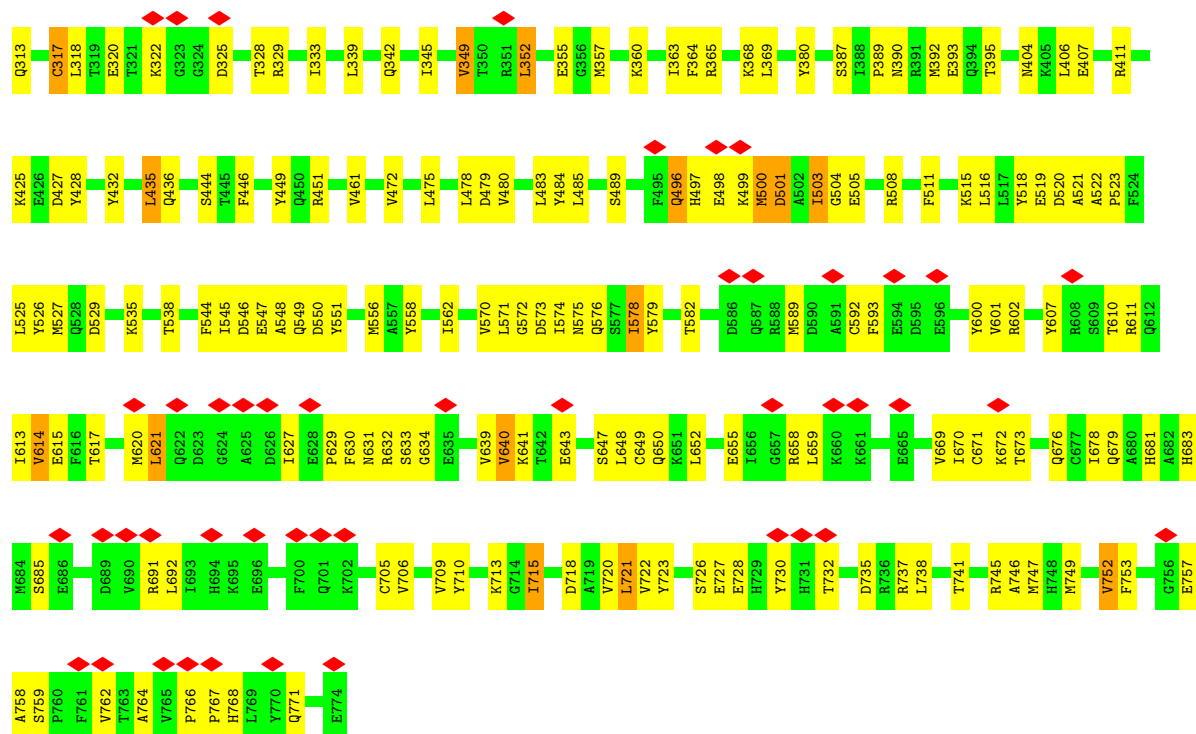
Chain H:  64% 33%



• Molecule 6: DNA helicase

Chain h:  9% 63% 34%





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 176374                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 96000                                   | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.914                                   | Depositor |
| Minimum map value                    | -0.463                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.1                                     | Depositor |
| Map size (Å)                         | 366.08002, 366.08002, 366.08002         | wwPDB     |
| Map dimensions                       | 280, 280, 280                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.3074286, 1.3074286, 1.3074286         | 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: ZN

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   | D     | 0.13         | 0/1013      | 0.36        | 1/1377 (0.1%)   |
| 1   | d     | 0.13         | 0/1013      | 0.36        | 1/1377 (0.1%)   |
| 2   | E     | 0.16         | 0/589       | 0.53        | 0/789           |
| 2   | e     | 0.16         | 0/589       | 0.53        | 0/789           |
| 3   | U     | 0.12         | 0/1801      | 0.32        | 0/2450          |
| 3   | V     | 0.11         | 0/1771      | 0.35        | 0/2409          |
| 3   | u     | 0.13         | 0/1801      | 0.34        | 0/2450          |
| 3   | v     | 0.12         | 0/1771      | 0.34        | 0/2409          |
| 4   | X     | 0.13         | 0/8627      | 0.37        | 4/11668 (0.0%)  |
| 4   | x     | 0.13         | 0/8620      | 0.36        | 4/11659 (0.0%)  |
| 5   | Y     | 0.14         | 0/9009      | 0.39        | 1/12155 (0.0%)  |
| 5   | y     | 0.14         | 0/9009      | 0.39        | 1/12155 (0.0%)  |
| 6   | H     | 0.14         | 0/6437      | 0.40        | 1/8662 (0.0%)   |
| 6   | h     | 0.14         | 0/6437      | 0.40        | 1/8662 (0.0%)   |
| All | All   | 0.13         | 0/58487     | 0.38        | 14/79011 (0.0%) |

There are no bond length outliers.

All (14) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | x     | 333  | PRO  | N-CA-CB | 7.53 | 111.15      | 103.25   |
| 4   | X     | 333  | PRO  | N-CA-CB | 7.52 | 111.15      | 103.25   |
| 1   | d     | 1001 | PRO  | N-CA-CB | 6.74 | 110.42      | 103.00   |
| 1   | D     | 1001 | PRO  | N-CA-CB | 6.72 | 110.39      | 103.00   |
| 4   | x     | 320  | PRO  | N-CA-CB | 6.55 | 110.13      | 103.25   |
| 4   | X     | 1055 | PRO  | N-CA-CB | 6.55 | 110.13      | 103.25   |
| 4   | x     | 1055 | PRO  | N-CA-CB | 6.52 | 110.10      | 103.25   |
| 4   | X     | 320  | PRO  | N-CA-CB | 6.50 | 110.08      | 103.25   |
| 4   | X     | 1063 | PRO  | N-CA-CB | 6.32 | 109.99      | 103.23   |
| 4   | x     | 1063 | PRO  | N-CA-CB | 6.30 | 109.97      | 103.23   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 5   | Y     | 1129 | GLU  | CA-CB-CG | 5.67  | 125.45      | 114.10   |
| 5   | y     | 1129 | GLU  | CA-CB-CG | 5.65  | 125.41      | 114.10   |
| 6   | H     | 107  | ILE  | N-CA-C   | -5.08 | 107.86      | 112.12   |
| 6   | h     | 107  | ILE  | N-CA-C   | -5.05 | 107.88      | 112.12   |

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   | D     | 998   | 0        | 842      | 22      | 0            |
| 1   | d     | 998   | 0        | 842      | 24      | 0            |
| 2   | E     | 580   | 0        | 585      | 22      | 0            |
| 2   | e     | 580   | 0        | 585      | 22      | 0            |
| 3   | U     | 1774  | 0        | 1781     | 49      | 0            |
| 3   | V     | 1745  | 0        | 1756     | 53      | 0            |
| 3   | u     | 1774  | 0        | 1781     | 48      | 0            |
| 3   | v     | 1745  | 0        | 1756     | 59      | 0            |
| 4   | X     | 8485  | 0        | 8312     | 211     | 0            |
| 4   | x     | 8478  | 0        | 8303     | 210     | 0            |
| 5   | Y     | 8867  | 0        | 9076     | 203     | 0            |
| 5   | y     | 8867  | 0        | 9081     | 216     | 0            |
| 6   | H     | 6306  | 0        | 6234     | 169     | 0            |
| 6   | h     | 6306  | 0        | 6234     | 173     | 0            |
| 7   | Y     | 1     | 0        | 0        | 0       | 0            |
| 7   | y     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 57505 | 0        | 57168    | 1397    | 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 12.

All (1397) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 5:y:809:GLN:HE22 | 5:y:1135:SER:HB3  | 1.24                     | 0.97              |
| 5:Y:809:GLN:HE22 | 5:Y:1135:SER:HB3  | 1.24                     | 0.97              |
| 5:y:413:ASN:O    | 5:y:455:MET:HA    | 1.77                     | 0.84              |
| 5:Y:413:ASN:O    | 5:Y:455:MET:HA    | 1.77                     | 0.84              |
| 1:d:48:LYS:HA    | 1:d:51:LEU:HB2    | 1.61                     | 0.83              |
| 1:D:48:LYS:HA    | 1:D:51:LEU:HB2    | 1.61                     | 0.82              |
| 4:x:109:GLN:HB3  | 4:x:446:GLN:HG2   | 1.61                     | 0.82              |
| 3:U:85:LEU:HA    | 3:U:122:ASN:HD21  | 1.45                     | 0.81              |
| 6:h:239:LYS:HB2  | 6:h:571:LEU:HD23  | 1.65                     | 0.78              |
| 1:d:34:GLN:O     | 1:d:38:ASN:ND2    | 2.16                     | 0.78              |
| 6:H:239:LYS:HB2  | 6:H:571:LEU:HD23  | 1.65                     | 0.78              |
| 1:D:34:GLN:O     | 1:D:38:ASN:ND2    | 2.16                     | 0.77              |
| 4:X:180:VAL:HG22 | 4:X:220:THR:HG21  | 1.67                     | 0.77              |
| 3:V:173:VAL:HA   | 3:V:200:THR:HA    | 1.68                     | 0.75              |
| 4:x:342:VAL:HG12 | 4:x:343:THR:HG23  | 1.66                     | 0.75              |
| 5:y:1007:ASN:OD1 | 5:y:1007:ASN:N    | 2.21                     | 0.74              |
| 5:Y:1131:ASP:OD1 | 5:Y:1131:ASP:N    | 2.19                     | 0.74              |
| 5:Y:578:MET:HE1  | 5:Y:586:ILE:HA    | 1.69                     | 0.74              |
| 3:V:121:LEU:HD22 | 3:V:203:SER:HB2   | 1.69                     | 0.73              |
| 6:H:194:LEU:HD12 | 6:H:632:ARG:HG3   | 1.70                     | 0.73              |
| 5:y:578:MET:HE1  | 5:y:586:ILE:HA    | 1.69                     | 0.73              |
| 6:H:726:SER:HB2  | 6:H:757:GLU:HB2   | 1.71                     | 0.73              |
| 6:h:194:LEU:HD12 | 6:h:632:ARG:HG3   | 1.70                     | 0.73              |
| 5:y:809:GLN:HE22 | 5:y:1135:SER:CB   | 2.00                     | 0.73              |
| 4:X:138:LEU:HD11 | 4:X:514:MET:HE1   | 1.70                     | 0.73              |
| 5:y:1131:ASP:OD1 | 5:y:1131:ASP:N    | 2.19                     | 0.73              |
| 4:X:600:ASN:HD21 | 5:Y:778:ILE:HD11  | 1.54                     | 0.72              |
| 4:x:208:LEU:HA   | 4:x:212:GLY:HA3   | 1.71                     | 0.72              |
| 4:x:544:GLU:HB3  | 4:x:563:TYR:HB3   | 1.72                     | 0.72              |
| 4:x:600:ASN:HD21 | 5:y:778:ILE:HD11  | 1.55                     | 0.72              |
| 1:d:61:ASP:OD1   | 5:y:822:ARG:NH1   | 2.23                     | 0.72              |
| 3:v:27:PRO:HG3   | 3:v:185:VAL:HG11  | 1.70                     | 0.72              |
| 4:x:995:ALA:HB1  | 4:x:999:ASP:HB3   | 1.72                     | 0.72              |
| 5:Y:809:GLN:HE22 | 5:Y:1135:SER:CB   | 2.00                     | 0.71              |
| 3:V:54:THR:HG22  | 3:V:168:SER:HB2   | 1.72                     | 0.71              |
| 4:X:155:LYS:HZ3  | 4:X:176:ALA:HA    | 1.55                     | 0.71              |
| 4:X:764:MET:HE3  | 4:X:1030:VAL:HG11 | 1.73                     | 0.71              |
| 6:h:726:SER:HB2  | 6:h:757:GLU:HB2   | 1.71                     | 0.71              |
| 2:E:34:ARG:HD2   | 4:X:1010:SER:HB3  | 1.71                     | 0.71              |
| 6:h:652:LEU:HD22 | 6:h:721:LEU:HD21  | 1.73                     | 0.71              |
| 3:v:173:VAL:HG23 | 3:v:200:THR:H     | 1.55                     | 0.71              |
| 6:H:652:LEU:HD22 | 6:H:721:LEU:HD21  | 1.73                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:y:673:LEU:HD21 | 5:y:764:LYS:HB3  | 1.72                     | 0.71              |
| 3:U:89:ILE:HG22  | 3:U:118:VAL:HG12 | 1.71                     | 0.71              |
| 6:h:496:GLN:HB3  | 6:h:500:MET:HG3  | 1.73                     | 0.71              |
| 4:x:180:VAL:HG22 | 4:x:220:THR:HG21 | 1.73                     | 0.70              |
| 4:X:557:VAL:HG22 | 4:X:585:GLY:HA2  | 1.73                     | 0.70              |
| 6:H:500:MET:HE3  | 6:H:501:ASP:H    | 1.57                     | 0.70              |
| 3:u:197:ASP:OD2  | 3:u:199:TRP:NE1  | 2.25                     | 0.70              |
| 4:x:556:LYS:HD3  | 4:x:586:ALA:H    | 1.57                     | 0.70              |
| 6:h:500:MET:HE3  | 6:h:501:ASP:H    | 1.57                     | 0.70              |
| 3:v:54:THR:HG22  | 3:v:168:SER:HB2  | 1.72                     | 0.69              |
| 6:H:195:GLN:HA   | 6:H:198:LEU:HB2  | 1.74                     | 0.69              |
| 3:V:38:ASN:ND2   | 4:X:1021:ARG:O   | 2.25                     | 0.69              |
| 6:h:227:LYS:HG2  | 6:h:228:ILE:HG13 | 1.75                     | 0.69              |
| 5:Y:1007:ASN:OD1 | 5:Y:1007:ASN:N   | 2.21                     | 0.69              |
| 1:D:51:LEU:HA    | 1:D:54:ARG:HB2   | 1.73                     | 0.69              |
| 1:d:51:LEU:HA    | 1:d:54:ARG:HB2   | 1.73                     | 0.69              |
| 6:h:308:GLU:HB2  | 6:h:515:LYS:HE2  | 1.74                     | 0.69              |
| 6:h:720:VAL:HG12 | 6:h:746:ALA:HB2  | 1.73                     | 0.69              |
| 1:D:79:ARG:HE    | 1:D:87:LEU:HD22  | 1.58                     | 0.69              |
| 4:X:28:ASN:HB3   | 4:X:31:GLU:HB2   | 1.75                     | 0.69              |
| 5:Y:673:LEU:HD21 | 5:Y:764:LYS:HB3  | 1.72                     | 0.69              |
| 6:H:720:VAL:HG12 | 6:H:746:ALA:HB2  | 1.73                     | 0.69              |
| 3:u:55:SER:HA    | 3:u:165:PRO:HA   | 1.73                     | 0.69              |
| 3:v:101:VAL:HG11 | 3:v:107:VAL:HG11 | 1.74                     | 0.69              |
| 3:v:130:LEU:HD11 | 3:v:136:PHE:HB2  | 1.74                     | 0.69              |
| 4:x:28:ASN:HB3   | 4:x:31:GLU:HB2   | 1.75                     | 0.69              |
| 6:H:308:GLU:HB2  | 6:H:515:LYS:HE2  | 1.74                     | 0.69              |
| 6:H:496:GLN:HB3  | 6:H:500:MET:HG3  | 1.73                     | 0.69              |
| 4:x:184:ILE:O    | 4:x:187:THR:OG1  | 2.11                     | 0.68              |
| 6:h:333:ILE:HG12 | 6:h:519:GLU:HG3  | 1.76                     | 0.68              |
| 4:X:1140:MET:HA  | 5:Y:23:TRP:HH2   | 1.57                     | 0.68              |
| 6:h:195:GLN:HA   | 6:h:198:LEU:HB2  | 1.73                     | 0.68              |
| 4:X:208:LEU:HD13 | 4:X:212:GLY:HA3  | 1.75                     | 0.68              |
| 6:H:578:ILE:HD11 | 6:H:737:ARG:HB3  | 1.75                     | 0.68              |
| 6:h:369:LEU:HD13 | 6:h:406:LEU:HD23 | 1.75                     | 0.68              |
| 6:h:575:ASN:HD22 | 6:h:621:LEU:HD11 | 1.58                     | 0.68              |
| 6:h:578:ILE:HD11 | 6:h:737:ARG:HB3  | 1.75                     | 0.68              |
| 5:Y:748:ARG:HD2  | 5:Y:763:ILE:HD12 | 1.75                     | 0.68              |
| 5:Y:949:ILE:HG13 | 5:Y:950:THR:HG23 | 1.76                     | 0.68              |
| 4:X:184:ILE:O    | 4:X:187:THR:OG1  | 2.11                     | 0.68              |
| 6:H:718:ASP:HA   | 6:H:747:MET:HG2  | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:H:369:LEU:HD13 | 6:H:406:LEU:HD23 | 1.76                     | 0.67              |
| 5:y:748:ARG:HD2  | 5:y:763:ILE:HD12 | 1.75                     | 0.67              |
| 6:h:718:ASP:HA   | 6:h:747:MET:HG2  | 1.76                     | 0.67              |
| 6:H:305:PHE:HE2  | 6:H:516:LEU:HB3  | 1.59                     | 0.67              |
| 3:u:63:HIS:HB2   | 4:x:886:ILE:HD12 | 1.77                     | 0.67              |
| 6:H:363:ILE:HA   | 6:H:368:LYS:HA   | 1.77                     | 0.67              |
| 5:y:949:ILE:HG13 | 5:y:950:THR:HG23 | 1.76                     | 0.67              |
| 6:H:227:LYS:HG2  | 6:H:228:ILE:HG13 | 1.75                     | 0.67              |
| 6:H:333:ILE:HG12 | 6:H:519:GLU:HG3  | 1.76                     | 0.67              |
| 3:u:222:ASN:HA   | 3:u:225:VAL:HG22 | 1.76                     | 0.67              |
| 6:H:575:ASN:HD22 | 6:H:621:LEU:HD11 | 1.58                     | 0.67              |
| 1:d:79:ARG:HE    | 1:d:87:LEU:HD22  | 1.58                     | 0.67              |
| 6:h:305:PHE:HE2  | 6:h:516:LEU:HB3  | 1.59                     | 0.66              |
| 6:h:363:ILE:HA   | 6:h:368:LYS:HA   | 1.77                     | 0.66              |
| 4:X:995:ALA:HB1  | 4:X:999:ASP:HB3  | 1.77                     | 0.66              |
| 4:X:554:THR:O    | 4:X:556:LYS:NZ   | 2.29                     | 0.66              |
| 5:Y:836:ILE:HG23 | 5:Y:1056:ARG:HG2 | 1.78                     | 0.66              |
| 6:H:100:TYR:HB2  | 6:H:118:TYR:HB3  | 1.78                     | 0.66              |
| 6:H:435:LEU:HD21 | 6:H:451:ARG:HD2  | 1.78                     | 0.66              |
| 6:h:500:MET:HE3  | 6:h:501:ASP:N    | 2.11                     | 0.66              |
| 4:X:473:GLN:HB2  | 4:X:718:SER:HB2  | 1.77                     | 0.66              |
| 4:X:773:ASP:OD2  | 4:X:965:ARG:NH1  | 2.29                     | 0.65              |
| 5:y:809:GLN:NE2  | 5:y:1135:SER:HB3 | 2.04                     | 0.65              |
| 6:h:100:TYR:HB2  | 6:h:118:TYR:HB3  | 1.78                     | 0.65              |
| 6:h:435:LEU:HD21 | 6:h:451:ARG:HD2  | 1.78                     | 0.65              |
| 6:H:500:MET:HE3  | 6:H:501:ASP:N    | 2.11                     | 0.65              |
| 3:v:91:SER:HB3   | 3:v:95:LYS:HZ1   | 1.60                     | 0.65              |
| 3:V:27:PRO:HB3   | 3:V:191:TYR:HB3  | 1.76                     | 0.65              |
| 4:X:420:PHE:HE1  | 4:X:458:ILE:HD11 | 1.62                     | 0.65              |
| 5:Y:583:LYS:HA   | 5:Y:586:ILE:HD12 | 1.79                     | 0.65              |
| 5:Y:809:GLN:NE2  | 5:Y:1135:SER:HB3 | 2.04                     | 0.65              |
| 5:y:836:ILE:HG23 | 5:y:1056:ARG:HG2 | 1.78                     | 0.65              |
| 3:U:55:SER:HB3   | 3:U:141:THR:HG22 | 1.79                     | 0.65              |
| 4:X:71:LEU:HA    | 4:X:92:LEU:HA    | 1.78                     | 0.65              |
| 4:X:342:VAL:HG12 | 4:X:343:THR:HG23 | 1.77                     | 0.65              |
| 5:Y:1121:LEU:HB2 | 5:Y:1126:ALA:HB2 | 1.79                     | 0.65              |
| 4:X:859:ARG:NH2  | 5:y:243:GLN:O    | 2.30                     | 0.64              |
| 4:x:190:LEU:HD12 | 4:x:191:PRO:HD2  | 1.79                     | 0.64              |
| 4:X:788:THR:HG22 | 4:X:918:LYS:HG2  | 1.79                     | 0.64              |
| 4:X:895:ARG:NH2  | 4:X:905:VAL:O    | 2.30                     | 0.64              |
| 4:X:208:LEU:HA   | 4:X:212:GLY:HA3  | 1.78                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:U:91:SER:OG     | 3:U:95:LYS:NZ    | 2.31                     | 0.64              |
| 4:X:144:VAL:HG12  | 4:X:162:VAL:HG22 | 1.79                     | 0.64              |
| 3:u:63:HIS:NE2    | 3:u:65:PHE:O     | 2.30                     | 0.64              |
| 4:X:227:GLU:H     | 4:X:231:LYS:HE3  | 1.63                     | 0.64              |
| 4:X:556:LYS:HD3   | 4:X:586:ALA:H    | 1.63                     | 0.64              |
| 4:x:895:ARG:NH2   | 4:x:905:VAL:O    | 2.31                     | 0.64              |
| 4:x:931:ASN:ND2   | 4:x:970:GLN:OE1  | 2.31                     | 0.64              |
| 1:D:61:ASP:OD1    | 5:Y:822:ARG:NH1  | 2.31                     | 0.64              |
| 5:Y:580:GLU:HB3   | 5:Y:582:THR:HG23 | 1.80                     | 0.64              |
| 3:v:28:LEU:HD13   | 3:v:36:LEU:HD21  | 1.80                     | 0.63              |
| 4:x:187:THR:HG22  | 4:x:188:ARG:H    | 1.63                     | 0.63              |
| 3:U:222:ASN:HA    | 3:U:225:VAL:HG12 | 1.79                     | 0.63              |
| 5:y:580:GLU:HB3   | 5:y:582:THR:HG23 | 1.80                     | 0.63              |
| 4:X:1142:VAL:HG12 | 4:X:1143:LYS:H   | 1.63                     | 0.63              |
| 3:U:41:ARG:HH22   | 4:X:952:PRO:HG3  | 1.63                     | 0.63              |
| 3:v:108:THR:HG23  | 3:v:110:ALA:H    | 1.64                     | 0.63              |
| 5:y:583:LYS:HA    | 5:y:586:ILE:HD12 | 1.79                     | 0.63              |
| 6:H:300:ARG:NH1   | 6:H:558:TYR:OH   | 2.32                     | 0.63              |
| 5:y:1121:LEU:HB2  | 5:y:1126:ALA:HB2 | 1.79                     | 0.63              |
| 6:h:105:ASP:HB2   | 6:h:167:VAL:HB   | 1.80                     | 0.63              |
| 4:X:615:PRO:O     | 4:X:616:LYS:HG2  | 1.99                     | 0.63              |
| 6:H:722:VAL:HB    | 6:H:752:VAL:HB   | 1.81                     | 0.63              |
| 4:x:149:LYS:NZ    | 4:x:151:ASP:OD2  | 2.25                     | 0.63              |
| 4:x:960:LEU:HD21  | 5:y:497:LEU:HD22 | 1.80                     | 0.62              |
| 4:x:842:LEU:HB2   | 4:x:877:LEU:HB2  | 1.82                     | 0.62              |
| 6:h:551:TYR:HB3   | 6:h:556:MET:HE3  | 1.81                     | 0.62              |
| 6:h:722:VAL:HB    | 6:h:752:VAL:HB   | 1.81                     | 0.62              |
| 3:V:58:ILE:HA     | 3:V:138:VAL:HG12 | 1.82                     | 0.62              |
| 4:x:64:LEU:HG     | 4:x:98:LEU:HD13  | 1.82                     | 0.62              |
| 6:h:300:ARG:NH1   | 6:h:558:TYR:OH   | 2.32                     | 0.62              |
| 4:x:513:ARG:HH22  | 4:x:566:ALA:HB2  | 1.63                     | 0.62              |
| 4:X:550:VAL:HA    | 4:X:557:VAL:HA   | 1.80                     | 0.62              |
| 4:x:504:ARG:HH22  | 4:x:527:LEU:HD12 | 1.64                     | 0.62              |
| 5:Y:49:GLU:OE2    | 5:Y:88:ARG:NH2   | 2.33                     | 0.62              |
| 4:x:420:PHE:HE1   | 4:x:458:ILE:HD11 | 1.64                     | 0.62              |
| 4:X:87:THR:HG22   | 4:X:127:ILE:HA   | 1.81                     | 0.62              |
| 6:H:105:ASP:HB2   | 6:H:167:VAL:HB   | 1.80                     | 0.61              |
| 5:Y:867:LEU:HD11  | 5:Y:905:ARG:HB2  | 1.82                     | 0.61              |
| 3:u:58:ILE:HG21   | 3:u:61:VAL:HB    | 1.82                     | 0.61              |
| 4:X:544:GLU:HB3   | 4:X:563:TYR:HB3  | 1.81                     | 0.61              |
| 3:U:227:LEU:HD13  | 3:V:12:VAL:HB    | 1.80                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:y:867:LEU:HD11 | 5:y:905:ARG:HB2   | 1.82                     | 0.61              |
| 3:U:156:ARG:NH1  | 3:U:159:GLN:O     | 2.34                     | 0.61              |
| 3:U:176:VAL:HG22 | 3:U:198:VAL:HG23  | 1.82                     | 0.61              |
| 4:X:968:ILE:HD11 | 5:Y:744:LEU:HD11  | 1.82                     | 0.61              |
| 4:x:473:GLN:HB2  | 4:x:718:SER:HB2   | 1.83                     | 0.61              |
| 5:y:49:GLU:OE2   | 5:y:88:ARG:NH2    | 2.33                     | 0.61              |
| 4:X:187:THR:HG22 | 4:X:188:ARG:H     | 1.64                     | 0.61              |
| 4:X:278:LYS:NZ   | 4:X:399:ASP:OD2   | 2.33                     | 0.61              |
| 4:x:62:LEU:HB3   | 4:x:98:LEU:HD11   | 1.82                     | 0.61              |
| 4:x:830:ILE:HD11 | 4:x:842:LEU:HA    | 1.82                     | 0.61              |
| 4:x:1140:MET:HA  | 5:y:23:TRP:HH2    | 1.66                     | 0.61              |
| 5:y:842:ARG:HH12 | 5:y:1048:LEU:HD21 | 1.66                     | 0.61              |
| 6:h:265:LEU:HG   | 6:h:544:PHE:HB2   | 1.82                     | 0.61              |
| 3:v:45:LEU:HD22  | 5:y:524:LEU:HD13  | 1.83                     | 0.61              |
| 3:V:130:LEU:HD11 | 3:V:136:PHE:HB2   | 1.81                     | 0.61              |
| 4:X:109:GLN:HB3  | 4:X:446:GLN:HG2   | 1.81                     | 0.61              |
| 6:H:551:TYR:HB3  | 6:H:556:MET:HE3   | 1.81                     | 0.61              |
| 6:H:640:VAL:HG22 | 6:H:753:PHE:CE1   | 2.36                     | 0.61              |
| 4:x:484:ARG:NH2  | 4:x:532:SER:O     | 2.34                     | 0.61              |
| 3:U:197:ASP:OD2  | 3:U:199:TRP:NE1   | 2.33                     | 0.60              |
| 5:Y:842:ARG:HH12 | 5:Y:1048:LEU:HD21 | 1.66                     | 0.60              |
| 3:u:42:ARG:NE    | 4:x:942:GLU:OE1   | 2.32                     | 0.60              |
| 4:X:804:LEU:O    | 4:X:870:ARG:NH2   | 2.33                     | 0.60              |
| 5:y:199:GLN:HA   | 5:y:203:ARG:HB2   | 1.83                     | 0.60              |
| 5:y:543:SER:O    | 5:y:543:SER:OG    | 2.19                     | 0.60              |
| 3:v:44:LEU:HD12  | 3:v:48:LEU:HD11   | 1.83                     | 0.60              |
| 6:h:640:VAL:HG22 | 6:h:753:PHE:CE1   | 2.36                     | 0.60              |
| 6:h:648:LEU:O    | 6:h:652:LEU:HG    | 2.01                     | 0.60              |
| 3:V:43:ILE:HD13  | 3:V:217:LEU:HD22  | 1.82                     | 0.60              |
| 5:Y:753:ASN:OD1  | 5:Y:754:PRO:HD2   | 2.02                     | 0.60              |
| 6:H:265:LEU:HG   | 6:H:544:PHE:HB2   | 1.82                     | 0.60              |
| 6:H:679:GLN:O    | 6:H:683:HIS:ND1   | 2.33                     | 0.60              |
| 4:x:278:LYS:NZ   | 4:x:399:ASP:OD2   | 2.32                     | 0.60              |
| 3:U:89:ILE:HD11  | 3:U:144:ARG:HB2   | 1.84                     | 0.60              |
| 5:Y:199:GLN:HA   | 5:Y:203:ARG:HB2   | 1.83                     | 0.60              |
| 6:H:60:GLU:O     | 6:H:64:THR:HG23   | 2.02                     | 0.60              |
| 4:X:636:ARG:NH1  | 4:X:639:MET:SD    | 2.75                     | 0.59              |
| 6:h:339:LEU:HD13 | 6:h:592:CYS:HB2   | 1.84                     | 0.59              |
| 4:X:642:ASN:OD1  | 4:X:645:ARG:NH1   | 2.35                     | 0.59              |
| 4:X:771:TYR:HD2  | 5:Y:346:VAL:HG11  | 1.68                     | 0.59              |
| 6:H:234:ALA:HA   | 6:H:573:ASP:HB3   | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:648:LEU:O     | 6:H:652:LEU:HG    | 2.01                     | 0.59              |
| 3:v:72:VAL:HG13   | 3:v:73:GLU:HG3    | 1.84                     | 0.59              |
| 6:H:339:LEU:HD13  | 6:H:592:CYS:HB2   | 1.84                     | 0.59              |
| 6:H:611:ARG:HG3   | 6:H:629:PRO:HG2   | 1.84                     | 0.59              |
| 6:H:39:ASP:OD2    | 6:H:78:ARG:NH1    | 2.35                     | 0.59              |
| 6:H:57:ASP:O      | 6:H:60:GLU:N      | 2.35                     | 0.59              |
| 3:v:90:TYR:O      | 3:v:144:ARG:NH1   | 2.35                     | 0.59              |
| 4:x:890:VAL:HG12  | 4:x:911:VAL:HG12  | 1.83                     | 0.59              |
| 3:V:47:SER:O      | 3:V:146:ARG:NH1   | 2.32                     | 0.59              |
| 5:y:753:ASN:OD1   | 5:y:754:PRO:HD2   | 2.02                     | 0.59              |
| 6:h:234:ALA:HA    | 6:h:573:ASP:HB3   | 1.83                     | 0.59              |
| 3:V:223:ILE:HG13  | 3:V:224:PHE:H     | 1.68                     | 0.59              |
| 6:h:60:GLU:O      | 6:h:64:THR:HG23   | 2.02                     | 0.59              |
| 4:X:849:LYS:HG3   | 4:X:873:ARG:HB2   | 1.85                     | 0.59              |
| 5:Y:753:ASN:HD22  | 5:Y:757:ARG:HB2   | 1.68                     | 0.59              |
| 4:x:1142:VAL:HG12 | 4:x:1143:LYS:H    | 1.67                     | 0.59              |
| 6:h:611:ARG:HG3   | 6:h:629:PRO:HG2   | 1.83                     | 0.59              |
| 6:h:57:ASP:O      | 6:h:60:GLU:N      | 2.36                     | 0.59              |
| 4:X:755:LEU:N     | 4:X:1036:TYR:OH   | 2.34                     | 0.59              |
| 4:x:924:LYS:HB3   | 4:x:1040:LEU:HD12 | 1.83                     | 0.59              |
| 5:Y:314:LYS:HG3   | 5:Y:318:HIS:HB2   | 1.85                     | 0.59              |
| 2:e:16:VAL:HG22   | 2:e:17:ARG:H      | 1.68                     | 0.59              |
| 6:h:39:ASP:OD2    | 6:h:78:ARG:NH1    | 2.35                     | 0.59              |
| 4:x:359:GLN:HG2   | 4:x:360:VAL:HG23  | 1.85                     | 0.58              |
| 5:y:240:PRO:O     | 5:y:252:SER:OG    | 2.16                     | 0.58              |
| 3:V:188:VAL:HG12  | 3:V:190:ASN:H     | 1.67                     | 0.58              |
| 4:X:427:MET:O     | 4:X:431:VAL:HG23  | 2.03                     | 0.58              |
| 4:X:14:ARG:HH12   | 4:X:656:PRO:HG2   | 1.68                     | 0.58              |
| 4:X:869:ALA:HB2   | 5:y:383:ILE:HG13  | 1.86                     | 0.58              |
| 3:u:95:LYS:HD2    | 3:u:115:ASP:HB3   | 1.86                     | 0.58              |
| 3:u:223:ILE:HD13  | 3:v:10:GLU:HB2    | 1.85                     | 0.58              |
| 5:y:63:GLY:O      | 5:y:66:LYS:NZ     | 2.37                     | 0.58              |
| 5:y:116:LEU:O     | 5:y:209:ARG:NH2   | 2.36                     | 0.58              |
| 5:y:375:VAL:HG11  | 5:y:383:ILE:HD13  | 1.85                     | 0.58              |
| 2:E:45:GLU:HG3    | 4:X:1016:VAL:HG11 | 1.85                     | 0.58              |
| 4:X:173:GLU:OE1   | 4:X:183:ARG:NH1   | 2.34                     | 0.58              |
| 2:e:34:ARG:HD2    | 4:x:1010:SER:HB2  | 1.85                     | 0.58              |
| 4:x:519:THR:HG21  | 4:x:525:ILE:HG23  | 1.85                     | 0.58              |
| 3:u:173:VAL:HA    | 3:u:200:THR:HA    | 1.86                     | 0.58              |
| 5:y:305:VAL:HG11  | 5:y:313:LEU:HD23  | 1.86                     | 0.58              |
| 3:V:44:LEU:HG     | 3:V:173:VAL:HG11  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:X:519:THR:HG21 | 4:X:525:ILE:HG23  | 1.85                     | 0.58              |
| 4:X:266:ASP:OD2  | 4:X:421:ARG:NH1   | 2.37                     | 0.58              |
| 5:Y:705:TRP:CE2  | 5:Y:762:PRO:HG3   | 2.39                     | 0.58              |
| 5:Y:748:ARG:NH1  | 6:H:73:GLU:OE2    | 2.37                     | 0.58              |
| 3:v:108:THR:OG1  | 3:v:123:PRO:O     | 2.20                     | 0.58              |
| 4:x:745:GLY:H    | 4:x:748:MET:HB2   | 1.68                     | 0.58              |
| 3:U:114:HIS:ND1  | 3:U:115:ASP:O     | 2.37                     | 0.57              |
| 4:X:573:VAL:HG12 | 4:X:596:PHE:HB2   | 1.86                     | 0.57              |
| 5:Y:807:VAL:HG22 | 5:Y:1127:SER:HB2  | 1.86                     | 0.57              |
| 4:x:691:TRP:CD1  | 4:x:709:LYS:HB3   | 2.39                     | 0.57              |
| 5:y:807:VAL:HG22 | 5:y:1127:SER:HB2  | 1.86                     | 0.57              |
| 4:x:71:LEU:HA    | 4:x:92:LEU:HA     | 1.87                     | 0.57              |
| 6:h:342:GLN:NE2  | 6:h:526:TYR:OH    | 2.33                     | 0.57              |
| 4:X:770:ASN:ND2  | 4:X:957:LEU:O     | 2.37                     | 0.57              |
| 4:X:980:ALA:O    | 4:X:984:GLY:N     | 2.33                     | 0.57              |
| 5:Y:63:GLY:O     | 5:Y:66:LYS:NZ     | 2.37                     | 0.57              |
| 5:Y:305:VAL:HG11 | 5:Y:313:LEU:HD23  | 1.86                     | 0.57              |
| 4:x:427:MET:O    | 4:x:431:VAL:HG23  | 2.04                     | 0.57              |
| 5:y:753:ASN:HD22 | 5:y:757:ARG:HB2   | 1.68                     | 0.57              |
| 2:E:16:VAL:HG22  | 2:E:17:ARG:H      | 1.68                     | 0.57              |
| 5:Y:116:LEU:O    | 5:Y:209:ARG:NH2   | 2.36                     | 0.57              |
| 2:e:45:GLU:HG3   | 4:x:1016:VAL:HG11 | 1.86                     | 0.57              |
| 6:h:484:TYR:HD2  | 6:h:511:PHE:HE2   | 1.51                     | 0.57              |
| 6:h:727:GLU:HG3  | 6:h:728:GLU:HG3   | 1.86                     | 0.57              |
| 4:x:354:ASP:OD1  | 4:x:355:GLN:N     | 2.37                     | 0.57              |
| 5:y:314:LYS:HG3  | 5:y:318:HIS:HB2   | 1.85                     | 0.57              |
| 5:y:1002:TYR:HE1 | 5:y:1024:LEU:HD21 | 1.70                     | 0.57              |
| 4:X:179:VAL:HA   | 4:X:220:THR:HG22  | 1.86                     | 0.57              |
| 5:Y:1123:ILE:O   | 5:Y:1127:SER:HB3  | 2.05                     | 0.57              |
| 4:x:1005:GLU:O   | 4:x:1010:SER:OG   | 2.20                     | 0.57              |
| 5:y:60:CYS:HA    | 5:y:80:VAL:HG21   | 1.87                     | 0.57              |
| 5:y:989:GLN:NE2  | 5:y:1005:PRO:O    | 2.37                     | 0.57              |
| 5:Y:851:GLN:NE2  | 5:Y:863:ASN:OD1   | 2.34                     | 0.57              |
| 5:Y:989:GLN:NE2  | 5:Y:1005:PRO:O    | 2.37                     | 0.57              |
| 6:H:727:GLU:HG3  | 6:H:728:GLU:HG3   | 1.87                     | 0.57              |
| 4:x:554:THR:O    | 4:x:556:LYS:NZ    | 2.31                     | 0.57              |
| 3:U:100:ASP:HA   | 3:U:136:PHE:O     | 2.05                     | 0.57              |
| 4:x:807:GLU:HG3  | 4:x:847:THR:HA    | 1.87                     | 0.57              |
| 6:h:217:GLN:O    | 6:h:221:ILE:HG12  | 2.05                     | 0.57              |
| 6:h:679:GLN:O    | 6:h:683:HIS:ND1   | 2.32                     | 0.57              |
| 5:y:519:THR:HG22 | 5:y:565:LEU:HD11  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:U:26:GLU:HB3   | 3:U:27:PRO:HD2    | 1.87                     | 0.56              |
| 5:y:705:TRP:CE2  | 5:y:762:PRO:HG3   | 2.39                     | 0.56              |
| 3:U:221:LEU:HD21 | 3:V:217:LEU:HB3   | 1.86                     | 0.56              |
| 5:Y:102:SER:H    | 5:Y:289:GLN:HE22  | 1.53                     | 0.56              |
| 5:Y:375:VAL:HG11 | 5:Y:383:ILE:HD13  | 1.85                     | 0.56              |
| 5:Y:1002:TYR:HE1 | 5:Y:1024:LEU:HD21 | 1.70                     | 0.56              |
| 6:H:484:TYR:HD2  | 6:H:511:PHE:HE2   | 1.51                     | 0.56              |
| 4:x:651:MET:HG2  | 4:x:790:ILE:HD11  | 1.85                     | 0.56              |
| 4:X:801:ASP:HA   | 4:X:806:PRO:HA    | 1.87                     | 0.56              |
| 5:Y:60:CYS:HA    | 5:Y:80:VAL:HG21   | 1.87                     | 0.56              |
| 5:y:851:GLN:NE2  | 5:y:863:ASN:OD1   | 2.34                     | 0.56              |
| 5:Y:519:THR:HG22 | 5:Y:565:LEU:HD11  | 1.87                     | 0.56              |
| 6:H:217:GLN:O    | 6:H:221:ILE:HG12  | 2.05                     | 0.56              |
| 5:y:1123:ILE:O   | 5:y:1127:SER:HB3  | 2.05                     | 0.56              |
| 5:Y:808:ALA:HB3  | 5:Y:924:ALA:HB2   | 1.87                     | 0.56              |
| 6:h:301:LEU:HD23 | 6:h:525:LEU:HD13  | 1.88                     | 0.56              |
| 5:Y:176:HIS:HB2  | 5:Y:227:ILE:HD11  | 1.87                     | 0.56              |
| 5:Y:896:HIS:NE2  | 5:Y:1131:ASP:OD2  | 2.38                     | 0.56              |
| 5:y:176:HIS:HB2  | 5:y:227:ILE:HD11  | 1.87                     | 0.56              |
| 5:y:191:LEU:HD21 | 5:y:209:ARG:HH11  | 1.71                     | 0.56              |
| 5:y:896:HIS:NE2  | 5:y:1131:ASP:OD2  | 2.38                     | 0.56              |
| 6:h:548:ALA:HB3  | 6:h:570:VAL:HG13  | 1.88                     | 0.56              |
| 3:U:12:VAL:HG12  | 3:U:25:VAL:HG12   | 1.87                     | 0.56              |
| 5:Y:383:ILE:HG13 | 4:x:869:ALA:HB2   | 1.88                     | 0.56              |
| 3:v:107:VAL:HG23 | 3:v:127:ILE:HB    | 1.87                     | 0.56              |
| 3:V:173:VAL:HG23 | 3:V:200:THR:H     | 1.71                     | 0.56              |
| 4:X:796:GLU:HG3  | 4:X:910:ARG:HG2   | 1.88                     | 0.56              |
| 5:y:808:ALA:HB3  | 5:y:924:ALA:HB2   | 1.87                     | 0.56              |
| 3:v:200:THR:OG1  | 3:v:204:THR:O     | 2.24                     | 0.55              |
| 4:X:604:SER:OG   | 4:X:606:ASN:OD1   | 2.18                     | 0.55              |
| 4:X:770:ASN:HD21 | 4:X:958:ASN:HA    | 1.71                     | 0.55              |
| 6:h:178:THR:HG22 | 6:h:180:LYS:HG3   | 1.89                     | 0.55              |
| 3:U:173:VAL:HG12 | 3:U:200:THR:HG22  | 1.89                     | 0.55              |
| 5:Y:240:PRO:O    | 5:Y:252:SER:OG    | 2.16                     | 0.55              |
| 1:d:84:TYR:OH    | 5:y:1036:LYS:NZ   | 2.38                     | 0.55              |
| 6:H:301:LEU:HD23 | 6:H:525:LEU:HD13  | 1.88                     | 0.55              |
| 2:e:16:VAL:HG21  | 5:y:529:GLY:CA    | 2.36                     | 0.55              |
| 3:u:221:LEU:HD23 | 3:v:218:THR:HB    | 1.88                     | 0.55              |
| 4:x:208:LEU:HD13 | 4:x:212:GLY:HA3   | 1.88                     | 0.55              |
| 2:e:57:TYR:CZ    | 3:u:13:GLU:HG3    | 2.41                     | 0.55              |
| 3:u:114:HIS:ND1  | 3:u:115:ASP:O     | 2.37                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:y:553:GLN:O     | 5:y:556:LYS:NZ    | 2.37                     | 0.55              |
| 4:X:1005:GLU:HA   | 4:X:1010:SER:HA   | 1.88                     | 0.55              |
| 3:v:49:PRO:HB3    | 3:v:146:ARG:HG2   | 1.88                     | 0.55              |
| 4:x:680:GLY:HA2   | 4:x:695:TYR:H     | 1.71                     | 0.55              |
| 6:H:257:VAL:HG22  | 6:H:258:ILE:HG12  | 1.88                     | 0.55              |
| 6:H:548:ALA:HB3   | 6:H:570:VAL:HG13  | 1.88                     | 0.55              |
| 4:x:636:ARG:NH1   | 4:x:639:MET:SD    | 2.80                     | 0.55              |
| 4:x:1132:ILE:HD12 | 4:x:1141:ASP:OD2  | 2.06                     | 0.55              |
| 5:y:305:VAL:HG22  | 5:y:307:GLY:H     | 1.72                     | 0.55              |
| 3:U:231:ALA:HB1   | 3:V:207:LYS:HD3   | 1.89                     | 0.55              |
| 5:Y:191:LEU:HD21  | 5:Y:209:ARG:HH11  | 1.71                     | 0.55              |
| 6:H:137:TRP:HE1   | 6:H:282:GLU:HB2   | 1.72                     | 0.55              |
| 5:y:102:SER:H     | 5:y:289:GLN:HE22  | 1.53                     | 0.55              |
| 3:U:127:ILE:HG22  | 3:U:128:ALA:H     | 1.71                     | 0.55              |
| 3:V:27:PRO:HG3    | 3:V:183:THR:HG21  | 1.89                     | 0.55              |
| 4:X:979:ALA:HB2   | 4:X:1004:LEU:HD12 | 1.89                     | 0.55              |
| 6:H:103:ARG:HD2   | 6:H:118:TYR:HE1   | 1.72                     | 0.55              |
| 4:x:714:LYS:NZ    | 4:x:726:GLN:O     | 2.32                     | 0.55              |
| 5:y:54:PRO:HG2    | 5:y:85:ALA:HA     | 1.89                     | 0.54              |
| 5:Y:136:VAL:HG11  | 5:Y:145:GLU:HA    | 1.89                     | 0.54              |
| 3:U:43:ILE:HD13   | 3:U:217:LEU:HB2   | 1.88                     | 0.54              |
| 3:U:44:LEU:HD12   | 3:U:173:VAL:HG11  | 1.89                     | 0.54              |
| 4:X:890:VAL:HG12  | 4:X:911:VAL:HG12  | 1.90                     | 0.54              |
| 5:Y:305:VAL:HG22  | 5:Y:307:GLY:H     | 1.72                     | 0.54              |
| 4:X:829:ILE:HA    | 4:X:843:VAL:HG12  | 1.88                     | 0.54              |
| 4:x:134:ILE:HB    | 4:x:412:VAL:HG12  | 1.90                     | 0.54              |
| 4:X:804:LEU:HD22  | 4:X:851:VAL:HG23  | 1.90                     | 0.54              |
| 5:Y:955:ARG:NH2   | 5:Y:1050:GLU:OE2  | 2.41                     | 0.54              |
| 3:v:154:ASN:O     | 3:v:159:GLN:NE2   | 2.41                     | 0.54              |
| 4:x:730:VAL:HG21  | 4:x:742:LEU:HD23  | 1.89                     | 0.54              |
| 1:D:69:LEU:N      | 1:D:77:GLY:O      | 2.39                     | 0.54              |
| 4:X:518:GLU:OE2   | 4:X:645:ARG:NH2   | 2.41                     | 0.54              |
| 4:x:546:PRO:HB2   | 4:x:613:VAL:HG21  | 1.90                     | 0.54              |
| 6:h:137:TRP:HE1   | 6:h:282:GLU:HB2   | 1.72                     | 0.54              |
| 2:E:2:ILE:HG23    | 2:E:50:VAL:HG11   | 1.89                     | 0.54              |
| 5:Y:306:THR:O     | 5:Y:311:ARG:N     | 2.38                     | 0.54              |
| 5:Y:809:GLN:HG3   | 5:Y:810:ASP:N     | 2.22                     | 0.54              |
| 6:H:178:THR:HG22  | 6:H:180:LYS:HG3   | 1.89                     | 0.54              |
| 6:H:360:LYS:HG3   | 6:H:479:ASP:HB2   | 1.89                     | 0.54              |
| 6:h:257:VAL:HG22  | 6:h:258:ILE:HG12  | 1.88                     | 0.54              |
| 3:U:12:VAL:HG22   | 3:V:227:LEU:HD23  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:69:LEU:N     | 1:d:77:GLY:O     | 2.39                     | 0.54              |
| 3:u:27:PRO:HB3   | 3:u:185:VAL:HG21 | 1.90                     | 0.54              |
| 6:h:655:GLU:OE2  | 6:h:658:ARG:NH1  | 2.41                     | 0.54              |
| 3:V:183:THR:HB   | 3:V:191:TYR:HB2  | 1.89                     | 0.54              |
| 5:Y:1136:ALA:O   | 5:Y:1140:GLN:HG2 | 2.08                     | 0.54              |
| 5:y:1136:ALA:O   | 5:y:1140:GLN:HG2 | 2.08                     | 0.54              |
| 6:h:103:ARG:HD2  | 6:h:118:TYR:HE1  | 1.72                     | 0.54              |
| 4:X:14:ARG:HD3   | 4:X:988:ALA:HB2  | 1.90                     | 0.53              |
| 4:X:188:ARG:O    | 4:X:239:ARG:NH2  | 2.41                     | 0.53              |
| 5:Y:54:PRO:HG2   | 5:Y:85:ALA:HA    | 1.89                     | 0.53              |
| 6:H:676:GLN:NE2  | 6:H:728:GLU:OE2  | 2.28                     | 0.53              |
| 5:y:955:ARG:NH2  | 5:y:1050:GLU:OE2 | 2.41                     | 0.53              |
| 4:X:978:MET:HE3  | 4:X:1033:GLY:HA2 | 1.91                     | 0.53              |
| 4:x:218:ARG:HA   | 4:x:221:LEU:HD12 | 1.89                     | 0.53              |
| 4:x:980:ALA:O    | 4:x:984:GLY:N    | 2.39                     | 0.53              |
| 5:y:809:GLN:HG3  | 5:y:810:ASP:N    | 2.22                     | 0.53              |
| 5:Y:543:SER:O    | 5:Y:543:SER:OG   | 2.19                     | 0.53              |
| 2:e:2:ILE:HG23   | 2:e:50:VAL:HG11  | 1.89                     | 0.53              |
| 3:v:41:ARG:HG3   | 3:v:176:VAL:HB   | 1.91                     | 0.53              |
| 5:y:241:MET:HA   | 5:y:250:ALA:HB3  | 1.89                     | 0.53              |
| 1:d:2:GLY:O      | 1:d:5:GLN:NE2    | 2.42                     | 0.53              |
| 4:x:197:ARG:NH2  | 4:x:226:THR:O    | 2.41                     | 0.53              |
| 4:x:279:LEU:O    | 4:x:366:ASN:ND2  | 2.38                     | 0.53              |
| 4:x:1125:PRO:HB2 | 4:x:1128:PHE:HB3 | 1.91                     | 0.53              |
| 6:h:387:SER:OG   | 6:h:389:PRO:HD2  | 2.09                     | 0.53              |
| 5:Y:895:PRO:O    | 5:Y:1097:HIS:NE2 | 2.42                     | 0.53              |
| 5:y:136:VAL:HG11 | 5:y:145:GLU:HA   | 1.89                     | 0.53              |
| 5:y:895:PRO:O    | 5:y:1097:HIS:NE2 | 2.42                     | 0.53              |
| 1:D:2:GLY:O      | 1:D:5:GLN:NE2    | 2.42                     | 0.53              |
| 4:X:348:LYS:HB3  | 4:X:369:ILE:HD13 | 1.90                     | 0.53              |
| 4:X:823:ASN:HA   | 4:X:831:ARG:HH11 | 1.72                     | 0.53              |
| 5:Y:468:GLU:HA   | 5:Y:471:ILE:HG23 | 1.91                     | 0.53              |
| 6:H:387:SER:OG   | 6:H:389:PRO:HD2  | 2.09                     | 0.53              |
| 4:x:226:THR:HG23 | 4:x:231:LYS:HG3  | 1.91                     | 0.53              |
| 6:h:360:LYS:HG3  | 6:h:479:ASP:HB2  | 1.89                     | 0.53              |
| 4:X:1078:MET:HE3 | 5:Y:244:LEU:HD11 | 1.90                     | 0.53              |
| 6:H:104:ILE:HD11 | 6:H:166:MET:HG2  | 1.91                     | 0.53              |
| 3:v:53:VAL:HG21  | 3:v:82:ILE:HG22  | 1.90                     | 0.53              |
| 4:x:160:ALA:HB3  | 4:x:172:TYR:HB2  | 1.90                     | 0.53              |
| 4:x:787:TYR:OH   | 4:x:1037:MET:O   | 2.19                     | 0.53              |
| 6:h:269:ASN:O    | 6:h:290:GLN:NE2  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:h:670:ILE:HD11 | 6:h:709:VAL:HA    | 1.90                     | 0.53              |
| 1:D:84:TYR:OH    | 5:Y:1036:LYS:NZ   | 2.36                     | 0.53              |
| 4:X:404:LEU:HD21 | 4:X:543:ILE:HD12  | 1.91                     | 0.53              |
| 4:X:842:LEU:HD13 | 4:X:911:VAL:HG21  | 1.89                     | 0.53              |
| 5:Y:876:ILE:HG23 | 5:Y:881:ILE:HD12  | 1.91                     | 0.53              |
| 6:h:435:LEU:HD11 | 6:h:451:ARG:HG2   | 1.91                     | 0.53              |
| 4:X:804:LEU:HD21 | 4:X:850:GLY:H     | 1.74                     | 0.53              |
| 5:Y:666:LEU:HD21 | 5:Y:716:LEU:HA    | 1.91                     | 0.53              |
| 6:H:655:GLU:OE2  | 6:H:658:ARG:NH1   | 2.41                     | 0.53              |
| 3:v:57:GLN:N     | 3:v:139:ARG:O     | 2.39                     | 0.53              |
| 5:y:257:LEU:HD13 | 5:y:295:LEU:HA    | 1.91                     | 0.53              |
| 5:y:341:ARG:HA   | 5:y:455:MET:HE2   | 1.91                     | 0.53              |
| 4:x:87:THR:HG22  | 4:x:128:ASN:H     | 1.74                     | 0.53              |
| 4:x:226:THR:OG1  | 4:x:235:GLU:OE1   | 2.27                     | 0.53              |
| 4:x:804:LEU:O    | 4:x:870:ARG:NH2   | 2.36                     | 0.53              |
| 5:y:876:ILE:HG23 | 5:y:881:ILE:HD12  | 1.91                     | 0.53              |
| 3:V:72:VAL:HG23  | 3:V:73:GLU:HG3    | 1.90                     | 0.52              |
| 4:X:95:LYS:NZ    | 4:X:110:ASP:OD2   | 2.41                     | 0.52              |
| 4:X:680:GLY:HA2  | 4:X:695:TYR:H     | 1.73                     | 0.52              |
| 5:Y:241:MET:HA   | 5:Y:250:ALA:HB3   | 1.89                     | 0.52              |
| 5:Y:295:LEU:O    | 5:Y:315:SER:OG    | 2.26                     | 0.52              |
| 6:H:269:ASN:O    | 6:H:290:GLN:NE2   | 2.42                     | 0.52              |
| 3:v:80:LEU:HA    | 3:v:83:LYS:HD3    | 1.90                     | 0.52              |
| 4:x:1128:PHE:O   | 4:x:1132:ILE:HG12 | 2.09                     | 0.52              |
| 5:y:295:LEU:O    | 5:y:315:SER:OG    | 2.26                     | 0.52              |
| 5:y:852:VAL:C    | 5:y:853:LYS:HZ3   | 2.18                     | 0.52              |
| 5:y:889:ALA:HB3  | 5:y:1068:GLU:HB3  | 1.91                     | 0.52              |
| 3:U:89:ILE:O     | 3:U:144:ARG:NH1   | 2.42                     | 0.52              |
| 3:V:38:ASN:HD21  | 4:X:1022:THR:HA   | 1.74                     | 0.52              |
| 3:v:56:ILE:HG12  | 3:v:166:ILE:HD11  | 1.92                     | 0.52              |
| 4:x:1048:LEU:O   | 5:y:341:ARG:N     | 2.42                     | 0.52              |
| 5:Y:257:LEU:HD13 | 5:Y:295:LEU:HA    | 1.91                     | 0.52              |
| 5:Y:462:SER:HB3  | 5:Y:465:ALA:HB3   | 1.92                     | 0.52              |
| 4:X:338:VAL:HB   | 4:X:346:SER:HB2   | 1.92                     | 0.52              |
| 5:Y:360:GLU:O    | 5:Y:364:GLU:HG2   | 2.10                     | 0.52              |
| 3:u:107:VAL:HG13 | 3:u:127:ILE:HB    | 1.92                     | 0.52              |
| 6:h:579:TYR:N    | 6:h:582:THR:OG1   | 2.43                     | 0.52              |
| 4:X:862:HIS:HA   | 4:X:869:ALA:HB3   | 1.92                     | 0.52              |
| 6:H:670:ILE:HD11 | 6:H:709:VAL:HA    | 1.90                     | 0.52              |
| 4:x:220:THR:O    | 4:x:224:ASP:N     | 2.43                     | 0.52              |
| 5:y:468:GLU:HA   | 5:y:471:ILE:HG23  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:Y:203:ARG:NH1  | 5:Y:1090:PRO:O    | 2.42                     | 0.52              |
| 5:Y:553:GLN:O    | 5:Y:556:LYS:NZ    | 2.37                     | 0.52              |
| 6:H:435:LEU:HD11 | 6:H:451:ARG:HG2   | 1.91                     | 0.52              |
| 6:H:759:SER:HB2  | 6:H:762:VAL:HG23  | 1.92                     | 0.52              |
| 4:x:15:ARG:HD3   | 4:x:985:ILE:HD11  | 1.92                     | 0.52              |
| 5:Y:264:ARG:HD2  | 5:Y:287:MET:HB3   | 1.92                     | 0.52              |
| 5:y:203:ARG:NH1  | 5:y:1090:PRO:O    | 2.42                     | 0.52              |
| 4:x:197:ARG:NH1  | 4:x:204:ASP:OD2   | 2.43                     | 0.52              |
| 5:y:350:LEU:HD11 | 5:y:437:ARG:HG3   | 1.92                     | 0.52              |
| 5:y:945:ALA:HB3  | 6:h:83:ARG:HG3    | 1.91                     | 0.52              |
| 6:h:104:ILE:HD11 | 6:h:166:MET:HG2   | 1.91                     | 0.52              |
| 3:V:110:ALA:HB2  | 3:V:123:PRO:HB2   | 1.91                     | 0.52              |
| 4:X:95:LYS:HG2   | 4:X:108:ASP:HB2   | 1.92                     | 0.52              |
| 6:H:14:ARG:HH21  | 6:H:118:TYR:HE2   | 1.57                     | 0.52              |
| 5:y:807:VAL:HG21 | 5:y:1123:ILE:HG13 | 1.92                     | 0.52              |
| 5:y:58:TRP:NE1   | 5:y:83:THR:O      | 2.43                     | 0.51              |
| 5:y:264:ARG:HD2  | 5:y:287:MET:HB3   | 1.92                     | 0.51              |
| 5:y:462:SER:HB3  | 5:y:465:ALA:HB3   | 1.92                     | 0.51              |
| 4:X:676:CYS:SG   | 4:X:677:LYS:N     | 2.83                     | 0.51              |
| 5:Y:297:ASP:OD1  | 5:Y:300:ARG:NE    | 2.43                     | 0.51              |
| 6:H:579:TYR:N    | 6:H:582:THR:OG1   | 2.43                     | 0.51              |
| 3:v:74:ASP:HB2   | 5:y:598:LYS:HD2   | 1.91                     | 0.51              |
| 5:y:839:LEU:HG   | 5:y:840:GLU:H     | 1.74                     | 0.51              |
| 6:h:212:THR:HA   | 6:h:215:LYS:HD2   | 1.92                     | 0.51              |
| 6:h:478:LEU:HB3  | 6:h:480:VAL:HG13  | 1.92                     | 0.51              |
| 5:Y:712:ILE:HD13 | 5:Y:747:MET:H     | 1.75                     | 0.51              |
| 5:Y:874:LEU:HA   | 5:Y:877:VAL:HG12  | 1.92                     | 0.51              |
| 4:x:731:SER:OG   | 4:x:732:VAL:N     | 2.42                     | 0.51              |
| 5:y:1129:GLU:OE1 | 5:y:1129:GLU:N    | 2.43                     | 0.51              |
| 3:U:172:PRO:HB3  | 3:U:203:SER:HB2   | 1.92                     | 0.51              |
| 5:Y:58:TRP:NE1   | 5:Y:83:THR:O      | 2.43                     | 0.51              |
| 5:Y:75:CYS:HB2   | 5:Y:80:VAL:HG22   | 1.92                     | 0.51              |
| 5:Y:852:VAL:C    | 5:Y:853:LYS:HZ3   | 2.18                     | 0.51              |
| 5:Y:1129:GLU:OE1 | 5:Y:1129:GLU:N    | 2.44                     | 0.51              |
| 5:y:989:GLN:NE2  | 5:y:1008:SER:O    | 2.43                     | 0.51              |
| 1:D:69:LEU:HB2   | 1:D:79:ARG:HD2    | 1.93                     | 0.51              |
| 4:X:166:ARG:NH2  | 4:X:266:ASP:OD2   | 2.41                     | 0.51              |
| 4:x:767:ASP:H    | 5:y:652:THR:HB    | 1.75                     | 0.51              |
| 5:y:75:CYS:HB2   | 5:y:80:VAL:HG22   | 1.92                     | 0.51              |
| 5:y:298:ASN:HD22 | 6:h:446:PHE:HE2   | 1.58                     | 0.51              |
| 5:y:1133:PHE:HB3 | 5:y:1154:LYS:HE3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:X:234:LEU:HD22 | 4:X:246:PRO:HB2   | 1.91                     | 0.51              |
| 5:Y:159:LEU:HD12 | 5:Y:163:GLY:HA2   | 1.93                     | 0.51              |
| 5:Y:889:ALA:HB3  | 5:Y:1068:GLU:HB3  | 1.91                     | 0.51              |
| 5:Y:1032:LYS:HA  | 5:Y:1120:LEU:HD21 | 1.91                     | 0.51              |
| 5:y:360:GLU:O    | 5:y:364:GLU:HG2   | 2.10                     | 0.51              |
| 5:y:874:LEU:HA   | 5:y:877:VAL:HG12  | 1.93                     | 0.51              |
| 6:h:738:LEU:O    | 6:h:741:THR:OG1   | 2.26                     | 0.51              |
| 3:V:45:LEU:HD11  | 5:Y:527:GLN:HG2   | 1.93                     | 0.51              |
| 5:Y:271:LEU:HD21 | 5:Y:280:ILE:HG22  | 1.92                     | 0.51              |
| 5:Y:341:ARG:HA   | 5:Y:455:MET:HE2   | 1.91                     | 0.51              |
| 5:Y:807:VAL:HG21 | 5:Y:1123:ILE:HG13 | 1.92                     | 0.51              |
| 3:u:220:HIS:CE1  | 3:v:6:LYS:HE2     | 2.46                     | 0.51              |
| 3:v:197:ASP:OD1  | 3:v:198:VAL:N     | 2.44                     | 0.51              |
| 5:y:666:LEU:HD21 | 5:y:716:LEU:HA    | 1.91                     | 0.51              |
| 5:y:1058:GLN:OE1 | 6:h:44:ARG:NH1    | 2.44                     | 0.51              |
| 5:Y:350:LEU:HD11 | 5:Y:437:ARG:HG3   | 1.92                     | 0.51              |
| 6:H:212:THR:HA   | 6:H:215:LYS:HD2   | 1.92                     | 0.51              |
| 3:v:27:PRO:HB3   | 3:v:183:THR:HG21  | 1.93                     | 0.51              |
| 5:y:803:ARG:HD2  | 5:y:1124:THR:HG22 | 1.93                     | 0.51              |
| 5:y:1032:LYS:HA  | 5:y:1120:LEU:HD21 | 1.91                     | 0.51              |
| 6:h:228:ILE:HD13 | 6:h:593:PHE:HZ    | 1.76                     | 0.51              |
| 6:h:298:GLU:OE2  | 6:h:307:CYS:HB3   | 2.11                     | 0.51              |
| 4:x:975:HIS:NE2  | 4:x:1013:ALA:O    | 2.42                     | 0.51              |
| 5:y:367:LYS:HE3  | 5:y:390:ILE:HG21  | 1.93                     | 0.51              |
| 5:y:712:ILE:HD13 | 5:y:747:MET:H     | 1.75                     | 0.51              |
| 5:y:853:LYS:HE3  | 5:y:860:VAL:HA    | 1.93                     | 0.51              |
| 1:D:51:LEU:O     | 1:D:55:ILE:HB     | 2.11                     | 0.51              |
| 3:U:74:ASP:OD1   | 3:U:75:VAL:N      | 2.41                     | 0.51              |
| 4:X:119:MET:HB2  | 4:X:125:PHE:HE1   | 1.76                     | 0.51              |
| 4:X:182:VAL:HB   | 4:X:192:VAL:HG12  | 1.93                     | 0.51              |
| 4:X:272:ARG:NH1  | 4:X:375:ASN:O     | 2.44                     | 0.51              |
| 5:Y:989:GLN:NE2  | 5:Y:1008:SER:O    | 2.43                     | 0.51              |
| 6:H:298:GLU:OE2  | 6:H:307:CYS:HB3   | 2.11                     | 0.51              |
| 5:y:271:LEU:HD21 | 5:y:280:ILE:HG22  | 1.92                     | 0.51              |
| 5:y:483:LYS:HD2  | 5:y:488:VAL:HG11  | 1.92                     | 0.51              |
| 3:V:98:GLU:HG2   | 3:V:139:ARG:HG2   | 1.92                     | 0.50              |
| 4:X:281:ILE:HG21 | 4:X:350:PHE:HD2   | 1.76                     | 0.50              |
| 4:X:344:LEU:HD22 | 4:X:378:PRO:HG3   | 1.92                     | 0.50              |
| 4:X:1043:MET:SD  | 4:X:1044:VAL:N    | 2.83                     | 0.50              |
| 5:Y:839:LEU:HG   | 5:Y:840:GLU:H     | 1.74                     | 0.50              |
| 6:H:496:GLN:O    | 6:H:497:HIS:HB2   | 2.11                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:y:571:LEU:HD13 | 5:y:575:PHE:HB2   | 1.93                     | 0.50              |
| 6:h:14:ARG:HH21  | 6:h:118:TYR:HE2   | 1.57                     | 0.50              |
| 3:v:70:GLY:HA3   | 3:v:134:ALA:HB2   | 1.93                     | 0.50              |
| 4:x:550:VAL:HA   | 4:x:557:VAL:HA    | 1.91                     | 0.50              |
| 4:x:960:LEU:HD23 | 5:y:729:MET:HE3   | 1.93                     | 0.50              |
| 5:y:709:LYS:HA   | 5:y:712:ILE:HG22  | 1.94                     | 0.50              |
| 6:h:12:GLN:HA    | 6:h:15:ILE:HD12   | 1.94                     | 0.50              |
| 3:U:41:ARG:NH2   | 4:X:952:PRO:HG3   | 2.25                     | 0.50              |
| 4:X:549:ARG:HD2  | 4:X:560:ARG:HH22  | 1.75                     | 0.50              |
| 5:Y:571:LEU:HD13 | 5:Y:575:PHE:HB2   | 1.93                     | 0.50              |
| 5:y:297:ASP:OD1  | 5:y:300:ARG:NE    | 2.43                     | 0.50              |
| 5:y:1104:LYS:O   | 5:y:1108:LEU:HG   | 2.11                     | 0.50              |
| 6:h:241:SER:HA   | 6:h:244:LEU:HB2   | 1.94                     | 0.50              |
| 4:X:220:THR:O    | 4:X:224:ASP:N     | 2.45                     | 0.50              |
| 6:H:342:GLN:NE2  | 6:H:526:TYR:OH    | 2.33                     | 0.50              |
| 4:x:42:ASP:OD1   | 4:x:69:TYR:OH     | 2.30                     | 0.50              |
| 4:x:228:ASN:HB3  | 4:x:231:LYS:HG2   | 1.92                     | 0.50              |
| 6:h:236:GLY:HA2  | 6:h:239:LYS:HE2   | 1.93                     | 0.50              |
| 6:h:558:TYR:O    | 6:h:562:ILE:HG12  | 2.12                     | 0.50              |
| 6:h:759:SER:HB2  | 6:h:762:VAL:HG23  | 1.92                     | 0.50              |
| 3:V:76:THR:HA    | 3:V:79:ILE:HD12   | 1.94                     | 0.50              |
| 5:Y:803:ARG:HD2  | 5:Y:1124:THR:HG22 | 1.93                     | 0.50              |
| 5:Y:1133:PHE:HB3 | 5:Y:1154:LYS:HE3  | 1.92                     | 0.50              |
| 6:H:228:ILE:HD13 | 6:H:593:PHE:HZ    | 1.76                     | 0.50              |
| 6:H:478:LEU:HB3  | 6:H:480:VAL:HG13  | 1.92                     | 0.50              |
| 3:v:11:THR:N     | 3:v:26:GLU:OE1    | 2.44                     | 0.50              |
| 5:y:315:SER:OG   | 5:y:316:LEU:N     | 2.45                     | 0.50              |
| 6:h:357:MET:N    | 6:h:380:TYR:OH    | 2.44                     | 0.50              |
| 6:h:549:GLN:OE1  | 6:h:572:GLY:HA3   | 2.12                     | 0.50              |
| 3:U:88:LYS:HG2   | 3:U:121:LEU:HD11  | 1.92                     | 0.50              |
| 4:X:15:ARG:HD2   | 4:X:985:ILE:HD12  | 1.93                     | 0.50              |
| 5:Y:483:LYS:HD2  | 5:Y:488:VAL:HG11  | 1.92                     | 0.50              |
| 6:H:558:TYR:O    | 6:H:562:ILE:HG12  | 2.12                     | 0.50              |
| 1:d:51:LEU:O     | 1:d:55:ILE:HB     | 2.11                     | 0.50              |
| 5:y:492:SER:OG   | 5:y:493:GLN:N     | 2.45                     | 0.50              |
| 6:h:496:GLN:O    | 6:h:497:HIS:HB2   | 2.11                     | 0.50              |
| 6:H:240:THR:HG23 | 6:H:241:SER:H     | 1.77                     | 0.50              |
| 4:x:153:ASN:OD1  | 4:x:155:LYS:HG2   | 2.12                     | 0.50              |
| 4:x:696:GLU:HB2  | 4:x:703:VAL:HG23  | 1.93                     | 0.50              |
| 4:X:244:GLU:HG2  | 4:X:245:PRO:HD2   | 1.93                     | 0.50              |
| 5:Y:441:LEU:HD21 | 5:Y:495:MET:HE1   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:H:549:GLN:OE1   | 6:H:572:GLY:HA3  | 2.12                     | 0.50              |
| 4:x:513:ARG:NH1   | 4:x:569:GLU:OE2  | 2.43                     | 0.50              |
| 4:x:785:ASP:OD1   | 4:x:788:THR:HG21 | 2.12                     | 0.50              |
| 5:y:306:THR:O     | 5:y:311:ARG:N    | 2.38                     | 0.50              |
| 3:V:31:GLY:O      | 3:V:34:THR:OG1   | 2.29                     | 0.50              |
| 5:Y:315:SER:OG    | 5:Y:316:LEU:N    | 2.45                     | 0.50              |
| 5:Y:853:LYS:HE3   | 5:Y:860:VAL:HA   | 1.93                     | 0.50              |
| 6:H:357:MET:N     | 6:H:380:TYR:OH   | 2.44                     | 0.50              |
| 5:Y:709:LYS:HA    | 5:Y:712:ILE:HG22 | 1.94                     | 0.49              |
| 5:Y:1104:LYS:O    | 5:Y:1108:LEU:HG  | 2.11                     | 0.49              |
| 3:u:137:ARG:HH12  | 3:u:139:ARG:HH11 | 1.60                     | 0.49              |
| 4:x:261:ASP:HB3   | 4:x:264:ARG:HB2  | 1.94                     | 0.49              |
| 5:y:475:ALA:O     | 5:y:479:ILE:HG12 | 2.12                     | 0.49              |
| 5:y:821:ASP:OD1   | 5:y:821:ASP:N    | 2.45                     | 0.49              |
| 4:X:197:ARG:NH2   | 4:X:226:THR:O    | 2.45                     | 0.49              |
| 4:x:272:ARG:NH1   | 4:x:375:ASN:O    | 2.45                     | 0.49              |
| 4:x:874:ASP:OD1   | 4:x:874:ASP:N    | 2.41                     | 0.49              |
| 5:y:895:PRO:HA    | 5:y:1097:HIS:CE1 | 2.47                     | 0.49              |
| 6:h:240:THR:HG23  | 6:h:241:SER:H    | 1.77                     | 0.49              |
| 6:h:669:VAL:HG22  | 6:h:721:LEU:HB3  | 1.94                     | 0.49              |
| 1:d:69:LEU:HB2    | 1:d:79:ARG:HD2   | 1.93                     | 0.49              |
| 2:e:16:VAL:HG21   | 5:y:529:GLY:HA2  | 1.92                     | 0.49              |
| 5:y:159:LEU:HD12  | 5:y:163:GLY:HA2  | 1.93                     | 0.49              |
| 6:h:293:PHE:O     | 6:h:297:ILE:HG12 | 2.13                     | 0.49              |
| 3:U:42:ARG:HE     | 3:V:35:THR:HB    | 1.77                     | 0.49              |
| 5:Y:728:MET:O     | 5:Y:732:SER:HB3  | 2.12                     | 0.49              |
| 6:H:425:LYS:HA    | 6:H:428:TYR:CD2  | 2.48                     | 0.49              |
| 6:H:671:CYS:HB2   | 6:H:723:TYR:HE1  | 1.77                     | 0.49              |
| 1:d:55:ILE:HA     | 1:d:58:PHE:HB3   | 1.94                     | 0.49              |
| 4:x:547:TYR:OH    | 4:x:595:ARG:NH1  | 2.43                     | 0.49              |
| 5:y:788:ALA:O     | 5:y:792:LEU:HG   | 2.13                     | 0.49              |
| 3:V:222:ASN:HA    | 3:V:225:VAL:HG12 | 1.93                     | 0.49              |
| 5:Y:1086:THR:HG21 | 5:Y:1106:VAL:HB  | 1.95                     | 0.49              |
| 6:H:669:VAL:HG22  | 6:H:721:LEU:HB3  | 1.94                     | 0.49              |
| 3:v:58:ILE:HA     | 3:v:138:VAL:HG12 | 1.95                     | 0.49              |
| 6:h:671:CYS:HB2   | 6:h:723:TYR:HE1  | 1.78                     | 0.49              |
| 3:V:176:VAL:HG12  | 3:V:198:VAL:HA   | 1.94                     | 0.49              |
| 5:Y:35:ASN:HB3    | 5:Y:38:THR:HG22  | 1.95                     | 0.49              |
| 5:Y:87:VAL:HG12   | 5:Y:91:ARG:HG2   | 1.95                     | 0.49              |
| 5:Y:475:ALA:O     | 5:Y:479:ILE:HG12 | 2.12                     | 0.49              |
| 6:H:293:PHE:O     | 6:H:297:ILE:HG12 | 2.13                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:e:18:GLU:O      | 2:e:19:LYS:HG2   | 2.13                     | 0.49              |
| 3:u:89:ILE:HD11   | 3:u:144:ARG:HB2  | 1.95                     | 0.49              |
| 3:v:74:ASP:O      | 3:v:77:THR:OG1   | 2.21                     | 0.49              |
| 4:x:777:MET:SD    | 4:x:781:LEU:HD23 | 2.53                     | 0.49              |
| 4:x:862:HIS:HA    | 4:x:869:ALA:HB3  | 1.95                     | 0.49              |
| 6:h:191:ASP:OD2   | 6:h:191:ASP:N    | 2.45                     | 0.49              |
| 6:h:475:LEU:HG    | 6:h:478:LEU:HD21 | 1.94                     | 0.49              |
| 3:U:66:SER:OG     | 3:U:67:THR:N     | 2.44                     | 0.49              |
| 3:V:30:ARG:HB2    | 3:V:190:ASN:HB3  | 1.95                     | 0.49              |
| 5:Y:788:ALA:O     | 5:Y:792:LEU:HG   | 2.13                     | 0.49              |
| 6:H:611:ARG:N     | 6:H:631:ASN:OD1  | 2.46                     | 0.49              |
| 4:x:234:LEU:HD22  | 4:x:246:PRO:HB2  | 1.93                     | 0.49              |
| 5:y:1086:THR:HG21 | 5:y:1106:VAL:HB  | 1.95                     | 0.49              |
| 3:U:225:VAL:O     | 3:U:228:THR:OG1  | 2.20                     | 0.49              |
| 4:X:424:LEU:HA    | 4:X:427:MET:HB3  | 1.95                     | 0.49              |
| 4:X:470:PHE:HD1   | 4:X:719:ASN:HD21 | 1.61                     | 0.49              |
| 5:Y:367:LYS:HE3   | 5:Y:390:ILE:HG21 | 1.93                     | 0.49              |
| 5:Y:895:PRO:HA    | 5:Y:1097:HIS:CE1 | 2.48                     | 0.49              |
| 4:x:403:HIS:HE1   | 4:x:566:ALA:HB1  | 1.78                     | 0.49              |
| 4:x:813:ILE:HD11  | 4:x:844:GLY:HA3  | 1.93                     | 0.49              |
| 5:y:728:MET:O     | 5:y:732:SER:HB3  | 2.12                     | 0.49              |
| 6:h:266:PHE:O     | 6:h:546:ASP:HB2  | 2.13                     | 0.49              |
| 3:U:53:VAL:HB     | 3:U:166:ILE:HD11 | 1.95                     | 0.49              |
| 4:X:787:TYR:OH    | 4:X:1037:MET:O   | 2.23                     | 0.49              |
| 6:H:191:ASP:OD2   | 6:H:191:ASP:N    | 2.45                     | 0.49              |
| 3:u:227:LEU:HD22  | 3:v:12:VAL:HG21  | 1.95                     | 0.49              |
| 4:x:64:LEU:HD22   | 4:x:96:VAL:HG12  | 1.94                     | 0.49              |
| 4:x:408:ARG:NH2   | 4:x:414:GLU:OE2  | 2.46                     | 0.49              |
| 4:x:681:ILE:HG12  | 4:x:695:TYR:HB2  | 1.95                     | 0.49              |
| 4:X:668:LYS:NZ    | 4:X:669:ASP:OD2  | 2.44                     | 0.49              |
| 5:Y:30:LYS:HB2    | 5:Y:45:GLY:HA2   | 1.95                     | 0.49              |
| 5:Y:668:ASP:OD1   | 5:Y:668:ASP:N    | 2.46                     | 0.49              |
| 6:H:639:VAL:HG12  | 6:H:641:LYS:H    | 1.78                     | 0.49              |
| 5:y:35:ASN:HB3    | 5:y:38:THR:HG22  | 1.95                     | 0.49              |
| 4:X:841:LEU:HB3   | 4:X:878:ARG:HD3  | 1.95                     | 0.48              |
| 5:Y:133:SER:OG    | 5:Y:134:TYR:N    | 2.46                     | 0.48              |
| 6:H:195:GLN:HG2   | 6:H:209:ILE:HD12 | 1.95                     | 0.48              |
| 3:v:38:ASN:ND2    | 4:x:1022:THR:HA  | 2.28                     | 0.48              |
| 4:X:92:LEU:HD22   | 4:X:116:PHE:HB2  | 1.95                     | 0.48              |
| 4:X:181:TYR:HA    | 4:X:191:PRO:HA   | 1.94                     | 0.48              |
| 4:X:581:LEU:HB3   | 4:X:587:PHE:CD1  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:Y:492:SER:OG   | 5:Y:493:GLN:N    | 2.45                     | 0.48              |
| 6:H:12:GLN:HA    | 6:H:15:ILE:HD12  | 1.94                     | 0.48              |
| 6:H:236:GLY:HA2  | 6:H:239:LYS:HE2  | 1.93                     | 0.48              |
| 6:H:475:LEU:HG   | 6:H:478:LEU:HD21 | 1.95                     | 0.48              |
| 1:d:79:ARG:HH21  | 1:d:87:LEU:HD13  | 1.78                     | 0.48              |
| 4:x:773:ASP:OD2  | 4:x:965:ARG:NH2  | 2.36                     | 0.48              |
| 5:y:87:VAL:HG12  | 5:y:91:ARG:HG2   | 1.95                     | 0.48              |
| 3:V:149:THR:HG23 | 3:V:153:ALA:HB3  | 1.95                     | 0.48              |
| 6:H:241:SER:HA   | 6:H:244:LEU:HB2  | 1.94                     | 0.48              |
| 3:u:47:SER:HB2   | 3:u:146:ARG:HD2  | 1.95                     | 0.48              |
| 6:h:195:GLN:HG2  | 6:h:209:ILE:HD12 | 1.95                     | 0.48              |
| 4:X:853:GLU:HB2  | 4:X:859:ARG:HD3  | 1.95                     | 0.48              |
| 4:x:166:ARG:HB2  | 4:x:266:ASP:HB3  | 1.94                     | 0.48              |
| 5:y:30:LYS:HB2   | 5:y:45:GLY:HA2   | 1.95                     | 0.48              |
| 5:y:75:CYS:HB3   | 5:y:80:VAL:H     | 1.78                     | 0.48              |
| 6:h:425:LYS:HA   | 6:h:428:TYR:CD2  | 2.48                     | 0.48              |
| 6:h:730:TYR:HB2  | 6:h:758:ALA:HB3  | 1.95                     | 0.48              |
| 2:E:7:TYR:CE1    | 2:E:21:ASP:HB2   | 2.48                     | 0.48              |
| 3:V:200:THR:OG1  | 3:V:204:THR:O    | 2.28                     | 0.48              |
| 5:Y:75:CYS:HB3   | 5:Y:80:VAL:H     | 1.78                     | 0.48              |
| 6:H:266:PHE:O    | 6:H:546:ASP:HB2  | 2.13                     | 0.48              |
| 6:H:300:ARG:NE   | 6:H:525:LEU:HD11 | 2.29                     | 0.48              |
| 6:H:730:TYR:HB2  | 6:H:758:ALA:HB3  | 1.96                     | 0.48              |
| 4:x:108:ASP:OD1  | 4:x:109:GLN:N    | 2.46                     | 0.48              |
| 4:x:454:VAL:O    | 4:x:457:SER:HB3  | 2.12                     | 0.48              |
| 5:Y:236:PRO:HA   | 5:Y:239:ARG:HG3  | 1.96                     | 0.48              |
| 5:Y:589:LYS:HA   | 5:Y:589:LYS:HD3  | 1.60                     | 0.48              |
| 4:x:779:GLU:HB2  | 4:x:941:GLU:HB2  | 1.94                     | 0.48              |
| 5:y:236:PRO:HA   | 5:y:239:ARG:HG3  | 1.95                     | 0.48              |
| 6:h:36:LEU:O     | 6:h:40:ILE:HG12  | 2.14                     | 0.48              |
| 3:U:26:GLU:O     | 3:U:28:LEU:HD12  | 2.13                     | 0.48              |
| 4:X:1048:LEU:O   | 5:Y:341:ARG:N    | 2.47                     | 0.48              |
| 6:H:106:PHE:HZ   | 6:H:144:LEU:HD21 | 1.79                     | 0.48              |
| 4:x:457:SER:O    | 4:x:460:GLU:HG3  | 2.12                     | 0.48              |
| 4:x:523:PRO:HA   | 6:h:62:ILE:HD12  | 1.95                     | 0.48              |
| 5:y:441:LEU:HD21 | 5:y:495:MET:HE1  | 1.94                     | 0.48              |
| 6:h:485:LEU:HD13 | 6:h:508:ARG:HG2  | 1.96                     | 0.48              |
| 4:X:1019:ASP:OD1 | 4:X:1020:GLY:N   | 2.46                     | 0.48              |
| 5:Y:505:GLU:HG2  | 5:Y:561:THR:HG21 | 1.95                     | 0.48              |
| 5:Y:821:ASP:OD1  | 5:Y:821:ASP:N    | 2.45                     | 0.48              |
| 6:h:143:SER:O    | 6:h:147:ASN:ND2  | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:55:ILE:HA    | 1:D:58:PHE:HB3   | 1.94                     | 0.48              |
| 4:X:928:ARG:NH2  | 4:X:973:GLU:OE2  | 2.39                     | 0.48              |
| 5:Y:1135:SER:O   | 5:Y:1138:SER:OG  | 2.22                     | 0.48              |
| 6:H:194:LEU:HD11 | 6:H:631:ASN:HB2  | 1.96                     | 0.48              |
| 6:H:497:HIS:ND1  | 6:H:499:LYS:HB2  | 2.29                     | 0.48              |
| 4:x:784:ASP:HB3  | 4:x:786:VAL:HG23 | 1.96                     | 0.48              |
| 4:x:839:GLY:H    | 4:x:879:VAL:HB   | 1.78                     | 0.48              |
| 6:h:355:GLU:O    | 6:h:380:TYR:OH   | 2.18                     | 0.48              |
| 6:h:611:ARG:N    | 6:h:631:ASN:OD1  | 2.46                     | 0.48              |
| 6:h:676:GLN:NE2  | 6:h:728:GLU:OE2  | 2.28                     | 0.48              |
| 5:Y:233:VAL:HG23 | 5:Y:258:TYR:CZ   | 2.49                     | 0.48              |
| 6:H:36:LEU:O     | 6:H:40:ILE:HG12  | 2.14                     | 0.48              |
| 6:H:578:ILE:HD13 | 6:H:741:THR:HG21 | 1.95                     | 0.48              |
| 6:H:738:LEU:O    | 6:H:741:THR:OG1  | 2.26                     | 0.48              |
| 4:x:564:LEU:HD22 | 4:x:568:GLU:HG2  | 1.95                     | 0.48              |
| 4:x:699:ASP:O    | 4:x:702:LYS:NZ   | 2.47                     | 0.48              |
| 5:y:505:GLU:HG2  | 5:y:561:THR:HG21 | 1.95                     | 0.48              |
| 6:h:671:CYS:SG   | 6:h:672:LYS:N    | 2.87                     | 0.48              |
| 6:H:485:LEU:HD13 | 6:H:508:ARG:HG2  | 1.95                     | 0.47              |
| 2:e:7:TYR:CE1    | 2:e:21:ASP:HB2   | 2.48                     | 0.47              |
| 3:U:64:GLU:HB2   | 3:U:164:ILE:HG12 | 1.96                     | 0.47              |
| 5:Y:110:ILE:HG12 | 6:H:449:TYR:HE1  | 1.79                     | 0.47              |
| 4:x:72:GLY:N     | 4:x:91:PRO:O     | 2.36                     | 0.47              |
| 5:y:211:GLU:HA   | 5:y:211:GLU:OE2  | 2.14                     | 0.47              |
| 6:h:231:VAL:HB   | 6:h:571:LEU:HG   | 1.96                     | 0.47              |
| 6:h:246:ARG:HH12 | 6:h:250:LEU:HD22 | 1.78                     | 0.47              |
| 1:D:23:LEU:O     | 1:D:27:HIS:HB2   | 2.15                     | 0.47              |
| 3:V:106:THR:HB   | 3:V:129:THR:HG23 | 1.96                     | 0.47              |
| 5:Y:692:ILE:HG23 | 5:Y:696:GLU:HB3  | 1.96                     | 0.47              |
| 6:H:246:ARG:HH12 | 6:H:250:LEU:HD22 | 1.78                     | 0.47              |
| 6:H:526:TYR:HD1  | 6:H:558:TYR:HD1  | 1.63                     | 0.47              |
| 3:u:161:ILE:HG21 | 4:x:834:ALA:HA   | 1.95                     | 0.47              |
| 3:u:222:ASN:HA   | 3:u:225:VAL:CG2  | 2.42                     | 0.47              |
| 4:x:800:ARG:HA   | 4:x:905:VAL:HA   | 1.95                     | 0.47              |
| 5:y:133:SER:OG   | 5:y:134:TYR:N    | 2.46                     | 0.47              |
| 5:y:233:VAL:HG23 | 5:y:258:TYR:CZ   | 2.49                     | 0.47              |
| 1:D:79:ARG:HH21  | 1:D:87:LEU:HD13  | 1.79                     | 0.47              |
| 3:V:74:ASP:HB2   | 5:Y:598:LYS:HD2  | 1.96                     | 0.47              |
| 5:Y:211:GLU:HA   | 5:Y:211:GLU:OE2  | 2.14                     | 0.47              |
| 5:Y:251:THR:HG1  | 5:y:36:TYR:HH    | 1.63                     | 0.47              |
| 1:d:23:LEU:O     | 1:d:27:HIS:HB2   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:x:338:VAL:HB   | 4:x:346:SER:HB2  | 1.96                     | 0.47              |
| 4:x:581:LEU:HA   | 4:x:587:PHE:HA   | 1.95                     | 0.47              |
| 5:y:462:SER:O    | 5:y:466:GLN:N    | 2.33                     | 0.47              |
| 6:h:497:HIS:ND1  | 6:h:499:LYS:HB2  | 2.29                     | 0.47              |
| 6:h:639:VAL:HG12 | 6:h:641:LYS:H    | 1.78                     | 0.47              |
| 2:E:18:GLU:O     | 2:E:19:LYS:HG2   | 2.13                     | 0.47              |
| 4:X:284:ARG:HD3  | 4:X:390:ASN:HD22 | 1.80                     | 0.47              |
| 4:X:974:LEU:HD12 | 4:X:1035:MET:HB2 | 1.97                     | 0.47              |
| 5:Y:88:ARG:HD2   | 5:Y:236:PRO:HG2  | 1.96                     | 0.47              |
| 6:H:143:SER:O    | 6:H:147:ASN:ND2  | 2.47                     | 0.47              |
| 3:u:12:VAL:HG21  | 3:v:227:LEU:HD22 | 1.96                     | 0.47              |
| 4:x:716:VAL:HG13 | 4:x:724:TYR:HB3  | 1.96                     | 0.47              |
| 5:y:88:ARG:HD2   | 5:y:236:PRO:HG2  | 1.96                     | 0.47              |
| 6:h:300:ARG:NE   | 6:h:525:LEU:HD11 | 2.29                     | 0.47              |
| 6:h:484:TYR:HD2  | 6:h:511:PHE:CE2  | 2.30                     | 0.47              |
| 6:H:671:CYS:SG   | 6:H:672:LYS:N    | 2.87                     | 0.47              |
| 3:v:149:THR:HB   | 3:v:168:SER:HB3  | 1.97                     | 0.47              |
| 4:x:32:ILE:HG13  | 4:x:33:GLN:N     | 2.29                     | 0.47              |
| 6:h:173:MET:HE2  | 6:h:181:ALA:HB2  | 1.97                     | 0.47              |
| 6:h:578:ILE:HD13 | 6:h:741:THR:HG21 | 1.95                     | 0.47              |
| 3:U:53:VAL:HG13  | 3:U:140:LEU:HD13 | 1.96                     | 0.47              |
| 4:X:62:LEU:HB3   | 4:X:98:LEU:HD11  | 1.95                     | 0.47              |
| 4:X:684:ARG:HB3  | 4:X:691:TRP:HB2  | 1.97                     | 0.47              |
| 4:X:811:ARG:HG2  | 4:X:821:LEU:HD11 | 1.97                     | 0.47              |
| 5:Y:191:LEU:HD11 | 5:Y:209:ARG:HE   | 1.80                     | 0.47              |
| 5:Y:486:LYS:HE3  | 5:Y:487:PRO:HD2  | 1.96                     | 0.47              |
| 6:H:231:VAL:HB   | 6:H:571:LEU:HG   | 1.96                     | 0.47              |
| 6:H:484:TYR:HD2  | 6:H:511:PHE:CE2  | 2.30                     | 0.47              |
| 6:H:610:THR:OG1  | 6:H:747:MET:O    | 2.30                     | 0.47              |
| 3:u:28:LEU:O     | 3:u:192:ASP:N    | 2.39                     | 0.47              |
| 4:x:266:ASP:OD2  | 4:x:421:ARG:NH1  | 2.47                     | 0.47              |
| 5:y:108:LYS:HE3  | 6:h:449:TYR:CE2  | 2.50                     | 0.47              |
| 5:y:751:MET:HG2  | 5:y:778:ILE:O    | 2.15                     | 0.47              |
| 3:v:173:VAL:HA   | 3:v:200:THR:HA   | 1.95                     | 0.47              |
| 4:x:159:THR:HG22 | 4:x:173:GLU:HG3  | 1.96                     | 0.47              |
| 4:x:955:ILE:HD11 | 4:x:1037:MET:HG3 | 1.97                     | 0.47              |
| 4:X:14:ARG:NH1   | 4:X:752:GLU:OE2  | 2.47                     | 0.47              |
| 4:X:457:SER:O    | 4:X:460:GLU:HG3  | 2.14                     | 0.47              |
| 4:X:777:MET:HE1  | 4:X:919:ILE:HG12 | 1.95                     | 0.47              |
| 3:u:66:SER:OG    | 3:u:67:THR:N     | 2.45                     | 0.47              |
| 4:x:513:ARG:HH12 | 4:x:566:ALA:HA   | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:y:802:ARG:HH21 | 5:y:1139:PHE:HA  | 1.80                     | 0.47              |
| 5:y:838:ARG:HG3  | 5:y:839:LEU:H    | 1.80                     | 0.47              |
| 6:h:194:LEU:HD11 | 6:h:631:ASN:HB2  | 1.96                     | 0.47              |
| 6:h:518:TYR:HA   | 6:h:521:ALA:HB3  | 1.97                     | 0.47              |
| 3:U:38:ASN:OD1   | 3:U:42:ARG:NH2   | 2.47                     | 0.47              |
| 4:X:254:LEU:HD11 | 4:X:258:ARG:HH11 | 1.80                     | 0.47              |
| 4:X:391:LEU:HG   | 4:X:396:GLY:HA3  | 1.97                     | 0.47              |
| 4:X:643:MET:HE3  | 4:X:932:LYS:HB3  | 1.96                     | 0.47              |
| 4:X:694:ARG:HB2  | 4:X:704:LYS:HB2  | 1.97                     | 0.47              |
| 4:X:696:GLU:HA   | 4:X:703:VAL:HA   | 1.96                     | 0.47              |
| 6:H:345:ILE:O    | 6:H:349:VAL:HG12 | 2.15                     | 0.47              |
| 3:v:97:LEU:HD21  | 3:v:118:VAL:HG11 | 1.96                     | 0.47              |
| 4:x:633:ASP:OD1  | 4:x:634:SER:N    | 2.44                     | 0.47              |
| 5:y:692:ILE:HG23 | 5:y:696:GLU:HB3  | 1.96                     | 0.47              |
| 4:X:620:SER:OG   | 4:X:621:ALA:N    | 2.47                     | 0.46              |
| 5:Y:751:MET:HG2  | 5:Y:778:ILE:O    | 2.15                     | 0.46              |
| 5:Y:787:LEU:O    | 5:Y:790:THR:OG1  | 2.23                     | 0.46              |
| 6:H:355:GLU:O    | 6:H:380:TYR:OH   | 2.18                     | 0.46              |
| 3:v:92:ASP:OD1   | 3:v:92:ASP:N     | 2.48                     | 0.46              |
| 3:v:221:LEU:O    | 3:v:225:VAL:HG23 | 2.14                     | 0.46              |
| 4:x:124:THR:OG1  | 4:x:132:ARG:O    | 2.30                     | 0.46              |
| 4:x:960:LEU:HA   | 5:y:729:MET:HE3  | 1.96                     | 0.46              |
| 4:x:991:VAL:HG23 | 4:x:992:PHE:HD1  | 1.80                     | 0.46              |
| 5:y:1038:THR:OG1 | 5:y:1039:ASP:N   | 2.48                     | 0.46              |
| 6:h:106:PHE:HZ   | 6:h:144:LEU:HD21 | 1.79                     | 0.46              |
| 4:X:46:ARG:HE    | 4:X:69:TYR:HE1   | 1.63                     | 0.46              |
| 6:H:518:TYR:HA   | 6:H:521:ALA:HB3  | 1.97                     | 0.46              |
| 3:v:122:ASN:ND2  | 3:v:125:LEU:HB2  | 2.31                     | 0.46              |
| 5:y:191:LEU:HD11 | 5:y:209:ARG:HE   | 1.80                     | 0.46              |
| 5:y:299:GLY:HA3  | 6:h:446:PHE:O    | 2.15                     | 0.46              |
| 4:X:480:LEU:HD22 | 4:X:670:SER:HB3  | 1.98                     | 0.46              |
| 4:X:997:GLU:OE1  | 5:Y:768:ARG:NH1  | 2.49                     | 0.46              |
| 5:Y:462:SER:O    | 5:Y:466:GLN:N    | 2.33                     | 0.46              |
| 6:H:647:SER:O    | 6:H:650:GLN:HG2  | 2.15                     | 0.46              |
| 4:x:475:ASN:HD22 | 4:x:647:ALA:HB3  | 1.80                     | 0.46              |
| 4:x:1005:GLU:HA  | 4:x:1010:SER:HA  | 1.98                     | 0.46              |
| 5:y:990:GLU:HA   | 5:y:1003:THR:HA  | 1.98                     | 0.46              |
| 5:y:1135:SER:O   | 5:y:1138:SER:OG  | 2.22                     | 0.46              |
| 6:h:647:SER:O    | 6:h:650:GLN:HG2  | 2.15                     | 0.46              |
| 6:h:691:ARG:HE   | 6:h:692:LEU:H    | 1.63                     | 0.46              |
| 2:E:25:ILE:HG21  | 2:E:33:VAL:HG13  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:V:8:LYS:HZ2     | 3:V:26:GLU:HG2    | 1.80                     | 0.46              |
| 4:X:132:ARG:NH1   | 4:X:468:SER:OG    | 2.49                     | 0.46              |
| 5:Y:990:GLU:HA    | 5:Y:1003:THR:HA   | 1.98                     | 0.46              |
| 6:H:173:MET:HE2   | 6:H:181:ALA:HB2   | 1.97                     | 0.46              |
| 1:d:9:GLU:HA      | 1:d:12:LYS:HD2    | 1.97                     | 0.46              |
| 4:x:829:ILE:HD12  | 4:x:890:VAL:HG21  | 1.97                     | 0.46              |
| 4:x:968:ILE:HD11  | 5:y:744:LEU:HD11  | 1.97                     | 0.46              |
| 6:h:526:TYR:HD1   | 6:h:558:TYR:HD1   | 1.63                     | 0.46              |
| 4:X:42:ASP:OD1    | 4:X:42:ASP:N      | 2.47                     | 0.46              |
| 6:H:263:ILE:HB    | 6:H:288:MET:HE1   | 1.98                     | 0.46              |
| 5:y:557:LEU:O     | 5:y:595:PHE:HB2   | 2.16                     | 0.46              |
| 3:V:13:GLU:OE2    | 3:V:15:SER:OG     | 2.33                     | 0.46              |
| 3:V:75:VAL:HA     | 3:V:78:ILE:HD12   | 1.97                     | 0.46              |
| 4:X:967:ASN:O     | 4:X:970:GLN:HG2   | 2.15                     | 0.46              |
| 4:X:1014:LYS:HD3  | 4:X:1030:VAL:C    | 2.41                     | 0.46              |
| 5:Y:802:ARG:HH21  | 5:Y:1139:PHE:HA   | 1.80                     | 0.46              |
| 5:Y:1120:LEU:HD23 | 5:Y:1120:LEU:H    | 1.81                     | 0.46              |
| 3:u:53:VAL:O      | 3:u:54:THR:HG22   | 2.16                     | 0.46              |
| 4:x:224:ASP:OD1   | 4:x:225:ASN:N     | 2.49                     | 0.46              |
| 5:y:486:LYS:HE3   | 5:y:487:PRO:HD2   | 1.96                     | 0.46              |
| 6:h:147:ASN:OD1   | 6:h:253:ARG:NH2   | 2.48                     | 0.46              |
| 6:h:345:ILE:O     | 6:h:349:VAL:HG12  | 2.15                     | 0.46              |
| 6:h:411:ARG:HA    | 6:h:461:VAL:HG11  | 1.98                     | 0.46              |
| 6:h:669:VAL:HB    | 6:h:706:VAL:HA    | 1.98                     | 0.46              |
| 3:U:27:PRO:HG3    | 3:U:185:VAL:HG11  | 1.98                     | 0.46              |
| 5:Y:256:ASP:OD1   | 5:Y:259:ARG:NH2   | 2.49                     | 0.46              |
| 5:Y:566:VAL:O     | 5:Y:569:GLU:HB3   | 2.16                     | 0.46              |
| 6:H:520:ASP:C     | 6:H:523:PRO:HD2   | 2.41                     | 0.46              |
| 6:H:613:ILE:O     | 6:H:617:THR:HG23  | 2.16                     | 0.46              |
| 6:H:669:VAL:HB    | 6:H:706:VAL:HA    | 1.98                     | 0.46              |
| 1:d:34:GLN:HA     | 1:d:37:LEU:HG     | 1.97                     | 0.46              |
| 2:e:25:ILE:HG21   | 2:e:33:VAL:HG13   | 1.97                     | 0.46              |
| 3:u:25:VAL:HG12   | 3:u:194:LEU:H     | 1.81                     | 0.46              |
| 4:x:764:MET:HE3   | 4:x:1030:VAL:HG11 | 1.96                     | 0.46              |
| 5:y:412:LEU:HD11  | 5:y:455:MET:HE3   | 1.98                     | 0.46              |
| 5:y:566:VAL:O     | 5:y:569:GLU:HB3   | 2.16                     | 0.46              |
| 5:y:993:VAL:O     | 5:y:999:THR:HA    | 2.16                     | 0.46              |
| 4:X:636:ARG:HA    | 4:X:636:ARG:HD3   | 1.65                     | 0.46              |
| 4:X:680:GLY:HA3   | 4:X:694:ARG:HA    | 1.98                     | 0.46              |
| 4:X:681:ILE:HG12  | 4:X:695:TYR:HB2   | 1.97                     | 0.46              |
| 5:Y:557:LEU:O     | 5:Y:595:PHE:HB2   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:x:547:TYR:HD2  | 4:x:564:LEU:HD12  | 1.81                     | 0.46              |
| 4:x:549:ARG:HD2  | 4:x:560:ARG:HH22  | 1.80                     | 0.46              |
| 4:x:658:VAL:HA   | 4:x:987:ILE:O     | 2.16                     | 0.46              |
| 6:H:147:ASN:OD1  | 6:H:253:ARG:NH2   | 2.48                     | 0.46              |
| 1:d:37:LEU:HD22  | 1:d:55:ILE:HD11   | 1.98                     | 0.46              |
| 4:x:1021:ARG:HG2 | 4:x:1022:THR:HG23 | 1.98                     | 0.46              |
| 1:D:34:GLN:HA    | 1:D:37:LEU:HG     | 1.98                     | 0.45              |
| 4:X:403:HIS:HE1  | 4:X:566:ALA:HB1   | 1.81                     | 0.45              |
| 6:H:329:ARG:NH2  | 6:H:519:GLU:OE2   | 2.49                     | 0.45              |
| 3:v:180:VAL:HG22 | 3:v:194:LEU:HB3   | 1.97                     | 0.45              |
| 4:x:404:LEU:HD23 | 4:x:513:ARG:HD2   | 1.97                     | 0.45              |
| 4:x:777:MET:HE3  | 4:x:777:MET:HB2   | 1.85                     | 0.45              |
| 5:y:465:ALA:HA   | 5:y:468:GLU:HG3   | 1.98                     | 0.45              |
| 1:D:9:GLU:HA     | 1:D:12:LYS:HD2    | 1.97                     | 0.45              |
| 3:V:70:GLY:HA3   | 3:V:134:ALA:HB2   | 1.97                     | 0.45              |
| 4:X:408:ARG:NH2  | 4:X:414:GLU:OE1   | 2.50                     | 0.45              |
| 4:X:807:GLU:HG2  | 4:X:847:THR:HA    | 1.99                     | 0.45              |
| 5:Y:884:VAL:HG12 | 5:Y:885:TRP:N     | 2.32                     | 0.45              |
| 6:H:522:ALA:HB3  | 6:H:523:PRO:HD3   | 1.98                     | 0.45              |
| 4:x:97:ARG:HA    | 4:x:108:ASP:HA    | 1.98                     | 0.45              |
| 6:h:613:ILE:O    | 6:h:617:THR:HG23  | 2.16                     | 0.45              |
| 2:E:8:GLN:OE1    | 2:E:15:PRO:HB3    | 2.16                     | 0.45              |
| 4:X:777:MET:HG3  | 4:X:781:LEU:HD12  | 1.98                     | 0.45              |
| 4:X:962:VAL:HB   | 4:X:963:PRO:HD3   | 1.98                     | 0.45              |
| 5:Y:465:ALA:HA   | 5:Y:468:GLU:HG3   | 1.98                     | 0.45              |
| 5:Y:838:ARG:HG3  | 5:Y:839:LEU:H     | 1.80                     | 0.45              |
| 6:H:610:THR:O    | 6:H:614:VAL:HG13  | 2.17                     | 0.45              |
| 3:v:53:VAL:HG12  | 3:v:140:LEU:HD13  | 1.97                     | 0.45              |
| 5:y:48:CYS:SG    | 5:y:50:ARG:HG2    | 2.56                     | 0.45              |
| 5:y:441:LEU:HD13 | 5:y:489:VAL:HG12  | 1.99                     | 0.45              |
| 6:h:520:ASP:C    | 6:h:523:PRO:HD2   | 2.41                     | 0.45              |
| 4:X:804:LEU:HD11 | 4:X:850:GLY:HA3   | 1.98                     | 0.45              |
| 5:Y:1082:ASP:OD1 | 5:Y:1082:ASP:N    | 2.46                     | 0.45              |
| 6:H:411:ARG:HA   | 6:H:461:VAL:HG11  | 1.98                     | 0.45              |
| 6:H:643:GLU:O    | 6:H:647:SER:OG    | 2.29                     | 0.45              |
| 4:x:426:ARG:HD2  | 4:x:453:PRO:HB3   | 1.97                     | 0.45              |
| 5:y:355:CYS:HG   | 5:y:426:PHE:HE2   | 1.63                     | 0.45              |
| 4:X:228:ASN:HB3  | 4:X:231:LYS:HG2   | 1.98                     | 0.45              |
| 5:Y:48:CYS:SG    | 5:Y:50:ARG:HG2    | 2.56                     | 0.45              |
| 5:Y:580:GLU:HG2  | 5:Y:594:PHE:CZ    | 2.51                     | 0.45              |
| 6:H:691:ARG:HE   | 6:H:692:LEU:H     | 1.64                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:8:GLN:OE1     | 2:e:15:PRO:HB3    | 2.16                     | 0.45              |
| 4:x:267:LEU:HD23  | 4:x:268:ALA:O     | 2.16                     | 0.45              |
| 4:x:1080:VAL:HA   | 4:x:1083:LEU:HG   | 1.98                     | 0.45              |
| 5:y:596:LEU:HD22  | 5:y:602:VAL:HG23  | 1.98                     | 0.45              |
| 5:y:884:VAL:HG12  | 5:y:885:TRP:N     | 2.32                     | 0.45              |
| 5:y:1120:LEU:H    | 5:y:1120:LEU:HD23 | 1.81                     | 0.45              |
| 6:h:363:ILE:HG12  | 6:h:368:LYS:HB3   | 1.99                     | 0.45              |
| 4:X:1142:VAL:HG12 | 4:X:1143:LYS:N    | 2.29                     | 0.45              |
| 4:x:226:THR:HG23  | 4:x:231:LYS:HE3   | 1.99                     | 0.45              |
| 4:x:887:ILE:HG22  | 4:x:913:ILE:HG22  | 1.99                     | 0.45              |
| 3:V:223:ILE:HG13  | 3:V:224:PHE:N     | 2.32                     | 0.45              |
| 4:X:760:MET:HG2   | 4:X:953:ILE:HG22  | 1.98                     | 0.45              |
| 4:X:832:ILE:HA    | 4:X:887:ILE:HD11  | 1.99                     | 0.45              |
| 1:D:37:LEU:HD22   | 1:D:55:ILE:HD11   | 1.98                     | 0.45              |
| 3:U:223:ILE:O     | 3:U:227:LEU:HG    | 2.16                     | 0.45              |
| 3:V:57:GLN:HB2    | 3:V:163:VAL:HG12  | 1.98                     | 0.45              |
| 5:y:256:ASP:OD1   | 5:y:259:ARG:NH2   | 2.49                     | 0.45              |
| 6:h:522:ALA:HB3   | 6:h:523:PRO:HD3   | 1.98                     | 0.45              |
| 6:h:610:THR:O     | 6:h:614:VAL:HG13  | 2.16                     | 0.45              |
| 4:X:420:PHE:CE1   | 4:X:458:ILE:HD11  | 2.46                     | 0.45              |
| 5:Y:993:VAL:O     | 5:Y:999:THR:HA    | 2.16                     | 0.45              |
| 2:e:40:LYS:HE3    | 2:e:40:LYS:HB2    | 1.81                     | 0.45              |
| 4:x:212:GLY:HA2   | 4:x:217:LEU:HD11  | 1.99                     | 0.45              |
| 4:x:573:VAL:HG12  | 4:x:596:PHE:HB2   | 1.98                     | 0.45              |
| 6:h:329:ARG:NH2   | 6:h:519:GLU:OE2   | 2.49                     | 0.45              |
| 4:X:160:ALA:HB3   | 4:X:172:TYR:HB2   | 1.98                     | 0.45              |
| 4:X:797:SER:HB2   | 4:X:877:LEU:HD21  | 1.99                     | 0.45              |
| 4:x:41:LEU:O      | 4:x:45:LEU:HB2    | 2.17                     | 0.45              |
| 4:x:562:ASP:OD1   | 4:x:562:ASP:N     | 2.47                     | 0.45              |
| 5:y:964:ASN:OD1   | 5:y:964:ASN:C     | 2.59                     | 0.45              |
| 5:y:984:VAL:HG12  | 5:y:990:GLU:OE1   | 2.17                     | 0.45              |
| 6:h:26:GLU:O      | 6:h:30:GLU:HG2    | 2.17                     | 0.45              |
| 3:U:228:THR:HB    | 3:V:211:ALA:HB2   | 1.99                     | 0.44              |
| 3:U:232:GLN:O     | 3:U:236:ILE:HG12  | 2.17                     | 0.44              |
| 4:X:55:ILE:HG23   | 4:X:435:MET:HE1   | 1.99                     | 0.44              |
| 4:X:547:TYR:OH    | 4:X:595:ARG:NH1   | 2.45                     | 0.44              |
| 4:X:1013:ALA:HB1  | 4:X:1014:LYS:NZ   | 2.31                     | 0.44              |
| 5:Y:840:GLU:O     | 5:Y:844:ILE:HB    | 2.17                     | 0.44              |
| 5:Y:964:ASN:OD1   | 5:Y:964:ASN:C     | 2.59                     | 0.44              |
| 6:H:264:VAL:HG13  | 6:H:289:GLU:HG3   | 1.99                     | 0.44              |
| 5:y:580:GLU:HG2   | 5:y:594:PHE:CZ    | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:h:615:GLU:HG3   | 6:h:629:PRO:HG3   | 1.99                     | 0.44              |
| 4:X:116:PHE:HE2   | 4:X:420:PHE:HZ    | 1.65                     | 0.44              |
| 4:X:451:ILE:O     | 4:X:454:VAL:HG12  | 2.17                     | 0.44              |
| 4:X:697:GLU:HB2   | 4:X:704:LYS:HE3   | 1.99                     | 0.44              |
| 5:Y:412:LEU:HD11  | 5:Y:455:MET:HE3   | 1.98                     | 0.44              |
| 6:H:26:GLU:O      | 6:H:30:GLU:HG2    | 2.18                     | 0.44              |
| 6:H:615:GLU:HG3   | 6:H:629:PRO:HG3   | 1.99                     | 0.44              |
| 3:u:42:ARG:NH1    | 3:v:34:THR:OG1    | 2.48                     | 0.44              |
| 4:x:978:MET:HE3   | 4:x:1009:MET:HE1  | 1.99                     | 0.44              |
| 5:y:890:PHE:CZ    | 5:y:1044:GLN:HB3  | 2.53                     | 0.44              |
| 6:h:263:ILE:HB    | 6:h:288:MET:HE1   | 1.98                     | 0.44              |
| 1:D:1:MET:HE3     | 1:D:2:GLY:H       | 1.83                     | 0.44              |
| 2:E:16:VAL:CG2    | 2:E:17:ARG:N      | 2.80                     | 0.44              |
| 4:X:1021:ARG:H    | 4:X:1021:ARG:HD3  | 1.82                     | 0.44              |
| 5:Y:596:LEU:HD22  | 5:Y:602:VAL:HG23  | 1.98                     | 0.44              |
| 1:d:1:MET:HE3     | 1:d:2:GLY:H       | 1.83                     | 0.44              |
| 2:e:12:ASP:O      | 2:e:14:VAL:HG22   | 2.18                     | 0.44              |
| 2:e:16:VAL:CG2    | 2:e:17:ARG:N      | 2.80                     | 0.44              |
| 3:u:23:PHE:HZ     | 3:u:210:ILE:HG13  | 1.82                     | 0.44              |
| 4:x:788:THR:HG22  | 4:x:918:LYS:HG2   | 1.98                     | 0.44              |
| 6:h:207:LYS:HA    | 6:h:207:LYS:HD3   | 1.86                     | 0.44              |
| 4:X:32:ILE:HG13   | 4:X:33:GLN:N      | 2.33                     | 0.44              |
| 5:Y:441:LEU:HD13  | 5:Y:489:VAL:HG12  | 1.99                     | 0.44              |
| 5:Y:536:ARG:HG2   | 5:Y:561:THR:HG22  | 1.98                     | 0.44              |
| 6:H:363:ILE:HG12  | 6:H:368:LYS:HB3   | 1.99                     | 0.44              |
| 3:u:42:ARG:CZ     | 3:v:35:THR:HB     | 2.48                     | 0.44              |
| 3:u:124:ASP:OD1   | 3:u:124:ASP:N     | 2.44                     | 0.44              |
| 4:x:980:ALA:HA    | 4:x:985:ILE:HG22  | 1.99                     | 0.44              |
| 4:X:744:ASP:OD1   | 4:X:744:ASP:N     | 2.51                     | 0.44              |
| 4:x:80:GLU:HA     | 4:x:83:GLU:HG3    | 2.00                     | 0.44              |
| 5:y:536:ARG:HG2   | 5:y:561:THR:HG22  | 1.99                     | 0.44              |
| 4:X:431:VAL:HG22  | 4:X:449:ILE:HD13  | 2.00                     | 0.44              |
| 4:X:819:ASP:OD1   | 4:X:819:ASP:N     | 2.51                     | 0.44              |
| 6:H:607:TYR:HE1   | 6:H:630:PHE:HD2   | 1.66                     | 0.44              |
| 6:H:741:THR:O     | 6:H:745:ARG:HG2   | 2.18                     | 0.44              |
| 6:h:607:TYR:HE1   | 6:h:630:PHE:HD2   | 1.66                     | 0.44              |
| 6:H:352:LEU:HD11  | 6:H:483:LEU:HD21  | 2.00                     | 0.44              |
| 2:e:2:ILE:HD13    | 2:e:55:LEU:HD11   | 2.00                     | 0.44              |
| 6:h:305:PHE:CE2   | 6:h:516:LEU:HB3   | 2.47                     | 0.44              |
| 4:X:1017:LEU:HD11 | 4:X:1032:VAL:HG11 | 1.99                     | 0.44              |
| 5:Y:890:PHE:CZ    | 5:Y:1044:GLN:HB3  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:H:320:GLU:O    | 6:H:325:ASP:N    | 2.51                     | 0.44              |
| 6:H:527:MET:HE3  | 6:H:527:MET:HB3  | 1.92                     | 0.44              |
| 4:x:475:ASN:HD22 | 4:x:755:LEU:HD22 | 1.83                     | 0.44              |
| 4:x:619:VAL:HB   | 4:x:623:THR:HG23 | 2.00                     | 0.44              |
| 4:x:620:SER:OG   | 4:x:621:ALA:N    | 2.51                     | 0.44              |
| 4:x:807:GLU:HB3  | 4:x:845:LYS:HE3  | 2.00                     | 0.44              |
| 4:x:862:HIS:CE1  | 4:x:867:GLU:HA   | 2.53                     | 0.44              |
| 6:h:545:ILE:HG21 | 6:h:556:MET:SD   | 2.58                     | 0.44              |
| 2:E:16:VAL:O     | 4:X:1025:PRO:HD2 | 2.17                     | 0.44              |
| 2:E:57:TYR:CE1   | 3:U:13:GLU:HG2   | 2.53                     | 0.44              |
| 6:H:208:ASN:O    | 6:H:212:THR:HG23 | 2.18                     | 0.44              |
| 6:H:766:PRO:HB2  | 6:H:767:PRO:HD3  | 2.00                     | 0.44              |
| 6:h:264:VAL:HG13 | 6:h:289:GLU:HG3  | 1.99                     | 0.44              |
| 6:h:320:GLU:O    | 6:h:325:ASP:N    | 2.51                     | 0.44              |
| 2:E:12:ASP:O     | 2:E:14:VAL:HG22  | 2.18                     | 0.43              |
| 4:X:356:GLU:HB2  | 4:X:360:VAL:HG13 | 1.99                     | 0.43              |
| 5:Y:980:GLU:HB3  | 5:Y:992:VAL:HG12 | 2.00                     | 0.43              |
| 6:H:30:GLU:HB3   | 6:H:89:LEU:HD13  | 2.00                     | 0.43              |
| 6:H:193:MET:HA   | 6:H:196:GLU:HB2  | 1.99                     | 0.43              |
| 6:H:545:ILE:HG21 | 6:H:556:MET:SD   | 2.58                     | 0.43              |
| 3:u:219:GLU:HA   | 3:u:222:ASN:OD1  | 2.18                     | 0.43              |
| 4:x:23:VAL:HG11  | 4:x:548:ARG:HE   | 1.83                     | 0.43              |
| 4:x:89:SER:HA    | 4:x:117:PRO:HA   | 2.00                     | 0.43              |
| 4:x:713:LEU:HD13 | 4:x:716:VAL:HG11 | 1.99                     | 0.43              |
| 4:x:770:ASN:O    | 4:x:958:ASN:ND2  | 2.51                     | 0.43              |
| 4:x:910:ARG:NH2  | 4:x:912:TYR:OH   | 2.45                     | 0.43              |
| 5:y:787:LEU:O    | 5:y:790:THR:OG1  | 2.23                     | 0.43              |
| 6:h:692:LEU:HB3  | 6:h:705:CYS:SG   | 2.58                     | 0.43              |
| 2:E:50:VAL:HG21  | 2:E:55:LEU:HD12  | 1.99                     | 0.43              |
| 3:V:38:ASN:ND2   | 4:X:1022:THR:HA  | 2.34                     | 0.43              |
| 4:X:505:ASP:OD1  | 4:X:505:ASP:N    | 2.47                     | 0.43              |
| 4:X:766:TRP:HA   | 5:Y:652:THR:OG1  | 2.18                     | 0.43              |
| 4:X:801:ASP:OD1  | 4:X:801:ASP:N    | 2.51                     | 0.43              |
| 4:X:962:VAL:HG22 | 4:X:970:GLN:HE21 | 1.83                     | 0.43              |
| 5:Y:355:CYS:HG   | 5:Y:426:PHE:HE2  | 1.63                     | 0.43              |
| 5:Y:984:VAL:HG12 | 5:Y:990:GLU:OE1  | 2.17                     | 0.43              |
| 3:v:156:ARG:HB2  | 3:v:159:GLN:HG3  | 2.01                     | 0.43              |
| 4:x:766:TRP:HA   | 5:y:652:THR:OG1  | 2.18                     | 0.43              |
| 6:h:352:LEU:HD11 | 6:h:483:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:47:LYS:HA    | 1:D:47:LYS:HD3   | 1.84                     | 0.43              |
| 3:V:97:LEU:HD12  | 3:V:112:ILE:HG22 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:X:480:LEU:HB2  | 4:X:670:SER:HB2   | 1.98                     | 0.43              |
| 4:X:731:SER:OG   | 4:X:734:ASP:OD2   | 2.35                     | 0.43              |
| 2:e:50:VAL:HG21  | 2:e:55:LEU:HD12   | 1.99                     | 0.43              |
| 4:x:70:SER:N     | 4:x:93:ARG:O      | 2.46                     | 0.43              |
| 5:y:789:ASP:O    | 5:y:793:LYS:HG2   | 2.18                     | 0.43              |
| 2:E:29:SER:O     | 2:E:33:VAL:HG23   | 2.18                     | 0.43              |
| 3:V:44:LEU:HD23  | 3:V:176:VAL:HG11  | 2.00                     | 0.43              |
| 4:X:489:LEU:HA   | 4:X:493:GLY:HA3   | 2.00                     | 0.43              |
| 5:Y:268:LEU:HD13 | 5:Y:284:GLU:HB3   | 2.00                     | 0.43              |
| 6:H:390:ASN:O    | 6:H:393:GLU:HG3   | 2.18                     | 0.43              |
| 6:H:574:ILE:HG22 | 6:H:589:MET:HG2   | 2.00                     | 0.43              |
| 5:y:78:CYS:HB2   | 5:y:80:VAL:HG13   | 2.00                     | 0.43              |
| 5:y:840:GLU:O    | 5:y:844:ILE:HB    | 2.17                     | 0.43              |
| 6:h:390:ASN:O    | 6:h:393:GLU:HG3   | 2.18                     | 0.43              |
| 4:X:472:ASP:N    | 4:X:472:ASP:OD1   | 2.52                     | 0.43              |
| 4:x:2:THR:OG1    | 4:x:3:GLY:N       | 2.51                     | 0.43              |
| 4:x:424:LEU:HA   | 4:x:427:MET:HB3   | 2.01                     | 0.43              |
| 1:D:70:ALA:HB2   | 5:Y:1115:THR:HG21 | 2.01                     | 0.43              |
| 5:Y:581:PRO:O    | 5:Y:619:ILE:HD12  | 2.19                     | 0.43              |
| 5:Y:789:ASP:O    | 5:Y:793:LYS:HG2   | 2.18                     | 0.43              |
| 3:u:52:ALA:HB1   | 3:u:168:SER:HB3   | 2.01                     | 0.43              |
| 3:u:122:ASN:OD1  | 3:u:122:ASN:N     | 2.52                     | 0.43              |
| 4:x:356:GLU:HB3  | 4:x:360:VAL:HB    | 2.00                     | 0.43              |
| 4:x:1014:LYS:HD3 | 4:x:1031:SER:N    | 2.33                     | 0.43              |
| 6:h:193:MET:HA   | 6:h:196:GLU:HB2   | 1.99                     | 0.43              |
| 6:h:766:PRO:HB2  | 6:h:767:PRO:HD3   | 2.00                     | 0.43              |
| 2:E:2:ILE:HD13   | 2:E:55:LEU:HD11   | 2.00                     | 0.43              |
| 3:U:224:PHE:O    | 3:U:228:THR:HG23  | 2.18                     | 0.43              |
| 4:X:425:SER:OG   | 4:X:426:ARG:N     | 2.51                     | 0.43              |
| 4:X:452:ARG:H    | 4:X:452:ARG:HG3   | 1.63                     | 0.43              |
| 5:Y:754:PRO:HD3  | 5:Y:781:HIS:HB3   | 2.01                     | 0.43              |
| 6:H:692:LEU:HB3  | 6:H:705:CYS:SG    | 2.58                     | 0.43              |
| 3:u:226:GLY:O    | 3:u:230:GLU:HG2   | 2.18                     | 0.43              |
| 3:v:156:ARG:H    | 3:v:159:GLN:CD    | 2.26                     | 0.43              |
| 4:x:425:SER:OG   | 4:x:426:ARG:N     | 2.51                     | 0.43              |
| 4:x:801:ASP:OD1  | 4:x:801:ASP:N     | 2.51                     | 0.43              |
| 4:x:971:VAL:O    | 4:x:974:LEU:HB3   | 2.18                     | 0.43              |
| 5:y:402:GLU:HG3  | 5:y:430:LEU:HD12  | 2.00                     | 0.43              |
| 6:h:655:GLU:O    | 6:h:659:LEU:HG    | 2.19                     | 0.43              |
| 6:h:768:HIS:HB3  | 6:h:771:GLN:HE22  | 1.84                     | 0.43              |
| 4:X:224:ASP:OD1  | 4:X:225:ASN:N     | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:610:THR:HG23  | 6:H:634:GLY:HA3   | 2.01                     | 0.43              |
| 6:H:655:GLU:O     | 6:H:659:LEU:HG    | 2.19                     | 0.43              |
| 3:u:47:SER:HB2    | 3:u:146:ARG:HH11  | 1.83                     | 0.43              |
| 3:u:87:LEU:H      | 3:u:87:LEU:HD23   | 1.84                     | 0.43              |
| 4:x:170:LEU:HD23  | 4:x:170:LEU:H     | 1.82                     | 0.43              |
| 4:x:511:TYR:OH    | 4:x:612:ASP:OD2   | 2.29                     | 0.43              |
| 5:y:671:GLU:O     | 5:y:674:GLU:HG2   | 2.19                     | 0.43              |
| 4:X:40:PHE:HB2    | 4:X:413:GLY:HA2   | 2.01                     | 0.43              |
| 4:X:777:MET:HE3   | 4:X:935:ILE:HG21  | 2.01                     | 0.43              |
| 5:Y:570:ILE:HG23  | 5:Y:639:MET:HE1   | 2.01                     | 0.43              |
| 6:H:205:GLN:O     | 6:H:209:ILE:HG12  | 2.19                     | 0.43              |
| 3:v:89:ILE:HA     | 3:v:117:ASP:O     | 2.19                     | 0.43              |
| 5:y:567:PHE:O     | 5:y:570:ILE:HG22  | 2.19                     | 0.43              |
| 6:h:741:THR:O     | 6:h:745:ARG:HG2   | 2.18                     | 0.43              |
| 3:U:42:ARG:HH22   | 4:X:1021:ARG:HA   | 1.84                     | 0.43              |
| 4:X:962:VAL:HG22  | 4:X:970:GLN:NE2   | 2.33                     | 0.43              |
| 5:Y:78:CYS:HB2    | 5:Y:80:VAL:HG13   | 2.00                     | 0.43              |
| 5:Y:1040:LEU:HD11 | 5:Y:1075:LEU:HD22 | 2.01                     | 0.43              |
| 5:Y:1079:ARG:HA   | 5:Y:1093:LEU:HA   | 2.01                     | 0.43              |
| 3:u:95:LYS:HG2    | 3:u:118:VAL:HG11  | 2.00                     | 0.43              |
| 4:x:127:ILE:HG22  | 4:x:128:ASN:ND2   | 2.33                     | 0.43              |
| 4:x:601:THR:OG1   | 4:x:602:VAL:N     | 2.52                     | 0.43              |
| 4:x:725:ASN:OD1   | 4:x:726:GLN:N     | 2.50                     | 0.43              |
| 5:y:507:ALA:HA    | 5:y:536:ARG:HH22  | 1.84                     | 0.43              |
| 5:y:933:GLN:HG3   | 6:h:48:TRP:CD1    | 2.54                     | 0.43              |
| 5:y:980:GLU:HB3   | 5:y:992:VAL:HG12  | 2.00                     | 0.43              |
| 5:y:1079:ARG:HA   | 5:y:1093:LEU:HA   | 2.01                     | 0.43              |
| 6:h:30:GLU:HB3    | 6:h:89:LEU:HD13   | 2.00                     | 0.43              |
| 6:h:574:ILE:HG22  | 6:h:589:MET:HG2   | 2.00                     | 0.43              |
| 6:h:643:GLU:O     | 6:h:647:SER:OG    | 2.29                     | 0.43              |
| 4:X:1018:TYR:CE1  | 4:X:1025:PRO:HG3  | 2.54                     | 0.42              |
| 5:Y:144:LEU:HD23  | 5:Y:158:TYR:HE2   | 1.84                     | 0.42              |
| 5:Y:808:ALA:O     | 5:Y:920:GLY:HA3   | 2.19                     | 0.42              |
| 5:Y:846:ARG:HH22  | 5:Y:1068:GLU:HG3  | 1.84                     | 0.42              |
| 4:x:41:LEU:HD12   | 4:x:42:ASP:N      | 2.34                     | 0.42              |
| 5:y:503:THR:HG21  | 5:y:615:PHE:HB2   | 2.01                     | 0.42              |
| 5:y:618:GLY:O     | 5:y:622:LYS:HG2   | 2.19                     | 0.42              |
| 5:y:693:THR:HG23  | 5:y:696:GLU:H     | 1.84                     | 0.42              |
| 5:y:846:ARG:HH22  | 5:y:1068:GLU:HG3  | 1.84                     | 0.42              |
| 5:y:987:LYS:HD2   | 5:y:987:LYS:HA    | 1.79                     | 0.42              |
| 4:X:194:VAL:HG12  | 4:X:236:ILE:HD11  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:57:ASP:O      | 6:H:59:HIS:N      | 2.52                     | 0.42              |
| 6:H:503:ILE:HG13  | 6:H:504:GLY:N     | 2.31                     | 0.42              |
| 6:H:550:ASP:HB2   | 6:H:579:TYR:CE2   | 2.54                     | 0.42              |
| 3:u:227:LEU:HA    | 3:u:230:GLU:HG2   | 2.01                     | 0.42              |
| 4:x:849:LYS:HE3   | 4:x:871:GLU:HG3   | 2.01                     | 0.42              |
| 6:h:208:ASN:O     | 6:h:212:THR:HG23  | 2.18                     | 0.42              |
| 6:h:328:THR:HG23  | 6:h:499:LYS:HD3   | 2.01                     | 0.42              |
| 6:h:550:ASP:HB2   | 6:h:579:TYR:CE2   | 2.54                     | 0.42              |
| 5:Y:253:ASP:OD2   | 5:Y:314:LYS:N     | 2.52                     | 0.42              |
| 5:Y:507:ALA:HA    | 5:Y:536:ARG:HH22  | 1.84                     | 0.42              |
| 5:Y:618:GLY:O     | 5:Y:622:LYS:HG2   | 2.19                     | 0.42              |
| 5:Y:671:GLU:O     | 5:Y:674:GLU:HG2   | 2.19                     | 0.42              |
| 6:H:768:HIS:HB3   | 6:H:771:GLN:HE22  | 1.84                     | 0.42              |
| 1:d:47:LYS:HD3    | 1:d:47:LYS:HA     | 1.84                     | 0.42              |
| 1:d:63:ASN:HD21   | 5:y:1115:THR:HA   | 1.84                     | 0.42              |
| 2:e:29:SER:O      | 2:e:33:VAL:HG23   | 2.18                     | 0.42              |
| 5:y:763:ILE:HG23  | 5:y:775:GLU:HG2   | 2.00                     | 0.42              |
| 6:h:715:ILE:HD13  | 6:h:715:ILE:HA    | 1.87                     | 0.42              |
| 6:h:728:GLU:HB2   | 6:h:735:ASP:OD2   | 2.19                     | 0.42              |
| 4:X:197:ARG:NH2   | 4:X:224:ASP:OD2   | 2.52                     | 0.42              |
| 4:X:267:LEU:HD23  | 4:X:268:ALA:O     | 2.19                     | 0.42              |
| 3:u:44:LEU:HD23   | 3:u:48:LEU:HD11   | 2.02                     | 0.42              |
| 3:v:101:VAL:HG13  | 3:v:136:PHE:HB3   | 2.02                     | 0.42              |
| 5:y:253:ASP:OD2   | 5:y:314:LYS:N     | 2.52                     | 0.42              |
| 5:y:1040:LEU:HD11 | 5:y:1075:LEU:HD22 | 2.01                     | 0.42              |
| 6:h:26:GLU:HB3    | 6:h:92:ILE:HG21   | 2.02                     | 0.42              |
| 3:U:227:LEU:HB3   | 3:V:12:VAL:HG11   | 2.02                     | 0.42              |
| 4:X:161:THR:HG23  | 4:X:171:GLU:HG2   | 2.01                     | 0.42              |
| 5:Y:402:GLU:HG3   | 5:Y:430:LEU:HD12  | 2.00                     | 0.42              |
| 5:Y:567:PHE:O     | 5:Y:570:ILE:HG22  | 2.19                     | 0.42              |
| 5:Y:763:ILE:HG23  | 5:Y:775:GLU:HG2   | 2.00                     | 0.42              |
| 5:Y:771:LEU:HD11  | 5:Y:776:TYR:HD2   | 1.84                     | 0.42              |
| 1:d:60:THR:O      | 1:d:64:ILE:HG12   | 2.19                     | 0.42              |
| 3:v:9:ILE:HD12    | 3:v:9:ILE:HA      | 1.91                     | 0.42              |
| 4:x:770:ASN:HD21  | 4:x:957:LEU:C     | 2.27                     | 0.42              |
| 5:y:549:PHE:O     | 5:y:550:THR:OG1   | 2.38                     | 0.42              |
| 5:y:570:ILE:HG23  | 5:y:639:MET:HE1   | 2.01                     | 0.42              |
| 3:U:50:GLY:HA3    | 3:U:170:TYR:O     | 2.20                     | 0.42              |
| 4:X:170:LEU:H     | 4:X:170:LEU:HD23  | 1.85                     | 0.42              |
| 4:X:261:ASP:HB3   | 4:X:264:ARG:HB2   | 2.01                     | 0.42              |
| 4:X:513:ARG:HH22  | 4:X:566:ALA:HB2   | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:580:ARG:NH1  | 4:X:589:ASP:OD1  | 2.52                     | 0.42              |
| 4:X:691:TRP:NE1  | 4:X:709:LYS:HB3  | 2.34                     | 0.42              |
| 6:H:404:ASN:O    | 6:H:407:GLU:HG3  | 2.20                     | 0.42              |
| 3:v:65:PHE:CE1   | 5:y:602:VAL:HG12 | 2.55                     | 0.42              |
| 3:v:67:THR:HG22  | 3:v:74:ASP:HA    | 2.02                     | 0.42              |
| 4:x:636:ARG:HA   | 4:x:636:ARG:HD3  | 1.83                     | 0.42              |
| 4:x:690:VAL:O    | 4:x:709:LYS:HA   | 2.19                     | 0.42              |
| 4:x:1125:PRO:HG2 | 4:x:1128:PHE:CD2 | 2.54                     | 0.42              |
| 5:y:668:ASP:OD1  | 5:y:668:ASP:N    | 2.46                     | 0.42              |
| 6:h:37:LYS:O     | 6:h:41:ILE:HG12  | 2.20                     | 0.42              |
| 6:h:119:ILE:HD12 | 6:h:142:SER:OG   | 2.20                     | 0.42              |
| 6:h:639:VAL:HG13 | 6:h:752:VAL:O    | 2.20                     | 0.42              |
| 1:D:60:THR:O     | 1:D:64:ILE:HG12  | 2.19                     | 0.42              |
| 5:Y:549:PHE:O    | 5:Y:550:THR:OG1  | 2.37                     | 0.42              |
| 4:x:62:LEU:HG    | 4:x:100:ASN:HB2  | 2.01                     | 0.42              |
| 5:y:108:LYS:HD2  | 5:y:108:LYS:HA   | 1.87                     | 0.42              |
| 6:h:205:GLN:O    | 6:h:209:ILE:HG12 | 2.19                     | 0.42              |
| 6:h:610:THR:OG1  | 6:h:747:MET:O    | 2.31                     | 0.42              |
| 3:U:182:ASN:HA   | 3:U:191:TYR:O    | 2.19                     | 0.42              |
| 4:X:450:ASN:O    | 4:X:453:PRO:HD2  | 2.20                     | 0.42              |
| 5:Y:130:TYR:OH   | 5:Y:293:ASP:OD1  | 2.29                     | 0.42              |
| 6:H:26:GLU:HB3   | 6:H:92:ILE:HG21  | 2.02                     | 0.42              |
| 6:H:230:ILE:HB   | 6:H:600:TYR:HB2  | 2.01                     | 0.42              |
| 6:H:764:ALA:C    | 6:H:767:PRO:HD2  | 2.45                     | 0.42              |
| 3:v:14:ILE:HG12  | 3:v:207:LYS:HE2  | 2.02                     | 0.42              |
| 5:y:580:GLU:HG2  | 5:y:594:PHE:CE2  | 2.55                     | 0.42              |
| 5:y:673:LEU:HD12 | 5:y:673:LEU:HA   | 1.95                     | 0.42              |
| 5:y:754:PRO:HD3  | 5:y:781:HIS:HB3  | 2.01                     | 0.42              |
| 3:U:42:ARG:NE    | 3:V:35:THR:HB    | 2.35                     | 0.42              |
| 4:X:53:SER:HA    | 4:X:54:PRO:HA    | 1.80                     | 0.42              |
| 4:X:204:ASP:O    | 4:X:208:LEU:HD23 | 2.20                     | 0.42              |
| 5:Y:503:THR:HG21 | 5:Y:615:PHE:HB2  | 2.01                     | 0.42              |
| 6:H:639:VAL:HG13 | 6:H:752:VAL:O    | 2.20                     | 0.42              |
| 4:x:57:ASP:OD1   | 4:x:57:ASP:N     | 2.50                     | 0.42              |
| 5:y:348:PRO:O    | 5:y:644:LYS:NZ   | 2.49                     | 0.42              |
| 6:h:527:MET:HE3  | 6:h:527:MET:HB3  | 1.92                     | 0.42              |
| 2:E:52:GLY:HA2   | 2:E:55:LEU:HB3   | 2.01                     | 0.42              |
| 3:V:98:GLU:O     | 3:V:113:THR:HG22 | 2.20                     | 0.42              |
| 5:Y:108:LYS:HD2  | 5:Y:108:LYS:HA   | 1.87                     | 0.42              |
| 5:Y:412:LEU:HD13 | 5:Y:457:VAL:HB   | 2.02                     | 0.42              |
| 5:Y:481:ASN:HB2  | 5:Y:482:PRO:HD3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:H:432:TYR:O    | 6:H:436:GLN:HG2  | 2.20                     | 0.42              |
| 3:u:185:VAL:HB   | 3:u:191:TYR:HD2  | 1.84                     | 0.42              |
| 3:v:74:ASP:OD1   | 3:v:75:VAL:N     | 2.53                     | 0.42              |
| 4:x:426:ARG:O    | 4:x:430:VAL:HG23 | 2.19                     | 0.42              |
| 4:x:761:VAL:HG22 | 4:x:955:ILE:HG13 | 2.01                     | 0.42              |
| 5:y:268:LEU:HD13 | 5:y:284:GLU:HB3  | 2.00                     | 0.42              |
| 5:y:481:ASN:HB2  | 5:y:482:PRO:HD3  | 2.02                     | 0.42              |
| 5:y:558:LEU:HA   | 5:y:595:PHE:HA   | 2.02                     | 0.42              |
| 4:X:68:ASP:HB2   | 4:X:95:LYS:HB2   | 2.01                     | 0.41              |
| 4:X:699:ASP:O    | 4:X:702:LYS:NZ   | 2.53                     | 0.41              |
| 5:Y:700:ARG:O    | 5:Y:704:ILE:HG12 | 2.20                     | 0.41              |
| 6:H:728:GLU:HB2  | 6:H:735:ASP:OD2  | 2.19                     | 0.41              |
| 3:u:116:SER:O    | 3:u:118:VAL:HG22 | 2.20                     | 0.41              |
| 3:v:10:GLU:OE2   | 3:v:10:GLU:N     | 2.53                     | 0.41              |
| 4:x:40:PHE:O     | 4:x:41:LEU:C     | 2.61                     | 0.41              |
| 5:y:144:LEU:HD23 | 5:y:158:TYR:HE2  | 1.84                     | 0.41              |
| 5:y:662:ASP:HB2  | 5:y:724:ASN:HD21 | 1.85                     | 0.41              |
| 5:y:808:ALA:O    | 5:y:920:GLY:HA3  | 2.19                     | 0.41              |
| 6:h:392:MET:O    | 6:h:395:THR:OG1  | 2.34                     | 0.41              |
| 4:X:682:VAL:HA   | 4:X:692:VAL:HA   | 2.02                     | 0.41              |
| 5:Y:580:GLU:HG2  | 5:Y:594:PHE:CE2  | 2.55                     | 0.41              |
| 5:Y:836:ILE:HD13 | 5:Y:1053:LYS:HA  | 2.02                     | 0.41              |
| 6:H:268:PRO:HD3  | 6:H:547:GLU:OE2  | 2.20                     | 0.41              |
| 2:e:50:VAL:HG22  | 2:e:55:LEU:HB2   | 2.02                     | 0.41              |
| 4:x:163:ILE:HG12 | 4:x:169:TRP:HE1  | 1.84                     | 0.41              |
| 4:x:451:ILE:O    | 4:x:454:VAL:HG22 | 2.20                     | 0.41              |
| 4:x:771:TYR:HD1  | 5:y:346:VAL:HG11 | 1.85                     | 0.41              |
| 5:y:581:PRO:O    | 5:y:619:ILE:HD12 | 2.19                     | 0.41              |
| 5:y:771:LEU:HD11 | 5:y:776:TYR:HD2  | 1.84                     | 0.41              |
| 6:h:57:ASP:O     | 6:h:59:HIS:N     | 2.52                     | 0.41              |
| 6:h:602:ARG:HH12 | 6:h:627:ILE:HD11 | 1.86                     | 0.41              |
| 6:h:691:ARG:HE   | 6:h:692:LEU:N    | 2.18                     | 0.41              |
| 3:V:24:VAL:HG22  | 3:V:195:THR:HG22 | 2.01                     | 0.41              |
| 4:X:40:PHE:O     | 4:X:41:LEU:C     | 2.62                     | 0.41              |
| 4:X:403:HIS:CE1  | 4:X:566:ALA:HB1  | 2.55                     | 0.41              |
| 4:X:625:CYS:HA   | 4:X:660:THR:HG21 | 2.02                     | 0.41              |
| 5:Y:1058:GLN:OE1 | 6:H:44:ARG:NH1   | 2.54                     | 0.41              |
| 6:H:369:LEU:HD23 | 6:H:369:LEU:HA   | 1.88                     | 0.41              |
| 6:H:602:ARG:HH12 | 6:H:627:ILE:HD11 | 1.85                     | 0.41              |
| 4:x:760:MET:HE3  | 4:x:760:MET:HB2  | 1.96                     | 0.41              |
| 4:x:763:PHE:HE1  | 4:x:957:LEU:HD12 | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:y:127:GLU:HB3   | 5:y:132:ALA:HB3   | 2.03                     | 0.41              |
| 6:h:78:ARG:HD2    | 6:h:78:ARG:HA     | 1.83                     | 0.41              |
| 6:h:317:CYS:SG    | 6:h:318:LEU:N     | 2.93                     | 0.41              |
| 6:h:432:TYR:O     | 6:h:436:GLN:HG2   | 2.20                     | 0.41              |
| 4:X:163:ILE:HA    | 4:X:169:TRP:HD1   | 1.85                     | 0.41              |
| 4:X:633:ASP:OD1   | 4:X:634:SER:N     | 2.50                     | 0.41              |
| 4:X:709:LYS:HB2   | 4:X:709:LYS:HE3   | 1.77                     | 0.41              |
| 5:Y:139:PRO:HG3   | 5:Y:146:LYS:HE2   | 2.02                     | 0.41              |
| 5:Y:558:LEU:HA    | 5:Y:595:PHE:HA    | 2.02                     | 0.41              |
| 6:H:103:ARG:HB3   | 6:H:170:ARG:HG2   | 2.03                     | 0.41              |
| 6:H:691:ARG:HE    | 6:H:692:LEU:N     | 2.18                     | 0.41              |
| 3:v:99:ILE:HG12   | 3:v:112:ILE:HG12  | 2.03                     | 0.41              |
| 5:y:412:LEU:HD13  | 5:y:457:VAL:HB    | 2.02                     | 0.41              |
| 5:y:836:ILE:HD13  | 5:y:1053:LYS:HA   | 2.02                     | 0.41              |
| 6:h:268:PRO:HD3   | 6:h:547:GLU:OE2   | 2.20                     | 0.41              |
| 6:h:610:THR:HG23  | 6:h:634:GLY:HA3   | 2.01                     | 0.41              |
| 6:h:764:ALA:C     | 6:h:767:PRO:HD2   | 2.45                     | 0.41              |
| 4:X:1128:PHE:CZ   | 5:Y:1158:LEU:HD11 | 2.56                     | 0.41              |
| 5:Y:84:ARG:C      | 5:Y:86:LYS:H      | 2.28                     | 0.41              |
| 5:Y:1047:LEU:HD23 | 5:Y:1047:LEU:HA   | 1.90                     | 0.41              |
| 6:H:37:LYS:O      | 6:H:41:ILE:HG12   | 2.20                     | 0.41              |
| 6:H:78:ARG:HA     | 6:H:78:ARG:HD2    | 1.83                     | 0.41              |
| 6:H:328:THR:HG23  | 6:H:499:LYS:HD3   | 2.01                     | 0.41              |
| 4:x:70:SER:O      | 4:x:93:ARG:N      | 2.50                     | 0.41              |
| 4:x:178:ASP:HB3   | 4:x:216:TYR:HD2   | 1.84                     | 0.41              |
| 4:x:550:VAL:HB    | 4:x:557:VAL:HG22  | 2.02                     | 0.41              |
| 4:x:796:GLU:HG3   | 4:x:910:ARG:HG2   | 2.02                     | 0.41              |
| 4:x:1126:GLU:OE2  | 5:y:89:ARG:NH1    | 2.54                     | 0.41              |
| 5:y:301:ARG:HA    | 5:y:301:ARG:HD3   | 1.85                     | 0.41              |
| 5:y:584:SER:C     | 5:y:589:LYS:HG2   | 2.46                     | 0.41              |
| 6:h:103:ARG:HB3   | 6:h:170:ARG:HG2   | 2.03                     | 0.41              |
| 3:V:40:LEU:O      | 3:V:44:LEU:HB2    | 2.20                     | 0.41              |
| 5:Y:127:GLU:HB3   | 5:Y:132:ALA:HB3   | 2.03                     | 0.41              |
| 5:Y:146:LYS:HA    | 5:Y:146:LYS:HD3   | 1.86                     | 0.41              |
| 6:H:305:PHE:CE2   | 6:H:516:LEU:HB3   | 2.47                     | 0.41              |
| 6:H:681:HIS:HB2   | 6:H:692:LEU:HD21  | 2.02                     | 0.41              |
| 2:e:52:GLY:HA2    | 2:e:55:LEU:HB3    | 2.01                     | 0.41              |
| 3:u:149:THR:HG23  | 3:u:167:ASP:HB2   | 2.03                     | 0.41              |
| 4:x:91:PRO:HA     | 4:x:115:ASP:HA    | 2.02                     | 0.41              |
| 4:x:356:GLU:HG3   | 4:x:357:GLY:H     | 1.86                     | 0.41              |
| 4:x:624:ALA:O     | 4:x:660:THR:HG21  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:h:230:ILE:HB   | 6:h:600:TYR:HB2  | 2.01                     | 0.41              |
| 6:h:501:ASP:O    | 6:h:505:GLU:HG2  | 2.21                     | 0.41              |
| 6:h:681:HIS:HB2  | 6:h:692:LEU:HD21 | 2.02                     | 0.41              |
| 2:E:51:ASN:O     | 2:E:54:PHE:N     | 2.53                     | 0.41              |
| 3:U:232:GLN:O    | 3:U:236:ILE:N    | 2.54                     | 0.41              |
| 4:X:445:PRO:HG2  | 4:X:448:LEU:HB2  | 2.02                     | 0.41              |
| 4:X:1014:LYS:HD3 | 4:X:1031:SER:N   | 2.35                     | 0.41              |
| 5:Y:662:ASP:HB2  | 5:Y:724:ASN:HD21 | 1.85                     | 0.41              |
| 5:Y:705:TRP:CD2  | 5:Y:762:PRO:HG3  | 2.56                     | 0.41              |
| 6:H:313:GLN:O    | 6:H:317:CYS:HB3  | 2.21                     | 0.41              |
| 6:H:710:TYR:HA   | 6:H:713:LYS:HD3  | 2.03                     | 0.41              |
| 2:e:20:THR:OG1   | 3:u:181:GLU:HA   | 2.20                     | 0.41              |
| 3:u:115:ASP:OD2  | 3:u:116:SER:N    | 2.53                     | 0.41              |
| 3:u:137:ARG:HH22 | 3:u:139:ARG:HH11 | 1.68                     | 0.41              |
| 4:x:346:SER:O    | 4:x:346:SER:OG   | 2.38                     | 0.41              |
| 4:x:424:LEU:HD22 | 4:x:454:VAL:HG11 | 2.03                     | 0.41              |
| 5:y:695:GLU:OE2  | 5:y:695:GLU:HA   | 2.20                     | 0.41              |
| 6:h:503:ILE:HG13 | 6:h:504:GLY:N    | 2.31                     | 0.41              |
| 6:h:576:GLN:HG3  | 6:h:741:THR:HG22 | 2.03                     | 0.41              |
| 6:h:640:VAL:HG23 | 6:h:640:VAL:O    | 2.21                     | 0.41              |
| 1:D:33:PHE:O     | 1:D:37:LEU:HG    | 2.21                     | 0.41              |
| 2:E:50:VAL:HG22  | 2:E:55:LEU:HB2   | 2.02                     | 0.41              |
| 3:V:74:ASP:OD1   | 3:V:75:VAL:N     | 2.54                     | 0.41              |
| 4:X:212:GLY:HA2  | 4:X:217:LEU:HD21 | 2.03                     | 0.41              |
| 5:Y:492:SER:H    | 5:Y:495:MET:HE3  | 1.86                     | 0.41              |
| 5:Y:695:GLU:OE2  | 5:Y:695:GLU:HA   | 2.20                     | 0.41              |
| 5:Y:1038:THR:OG1 | 5:Y:1039:ASP:N   | 2.48                     | 0.41              |
| 6:H:317:CYS:SG   | 6:H:318:LEU:N    | 2.93                     | 0.41              |
| 6:H:501:ASP:O    | 6:H:505:GLU:HG2  | 2.21                     | 0.41              |
| 6:H:531:ILE:HD12 | 6:H:531:ILE:HA   | 1.92                     | 0.41              |
| 6:H:576:GLN:HG3  | 6:H:741:THR:HG22 | 2.03                     | 0.41              |
| 3:u:228:THR:O    | 3:u:232:GLN:HG2  | 2.21                     | 0.41              |
| 3:v:83:LYS:HE2   | 5:y:517:LYS:HB2  | 2.02                     | 0.41              |
| 5:y:130:TYR:OH   | 5:y:293:ASP:OD1  | 2.29                     | 0.41              |
| 5:y:390:ILE:HD13 | 5:y:390:ILE:HA   | 1.87                     | 0.41              |
| 6:h:318:LEU:HB3  | 6:h:672:LYS:HZ3  | 1.85                     | 0.41              |
| 2:E:1:MET:N      | 2:E:27:GLY:O     | 2.40                     | 0.41              |
| 3:V:41:ARG:NH2   | 5:Y:527:GLN:OE1  | 2.42                     | 0.41              |
| 3:V:221:LEU:HD23 | 3:V:224:PHE:HE1  | 1.85                     | 0.41              |
| 4:X:190:LEU:HD11 | 4:X:194:VAL:HG11 | 2.03                     | 0.41              |
| 4:X:267:LEU:O    | 4:X:374:LYS:HG2  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:X:402:ASP:OD1   | 4:X:402:ASP:N     | 2.52                     | 0.41              |
| 4:X:595:ARG:HA    | 4:X:600:ASN:HA    | 2.03                     | 0.41              |
| 4:X:651:MET:HG2   | 4:X:790:ILE:HD11  | 2.03                     | 0.41              |
| 4:X:847:THR:OG1   | 4:X:873:ARG:HB3   | 2.21                     | 0.41              |
| 5:Y:140:ALA:HB3   | 5:Y:165:LYS:O     | 2.21                     | 0.41              |
| 5:Y:693:THR:HG23  | 5:Y:696:GLU:H     | 1.84                     | 0.41              |
| 5:Y:1137:ALA:HA   | 5:Y:1145:VAL:HG11 | 2.03                     | 0.41              |
| 6:H:119:ILE:HD12  | 6:H:142:SER:OG    | 2.20                     | 0.41              |
| 6:H:640:VAL:O     | 6:H:640:VAL:HG23  | 2.21                     | 0.41              |
| 3:u:74:ASP:OD1    | 3:u:75:VAL:N      | 2.52                     | 0.41              |
| 3:v:56:ILE:HA     | 3:v:140:LEU:HA    | 2.02                     | 0.41              |
| 4:x:415:LEU:HD13  | 4:x:467:LEU:HD13  | 2.03                     | 0.41              |
| 4:x:416:LEU:HD23  | 4:x:416:LEU:HA    | 1.91                     | 0.41              |
| 4:x:573:VAL:HG23  | 4:x:608:VAL:HA    | 2.03                     | 0.41              |
| 4:x:605:ARG:O     | 4:x:608:VAL:HG22  | 2.21                     | 0.41              |
| 4:x:1032:VAL:HG22 | 4:x:1033:GLY:N    | 2.36                     | 0.41              |
| 5:y:108:LYS:HE3   | 6:h:449:TYR:HE2   | 1.84                     | 0.41              |
| 5:y:872:LYS:HA    | 5:y:875:GLU:HG2   | 2.03                     | 0.41              |
| 6:h:404:ASN:O     | 6:h:407:GLU:HG3   | 2.20                     | 0.41              |
| 6:h:529:ASP:OD2   | 6:h:535:LYS:HB3   | 2.21                     | 0.41              |
| 4:X:920:SER:OG    | 4:X:921:GLU:N     | 2.53                     | 0.41              |
| 6:H:32:SER:OG     | 6:H:85:MET:HE1    | 2.21                     | 0.41              |
| 6:H:240:THR:HG23  | 6:H:241:SER:N     | 2.36                     | 0.41              |
| 1:d:62:LEU:HG     | 1:d:68:PHE:CD2    | 2.56                     | 0.41              |
| 4:x:583:ASP:OD1   | 4:x:583:ASP:N     | 2.53                     | 0.41              |
| 4:x:1019:ASP:OD1  | 4:x:1021:ARG:NH1  | 2.54                     | 0.41              |
| 5:y:824:ILE:HD13  | 5:y:824:ILE:HA    | 1.94                     | 0.41              |
| 5:y:994:GLN:HE21  | 5:y:994:GLN:HB3   | 1.71                     | 0.41              |
| 6:h:659:LEU:HD22  | 6:h:749:MET:HE3   | 2.03                     | 0.41              |
| 3:V:45:LEU:HA     | 3:V:171:THR:HG21  | 2.02                     | 0.40              |
| 4:X:546:PRO:HB2   | 4:X:613:VAL:HG11  | 2.03                     | 0.40              |
| 5:Y:357:LEU:HD23  | 5:Y:357:LEU:HA    | 1.92                     | 0.40              |
| 5:Y:884:VAL:HG12  | 5:Y:885:TRP:H     | 1.87                     | 0.40              |
| 6:H:364:PHE:CG    | 6:H:365:ARG:N     | 2.89                     | 0.40              |
| 6:H:560:ARG:HD2   | 6:H:560:ARG:HA    | 1.91                     | 0.40              |
| 4:x:516:PRO:HB2   | 5:y:780:THR:HG21  | 2.04                     | 0.40              |
| 5:y:700:ARG:O     | 5:y:704:ILE:HG12  | 2.20                     | 0.40              |
| 5:y:720:LEU:HG    | 5:y:727:TYR:HB2   | 2.03                     | 0.40              |
| 6:h:520:ASP:HA    | 6:h:523:PRO:HD2   | 2.03                     | 0.40              |
| 6:h:710:TYR:HA    | 6:h:713:LYS:HD3   | 2.03                     | 0.40              |
| 1:D:66:GLY:O      | 1:D:79:ARG:NH1    | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:9:GLU:OE1    | 2:E:10:LYS:N     | 2.54                     | 0.40              |
| 2:E:40:LYS:HE3   | 2:E:40:LYS:HB2   | 1.81                     | 0.40              |
| 3:U:29:GLU:HG3   | 3:U:30:ARG:H     | 1.86                     | 0.40              |
| 4:X:745:GLY:H    | 4:X:748:MET:HB2  | 1.85                     | 0.40              |
| 4:X:748:MET:HE2  | 4:X:748:MET:HB3  | 1.96                     | 0.40              |
| 4:X:750:LEU:HD12 | 4:X:750:LEU:HA   | 1.93                     | 0.40              |
| 5:Y:1055:TYR:HD1 | 5:Y:1055:TYR:HA  | 1.78                     | 0.40              |
| 6:H:536:LYS:HE2  | 6:H:536:LYS:HB3  | 1.89                     | 0.40              |
| 3:v:77:THR:O     | 3:v:80:LEU:HG    | 2.21                     | 0.40              |
| 4:x:100:ASN:ND2  | 4:x:103:THR:OG1  | 2.55                     | 0.40              |
| 4:x:201:PHE:HB3  | 4:x:206:GLU:HB3  | 2.02                     | 0.40              |
| 4:x:507:HIS:O    | 4:x:509:SER:N    | 2.55                     | 0.40              |
| 5:y:84:ARG:C     | 5:y:86:LYS:H     | 2.28                     | 0.40              |
| 5:y:492:SER:H    | 5:y:495:MET:HE3  | 1.86                     | 0.40              |
| 5:Y:390:ILE:HD13 | 5:Y:390:ILE:HA   | 1.88                     | 0.40              |
| 6:H:640:VAL:HG22 | 6:H:753:PHE:HE1  | 1.85                     | 0.40              |
| 1:d:85:ASP:O     | 1:d:88:ASP:HB2   | 2.21                     | 0.40              |
| 2:e:29:SER:OG    | 2:e:30:GLU:N     | 2.54                     | 0.40              |
| 5:y:139:PRO:HG3  | 5:y:146:LYS:HE2  | 2.02                     | 0.40              |
| 5:y:772:THR:HB   | 5:y:775:GLU:OE1  | 2.21                     | 0.40              |
| 6:h:322:LYS:HZ1  | 6:h:673:THR:HG21 | 1.85                     | 0.40              |
| 6:h:364:PHE:CG   | 6:h:365:ARG:N    | 2.89                     | 0.40              |
| 4:X:30:ILE:HG21  | 4:X:483:LYS:HD2  | 2.03                     | 0.40              |
| 5:Y:632:HIS:CG   | 5:Y:633:ILE:H    | 2.40                     | 0.40              |
| 5:Y:872:LYS:HA   | 5:Y:875:GLU:HG2  | 2.03                     | 0.40              |
| 6:H:520:ASP:HA   | 6:H:523:PRO:HD2  | 2.03                     | 0.40              |
| 1:d:33:PHE:O     | 1:d:37:LEU:HG    | 2.21                     | 0.40              |
| 4:x:76:TYR:CD2   | 4:x:80:GLU:HB2   | 2.56                     | 0.40              |
| 5:y:20:ILE:HD12  | 5:y:232:PRO:HG3  | 2.04                     | 0.40              |
| 5:y:583:LYS:HE2  | 5:y:583:LYS:HB3  | 1.86                     | 0.40              |
| 5:y:705:TRP:CD2  | 5:y:762:PRO:HG3  | 2.56                     | 0.40              |
| 5:y:748:ARG:HB3  | 5:y:763:ILE:HB   | 2.04                     | 0.40              |
| 2:E:14:VAL:N     | 2:E:15:PRO:HD3   | 2.37                     | 0.40              |
| 3:U:68:ILE:HG12  | 3:U:75:VAL:HG22  | 2.03                     | 0.40              |
| 4:X:89:SER:OG    | 4:X:115:ASP:HB3  | 2.21                     | 0.40              |
| 5:Y:398:TRP:O    | 5:Y:402:GLU:HB2  | 2.22                     | 0.40              |
| 6:H:265:LEU:HD22 | 6:H:272:PHE:CE1  | 2.57                     | 0.40              |
| 1:d:66:GLY:O     | 1:d:79:ARG:NH1   | 2.54                     | 0.40              |
| 2:e:51:ASN:O     | 2:e:54:PHE:N     | 2.53                     | 0.40              |
| 4:x:400:ASP:OD2  | 4:x:403:HIS:N    | 2.54                     | 0.40              |
| 4:x:658:VAL:HG11 | 4:x:973:GLU:HG3  | 2.03                     | 0.40              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 5:y:853:LYS:O | 5:y:857:THR:HA  | 2.22                     | 0.40              |
| 6:h:313:GLN:O | 6:h:317:CYS:HB3 | 2.21                     | 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   | D     | 135/139 (97%)   | 116 (86%)  | 19 (14%) | 0        | 100         | 100 |
| 1   | d     | 135/139 (97%)   | 116 (86%)  | 19 (14%) | 0        | 100         | 100 |
| 2   | E     | 67/69 (97%)     | 57 (85%)   | 9 (13%)  | 1 (2%)   | 8           | 37  |
| 2   | e     | 67/69 (97%)     | 57 (85%)   | 9 (13%)  | 1 (2%)   | 8           | 37  |
| 3   | U     | 229/314 (73%)   | 213 (93%)  | 16 (7%)  | 0        | 100         | 100 |
| 3   | V     | 225/314 (72%)   | 201 (89%)  | 23 (10%) | 1 (0%)   | 30          | 64  |
| 3   | u     | 229/314 (73%)   | 204 (89%)  | 25 (11%) | 0        | 100         | 100 |
| 3   | v     | 225/314 (72%)   | 209 (93%)  | 16 (7%)  | 0        | 100         | 100 |
| 4   | X     | 1085/1193 (91%) | 993 (92%)  | 90 (8%)  | 2 (0%)   | 43          | 74  |
| 4   | x     | 1084/1193 (91%) | 1001 (92%) | 80 (7%)  | 3 (0%)   | 36          | 69  |
| 5   | Y     | 1121/1199 (94%) | 1030 (92%) | 89 (8%)  | 2 (0%)   | 43          | 74  |
| 5   | y     | 1121/1199 (94%) | 1030 (92%) | 89 (8%)  | 2 (0%)   | 43          | 74  |
| 6   | H     | 769/774 (99%)   | 701 (91%)  | 66 (9%)  | 2 (0%)   | 36          | 69  |
| 6   | h     | 769/774 (99%)   | 702 (91%)  | 65 (8%)  | 2 (0%)   | 36          | 69  |
| All | All   | 7261/8004 (91%) | 6630 (91%) | 615 (8%) | 16 (0%)  | 44          | 74  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | X     | 333  | PRO  |
| 4   | x     | 333  | PRO  |
| 4   | X     | 332  | TYR  |
| 2   | E     | 52   | GLY  |
| 5   | Y     | 1087 | ASP  |
| 2   | e     | 52   | GLY  |
| 4   | x     | 332  | TYR  |
| 5   | y     | 1087 | ASP  |
| 6   | H     | 496  | GLN  |
| 6   | h     | 496  | GLN  |
| 5   | Y     | 572  | PRO  |
| 6   | H     | 58   | ALA  |
| 5   | y     | 572  | PRO  |
| 6   | h     | 58   | ALA  |
| 4   | x     | 1055 | PRO  |
| 3   | V     | 161  | ILE  |

### 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   | D     | 82/126 (65%)   | 78 (95%)   | 4 (5%)   | 22          | 47  |
| 1   | d     | 82/126 (65%)   | 78 (95%)   | 4 (5%)   | 22          | 47  |
| 2   | E     | 65/65 (100%)   | 61 (94%)   | 4 (6%)   | 16          | 43  |
| 2   | e     | 65/65 (100%)   | 61 (94%)   | 4 (6%)   | 16          | 43  |
| 3   | U     | 197/273 (72%)  | 197 (100%) | 0        | 100         | 100 |
| 3   | V     | 195/273 (71%)  | 195 (100%) | 0        | 100         | 100 |
| 3   | u     | 197/273 (72%)  | 197 (100%) | 0        | 100         | 100 |
| 3   | v     | 195/273 (71%)  | 195 (100%) | 0        | 100         | 100 |
| 4   | X     | 902/1026 (88%) | 902 (100%) | 0        | 100         | 100 |
| 4   | x     | 901/1026 (88%) | 901 (100%) | 0        | 100         | 100 |
| 5   | Y     | 965/1027 (94%) | 894 (93%)  | 71 (7%)  | 13          | 38  |
| 5   | y     | 965/1027 (94%) | 894 (93%)  | 71 (7%)  | 13          | 38  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 6   | H     | 679/682 (100%)  | 634 (93%)  | 45 (7%)  | 15          | 41 |
| 6   | h     | 679/682 (100%)  | 634 (93%)  | 45 (7%)  | 15          | 41 |
| All | All   | 6169/6944 (89%) | 5921 (96%) | 248 (4%) | 29          | 51 |

All (248) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 61  | ASP  |
| 1   | D     | 72  | SER  |
| 1   | D     | 88  | ASP  |
| 1   | D     | 92  | GLN  |
| 2   | E     | 16  | VAL  |
| 2   | E     | 28  | VAL  |
| 2   | E     | 61  | SER  |
| 2   | E     | 66  | VAL  |
| 5   | Y     | 32  | GLU  |
| 5   | Y     | 33  | THR  |
| 5   | Y     | 81  | GLU  |
| 5   | Y     | 83  | THR  |
| 5   | Y     | 102 | SER  |
| 5   | Y     | 127 | GLU  |
| 5   | Y     | 133 | SER  |
| 5   | Y     | 151 | SER  |
| 5   | Y     | 185 | VAL  |
| 5   | Y     | 193 | GLU  |
| 5   | Y     | 211 | GLU  |
| 5   | Y     | 242 | VAL  |
| 5   | Y     | 278 | SER  |
| 5   | Y     | 287 | MET  |
| 5   | Y     | 293 | ASP  |
| 5   | Y     | 306 | THR  |
| 5   | Y     | 345 | VAL  |
| 5   | Y     | 346 | VAL  |
| 5   | Y     | 370 | VAL  |
| 5   | Y     | 400 | VAL  |
| 5   | Y     | 402 | GLU  |
| 5   | Y     | 403 | SER  |
| 5   | Y     | 411 | LEU  |
| 5   | Y     | 462 | SER  |
| 5   | Y     | 464 | GLU  |
| 5   | Y     | 471 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Y     | 489  | VAL  |
| 5   | Y     | 490  | THR  |
| 5   | Y     | 496  | VAL  |
| 5   | Y     | 515  | VAL  |
| 5   | Y     | 543  | SER  |
| 5   | Y     | 569  | GLU  |
| 5   | Y     | 582  | THR  |
| 5   | Y     | 637  | SER  |
| 5   | Y     | 651  | SER  |
| 5   | Y     | 658  | VAL  |
| 5   | Y     | 661  | SER  |
| 5   | Y     | 695  | GLU  |
| 5   | Y     | 699  | GLU  |
| 5   | Y     | 703  | SER  |
| 5   | Y     | 706  | SER  |
| 5   | Y     | 710  | ASP  |
| 5   | Y     | 711  | VAL  |
| 5   | Y     | 794  | THR  |
| 5   | Y     | 796  | ASP  |
| 5   | Y     | 797  | SER  |
| 5   | Y     | 815  | GLU  |
| 5   | Y     | 816  | THR  |
| 5   | Y     | 830  | LYS  |
| 5   | Y     | 833  | THR  |
| 5   | Y     | 835  | THR  |
| 5   | Y     | 841  | GLU  |
| 5   | Y     | 860  | VAL  |
| 5   | Y     | 882  | GLU  |
| 5   | Y     | 912  | ASP  |
| 5   | Y     | 915  | VAL  |
| 5   | Y     | 964  | ASN  |
| 5   | Y     | 972  | THR  |
| 5   | Y     | 977  | THR  |
| 5   | Y     | 982  | ASN  |
| 5   | Y     | 984  | VAL  |
| 5   | Y     | 993  | VAL  |
| 5   | Y     | 1003 | THR  |
| 5   | Y     | 1007 | ASN  |
| 5   | Y     | 1010 | LEU  |
| 5   | Y     | 1127 | SER  |
| 5   | Y     | 1129 | GLU  |
| 5   | Y     | 1131 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | Y     | 1132 | SER  |
| 5   | Y     | 1148 | ASP  |
| 5   | Y     | 1152 | LYS  |
| 6   | H     | 13   | SER  |
| 6   | H     | 17   | GLU  |
| 6   | H     | 51   | VAL  |
| 6   | H     | 64   | THR  |
| 6   | H     | 76   | SER  |
| 6   | H     | 77   | ASP  |
| 6   | H     | 107  | ILE  |
| 6   | H     | 149  | SER  |
| 6   | H     | 198  | LEU  |
| 6   | H     | 199  | SER  |
| 6   | H     | 204  | THR  |
| 6   | H     | 225  | LYS  |
| 6   | H     | 226  | SER  |
| 6   | H     | 241  | SER  |
| 6   | H     | 257  | VAL  |
| 6   | H     | 276  | VAL  |
| 6   | H     | 286  | GLU  |
| 6   | H     | 308  | GLU  |
| 6   | H     | 317  | CYS  |
| 6   | H     | 349  | VAL  |
| 6   | H     | 352  | LEU  |
| 6   | H     | 427  | ASP  |
| 6   | H     | 435  | LEU  |
| 6   | H     | 444  | SER  |
| 6   | H     | 472  | VAL  |
| 6   | H     | 489  | SER  |
| 6   | H     | 498  | GLU  |
| 6   | H     | 500  | MET  |
| 6   | H     | 501  | ASP  |
| 6   | H     | 503  | ILE  |
| 6   | H     | 538  | THR  |
| 6   | H     | 578  | ILE  |
| 6   | H     | 601  | VAL  |
| 6   | H     | 614  | VAL  |
| 6   | H     | 620  | MET  |
| 6   | H     | 621  | LEU  |
| 6   | H     | 633  | SER  |
| 6   | H     | 640  | VAL  |
| 6   | H     | 649  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 678 | ILE  |
| 6   | H     | 685 | SER  |
| 6   | H     | 715 | ILE  |
| 6   | H     | 721 | LEU  |
| 6   | H     | 732 | THR  |
| 6   | H     | 752 | VAL  |
| 1   | d     | 61  | ASP  |
| 1   | d     | 72  | SER  |
| 1   | d     | 88  | ASP  |
| 1   | d     | 92  | GLN  |
| 2   | e     | 16  | VAL  |
| 2   | e     | 28  | VAL  |
| 2   | e     | 61  | SER  |
| 2   | e     | 66  | VAL  |
| 5   | y     | 32  | GLU  |
| 5   | y     | 33  | THR  |
| 5   | y     | 81  | GLU  |
| 5   | y     | 83  | THR  |
| 5   | y     | 102 | SER  |
| 5   | y     | 127 | GLU  |
| 5   | y     | 133 | SER  |
| 5   | y     | 151 | SER  |
| 5   | y     | 185 | VAL  |
| 5   | y     | 193 | GLU  |
| 5   | y     | 211 | GLU  |
| 5   | y     | 242 | VAL  |
| 5   | y     | 278 | SER  |
| 5   | y     | 287 | MET  |
| 5   | y     | 293 | ASP  |
| 5   | y     | 306 | THR  |
| 5   | y     | 345 | VAL  |
| 5   | y     | 346 | VAL  |
| 5   | y     | 370 | VAL  |
| 5   | y     | 400 | VAL  |
| 5   | y     | 402 | GLU  |
| 5   | y     | 403 | SER  |
| 5   | y     | 411 | LEU  |
| 5   | y     | 462 | SER  |
| 5   | y     | 464 | GLU  |
| 5   | y     | 471 | ILE  |
| 5   | y     | 489 | VAL  |
| 5   | y     | 490 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | y     | 496  | VAL  |
| 5   | y     | 515  | VAL  |
| 5   | y     | 543  | SER  |
| 5   | y     | 569  | GLU  |
| 5   | y     | 582  | THR  |
| 5   | y     | 637  | SER  |
| 5   | y     | 651  | SER  |
| 5   | y     | 658  | VAL  |
| 5   | y     | 661  | SER  |
| 5   | y     | 695  | GLU  |
| 5   | y     | 699  | GLU  |
| 5   | y     | 703  | SER  |
| 5   | y     | 706  | SER  |
| 5   | y     | 710  | ASP  |
| 5   | y     | 711  | VAL  |
| 5   | y     | 794  | THR  |
| 5   | y     | 796  | ASP  |
| 5   | y     | 797  | SER  |
| 5   | y     | 815  | GLU  |
| 5   | y     | 816  | THR  |
| 5   | y     | 830  | LYS  |
| 5   | y     | 833  | THR  |
| 5   | y     | 835  | THR  |
| 5   | y     | 841  | GLU  |
| 5   | y     | 860  | VAL  |
| 5   | y     | 882  | GLU  |
| 5   | y     | 912  | ASP  |
| 5   | y     | 915  | VAL  |
| 5   | y     | 964  | ASN  |
| 5   | y     | 972  | THR  |
| 5   | y     | 977  | THR  |
| 5   | y     | 982  | ASN  |
| 5   | y     | 984  | VAL  |
| 5   | y     | 993  | VAL  |
| 5   | y     | 1003 | THR  |
| 5   | y     | 1007 | ASN  |
| 5   | y     | 1010 | LEU  |
| 5   | y     | 1127 | SER  |
| 5   | y     | 1129 | GLU  |
| 5   | y     | 1131 | ASP  |
| 5   | y     | 1132 | SER  |
| 5   | y     | 1148 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | y     | 1152 | LYS  |
| 6   | h     | 13   | SER  |
| 6   | h     | 17   | GLU  |
| 6   | h     | 51   | VAL  |
| 6   | h     | 64   | THR  |
| 6   | h     | 76   | SER  |
| 6   | h     | 77   | ASP  |
| 6   | h     | 107  | ILE  |
| 6   | h     | 149  | SER  |
| 6   | h     | 198  | LEU  |
| 6   | h     | 199  | SER  |
| 6   | h     | 204  | THR  |
| 6   | h     | 225  | LYS  |
| 6   | h     | 226  | SER  |
| 6   | h     | 241  | SER  |
| 6   | h     | 257  | VAL  |
| 6   | h     | 276  | VAL  |
| 6   | h     | 286  | GLU  |
| 6   | h     | 308  | GLU  |
| 6   | h     | 317  | CYS  |
| 6   | h     | 349  | VAL  |
| 6   | h     | 352  | LEU  |
| 6   | h     | 427  | ASP  |
| 6   | h     | 435  | LEU  |
| 6   | h     | 444  | SER  |
| 6   | h     | 472  | VAL  |
| 6   | h     | 489  | SER  |
| 6   | h     | 498  | GLU  |
| 6   | h     | 500  | MET  |
| 6   | h     | 501  | ASP  |
| 6   | h     | 503  | ILE  |
| 6   | h     | 538  | THR  |
| 6   | h     | 578  | ILE  |
| 6   | h     | 601  | VAL  |
| 6   | h     | 614  | VAL  |
| 6   | h     | 620  | MET  |
| 6   | h     | 621  | LEU  |
| 6   | h     | 633  | SER  |
| 6   | h     | 640  | VAL  |
| 6   | h     | 649  | CYS  |
| 6   | h     | 678  | ILE  |
| 6   | h     | 685  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | h     | 715 | ILE  |
| 6   | h     | 721 | LEU  |
| 6   | h     | 732 | THR  |
| 6   | h     | 752 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 86   | GLN  |
| 1   | D     | 92   | GLN  |
| 3   | U     | 190  | ASN  |
| 3   | V     | 81   | HIS  |
| 3   | V     | 190  | ASN  |
| 4   | X     | 390  | ASN  |
| 4   | X     | 576  | GLN  |
| 4   | X     | 617  | GLN  |
| 4   | X     | 719  | ASN  |
| 4   | X     | 770  | ASN  |
| 4   | X     | 881  | HIS  |
| 4   | X     | 970  | GLN  |
| 4   | X     | 975  | HIS  |
| 5   | Y     | 298  | ASN  |
| 5   | Y     | 478  | ASN  |
| 5   | Y     | 542  | ASN  |
| 5   | Y     | 579  | ASN  |
| 5   | Y     | 724  | ASN  |
| 5   | Y     | 809  | GLN  |
| 5   | Y     | 854  | HIS  |
| 5   | Y     | 982  | ASN  |
| 5   | Y     | 994  | GLN  |
| 5   | Y     | 1049 | HIS  |
| 6   | H     | 88   | GLN  |
| 6   | H     | 147  | ASN  |
| 6   | H     | 290  | GLN  |
| 6   | H     | 394  | GLN  |
| 6   | H     | 497  | HIS  |
| 6   | H     | 581  | HIS  |
| 6   | H     | 698  | GLN  |
| 1   | d     | 63   | ASN  |
| 1   | d     | 92   | GLN  |
| 3   | u     | 190  | ASN  |
| 3   | v     | 38   | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | v     | 114  | HIS  |
| 3   | v     | 122  | ASN  |
| 3   | v     | 222  | ASN  |
| 4   | x     | 100  | ASN  |
| 4   | x     | 375  | ASN  |
| 4   | x     | 576  | GLN  |
| 4   | x     | 617  | GLN  |
| 4   | x     | 720  | GLN  |
| 4   | x     | 1042 | HIS  |
| 5   | y     | 255  | ASN  |
| 5   | y     | 298  | ASN  |
| 5   | y     | 542  | ASN  |
| 5   | y     | 579  | ASN  |
| 5   | y     | 740  | ASN  |
| 5   | y     | 809  | GLN  |
| 5   | y     | 854  | HIS  |
| 5   | y     | 982  | ASN  |
| 5   | y     | 994  | GLN  |
| 5   | y     | 1049 | HIS  |
| 6   | h     | 88   | GLN  |
| 6   | h     | 147  | ASN  |
| 6   | h     | 273  | ASN  |
| 6   | h     | 290  | GLN  |
| 6   | h     | 342  | GLN  |
| 6   | h     | 394  | GLN  |
| 6   | h     | 497  | HIS  |
| 6   | h     | 581  | HIS  |
| 6   | h     | 698  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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 |
|-----|-------|------------------|
| 1   | D     | 1                |
| 1   | d     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | D     | 92:GLN    | C      | 1001:PRO  | N      | 26.80        |
| 1     | d     | 92:GLN    | C      | 1001:PRO  | N      | 26.80        |

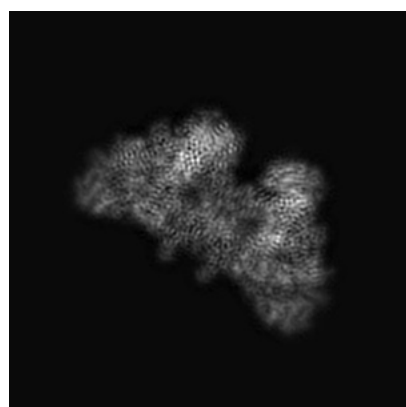
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11105. These allow visual inspection of the internal detail of the map and identification of artifacts.

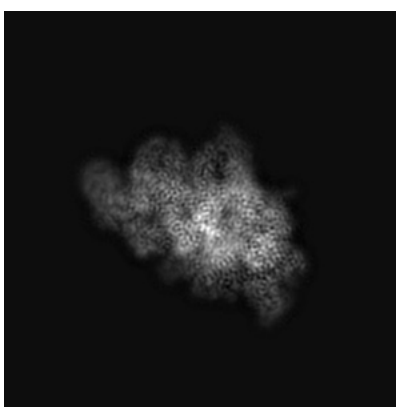
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

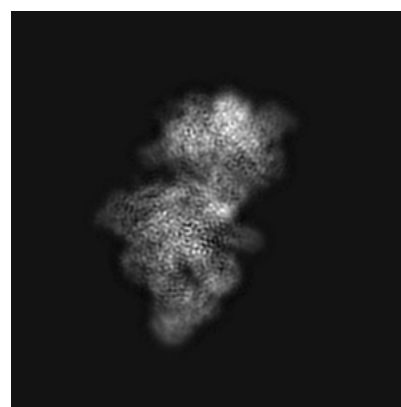
#### 6.1.1 Primary map



X



Y

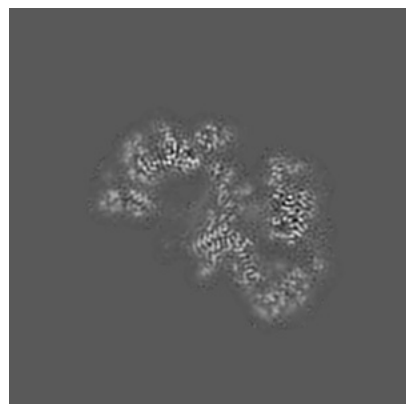


Z

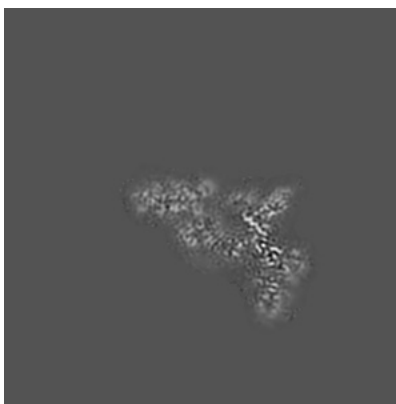
The images above show the map projected in three orthogonal directions.

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

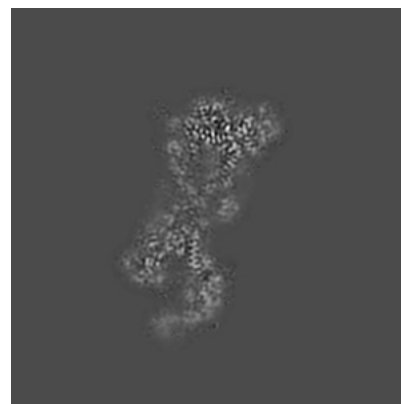
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

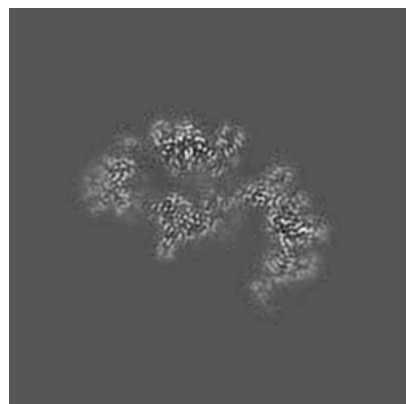


Z Index: 140

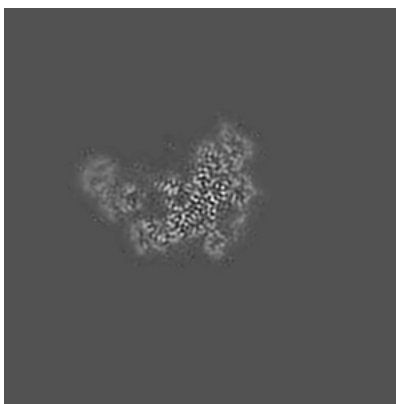
The images above show central slices of the map in three orthogonal directions.

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

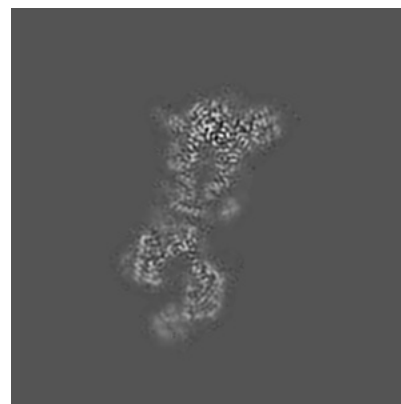
### 6.3.1 Primary map



X Index: 125



Y Index: 198

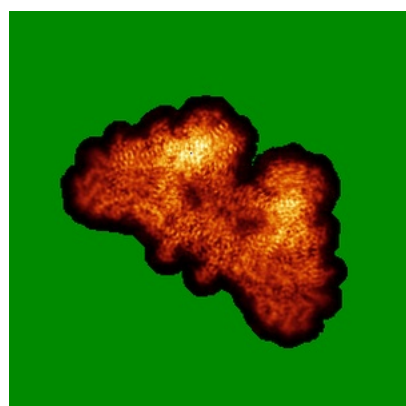


Z Index: 143

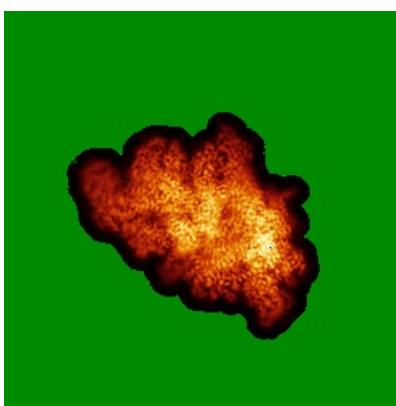
The images above show the largest variance slices of the map in three orthogonal directions.

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

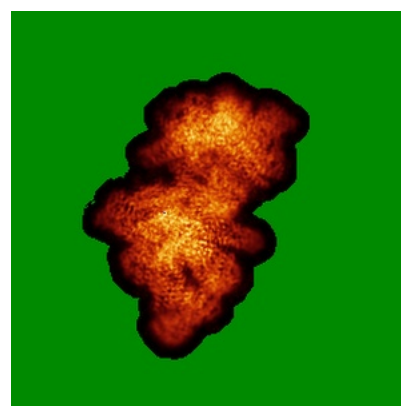
### 6.4.1 Primary map



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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

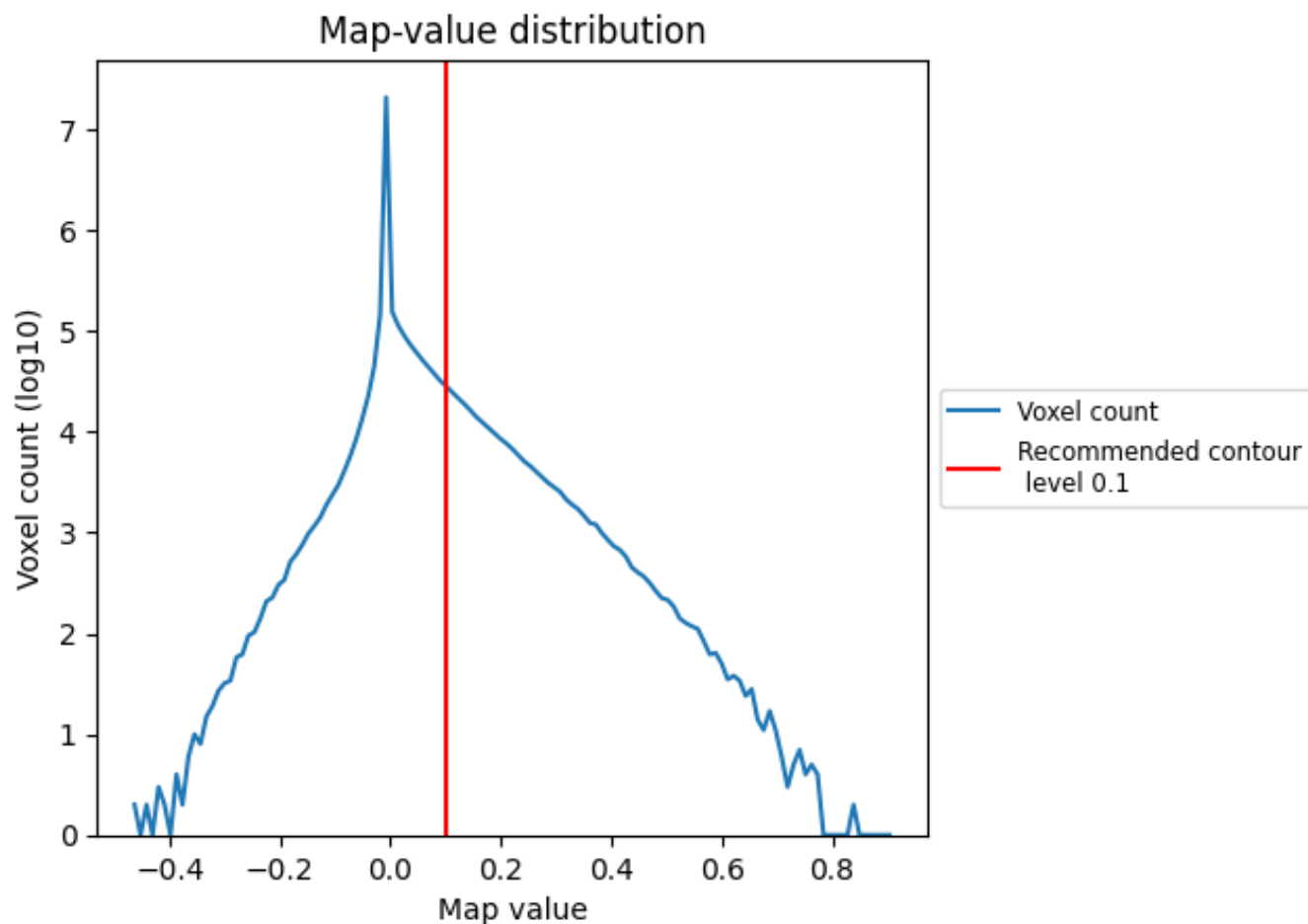
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

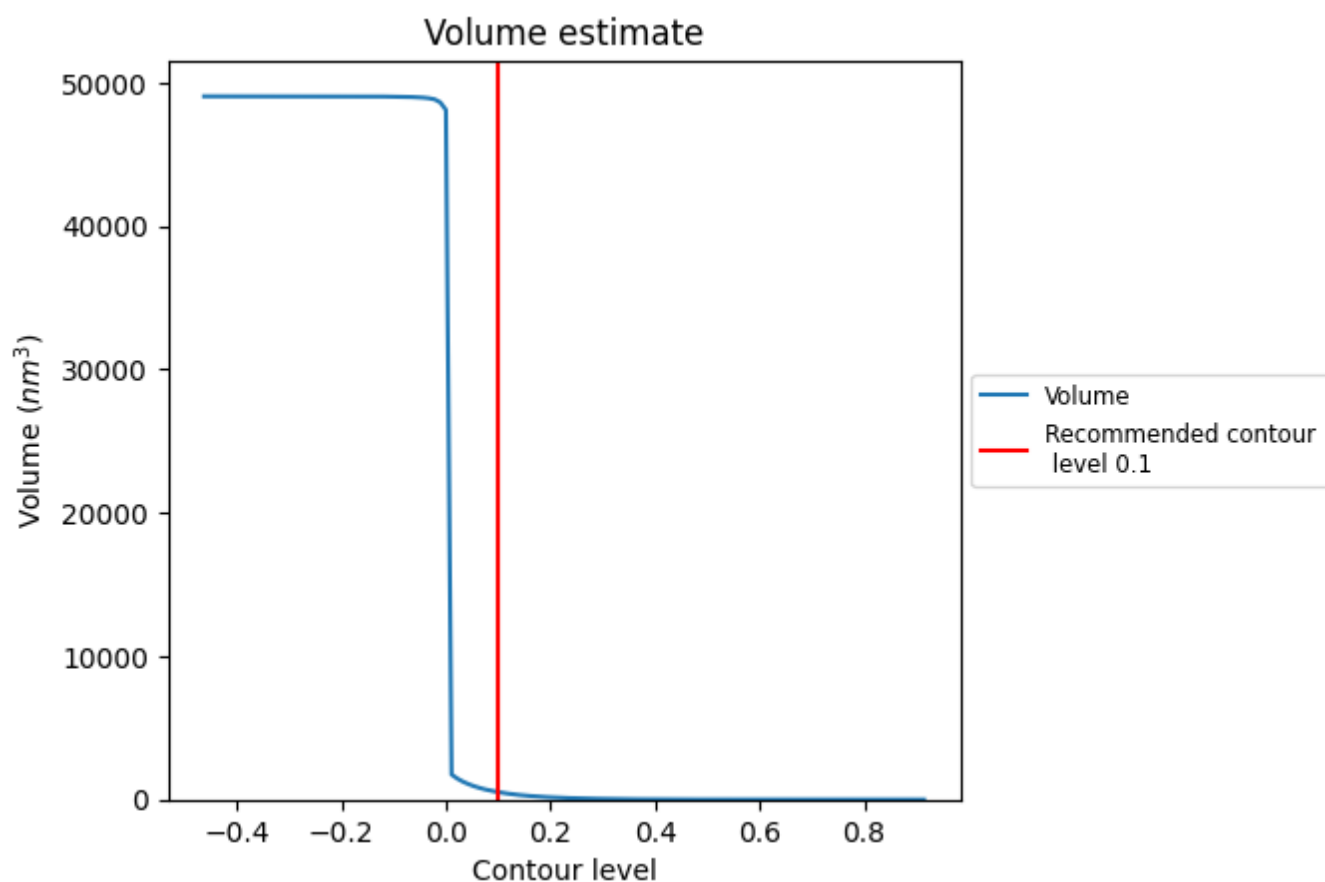
This section contains the results of statistical analysis of the map.

### 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.

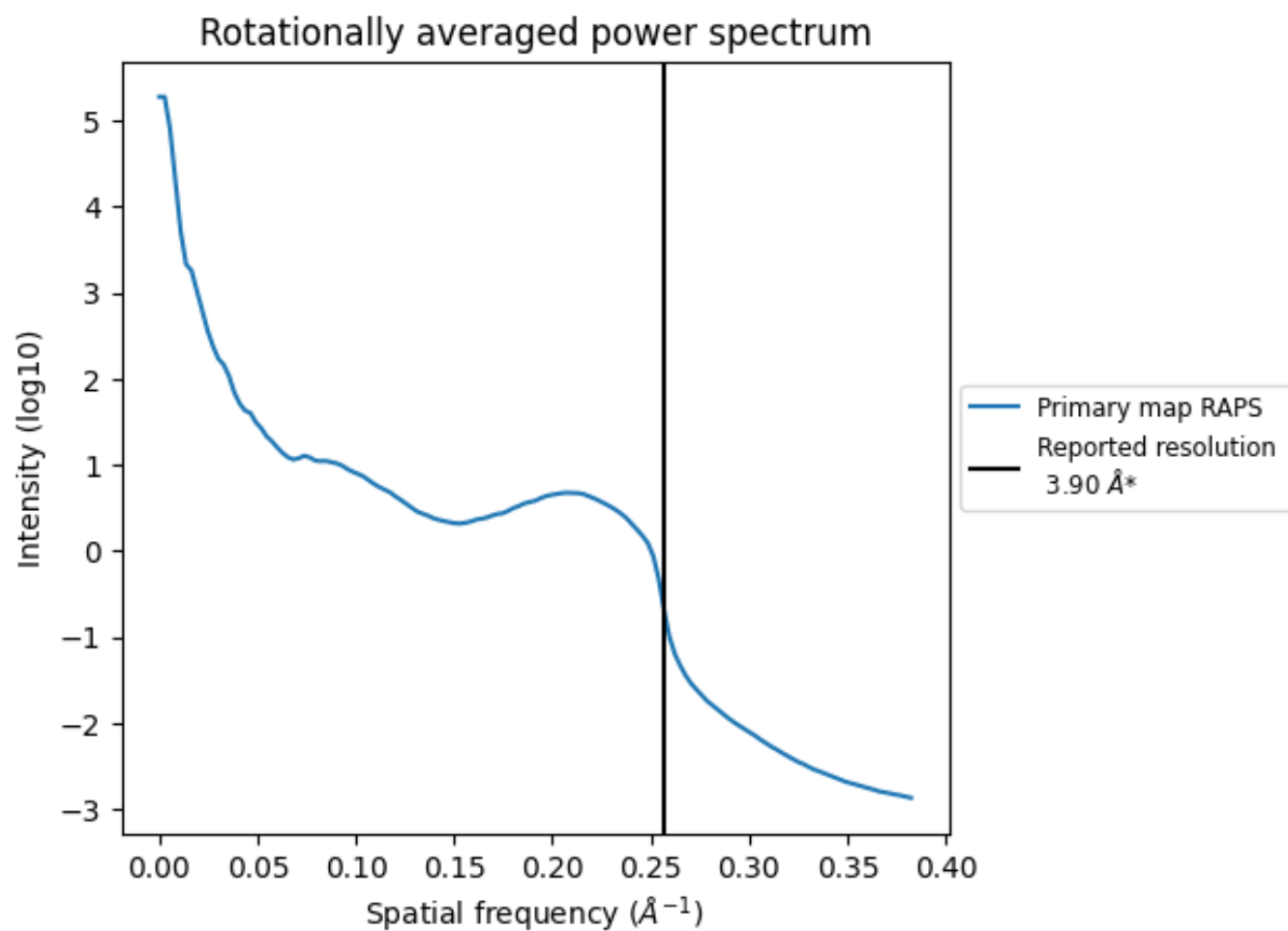
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 519 nm<sup>3</sup>; this corresponds to an approximate mass of 469 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 ⓘ

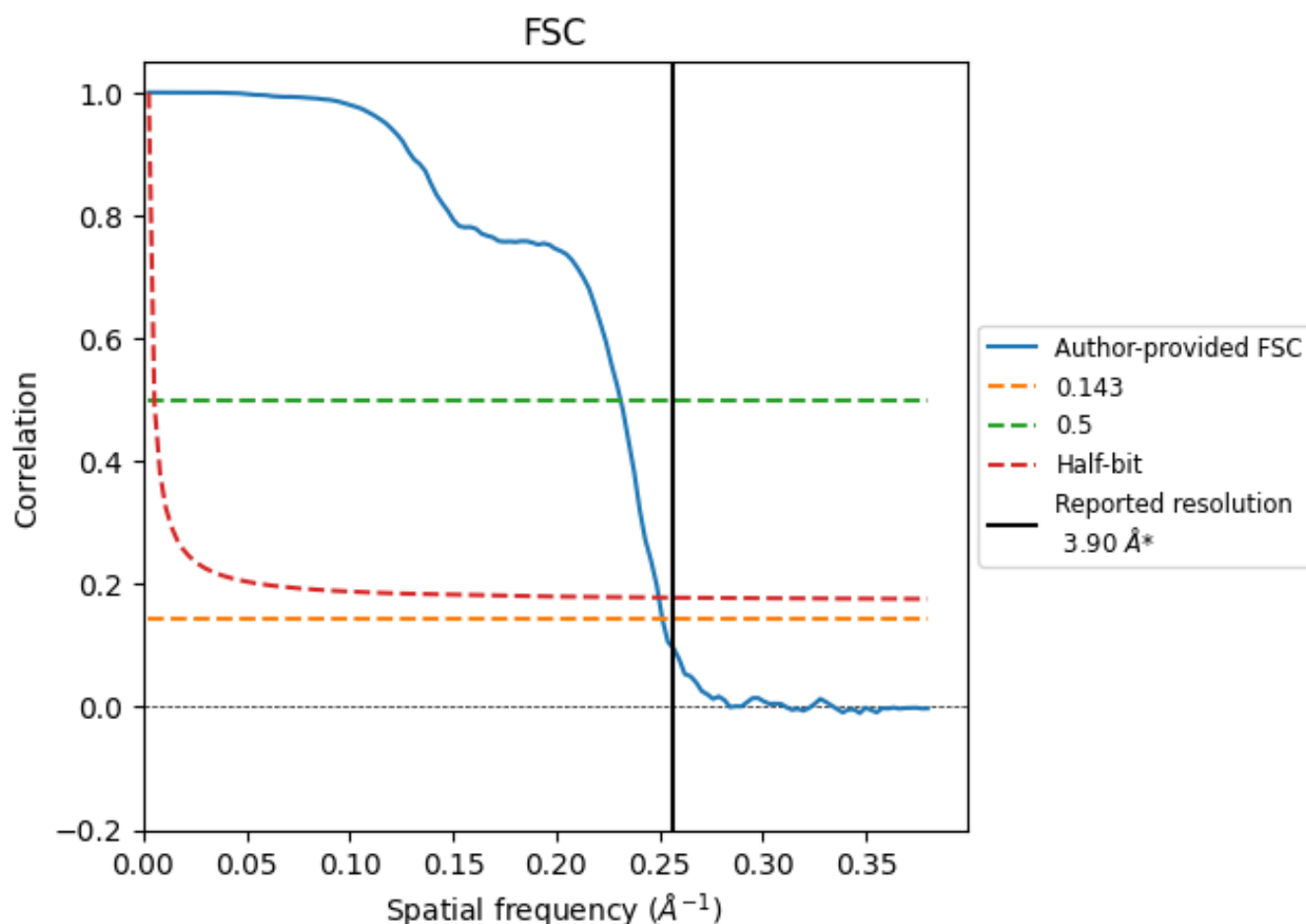


\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

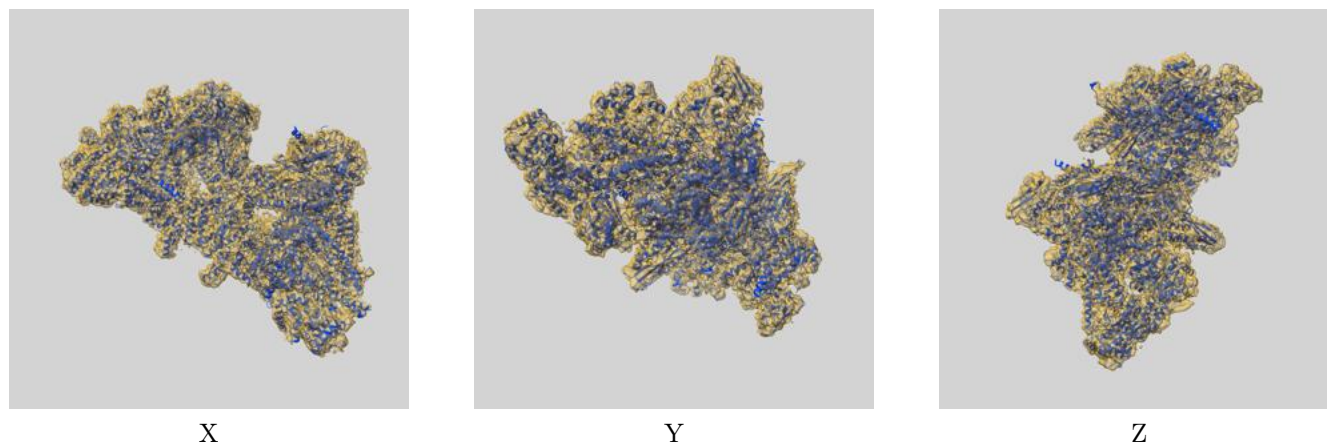
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.90                               | -    | -        |
| Author-provided FSC curve | 3.98                               | 4.33 | 4.01     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

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

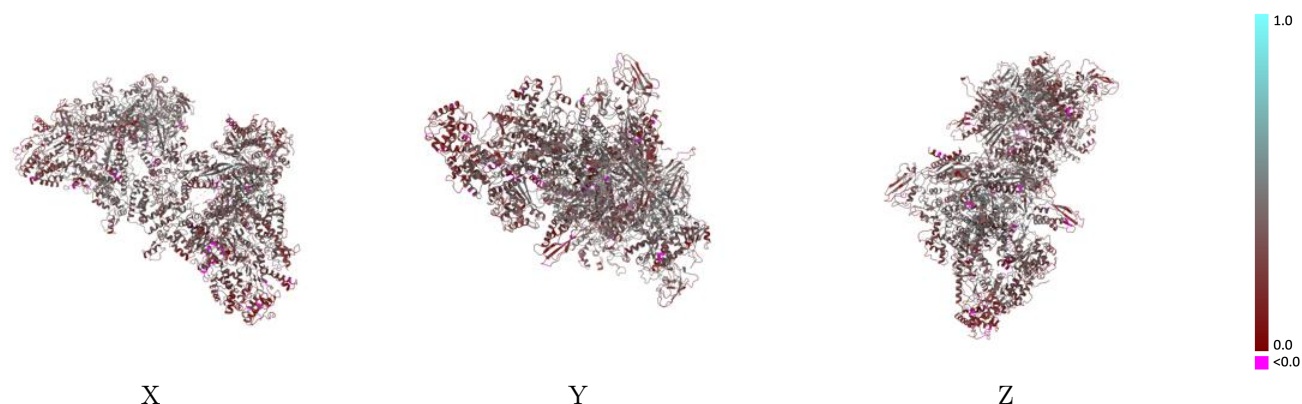
This section contains information regarding the fit between EMDB map EMD-11105 and PDB model 6ZFB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



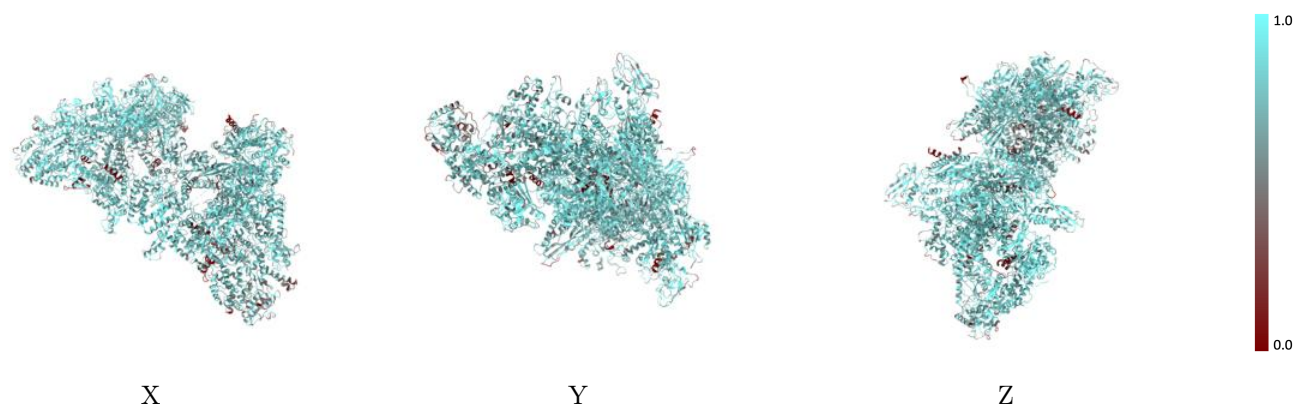
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



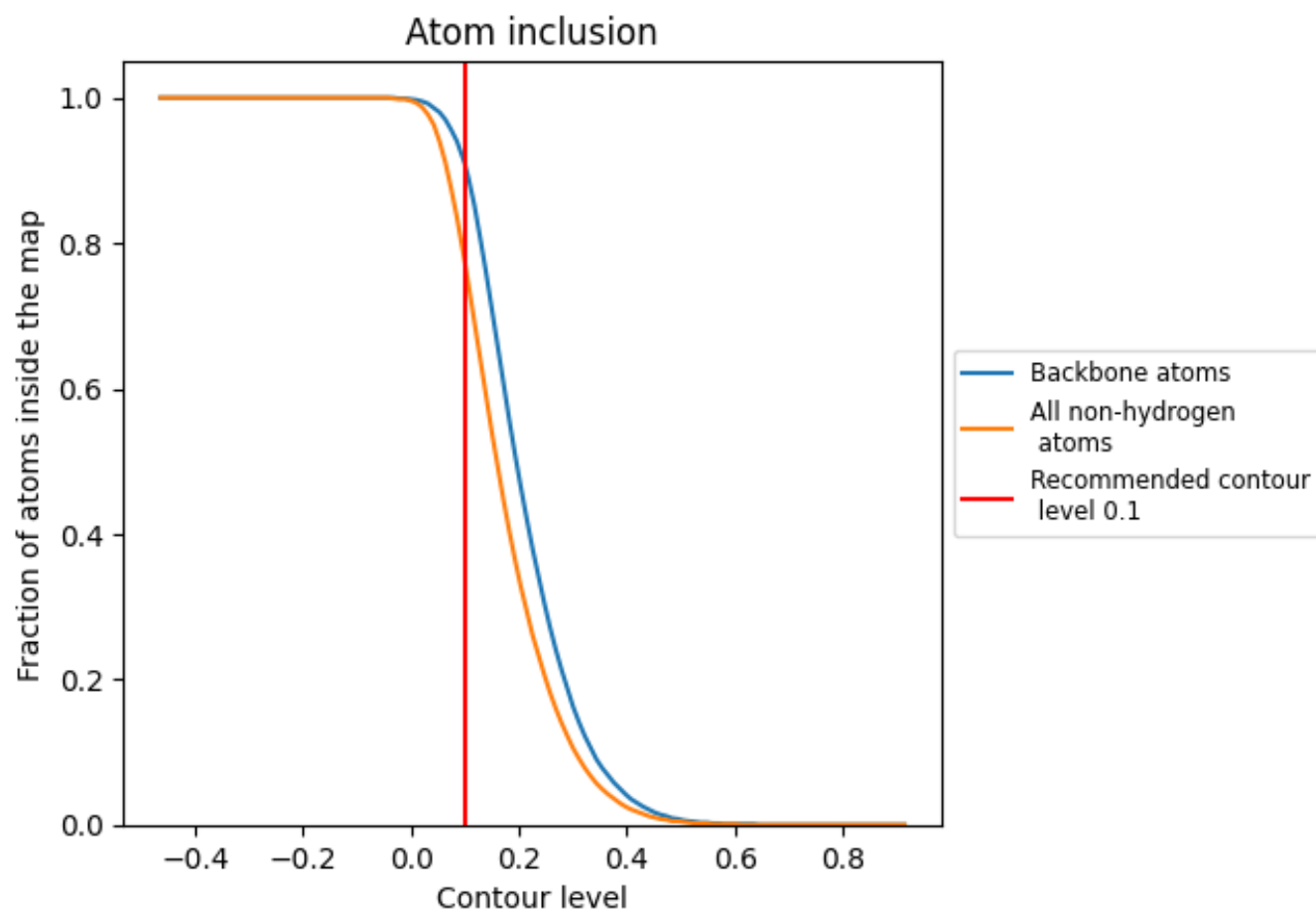
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                            | Q-score                                                                                   |
|-------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| All   |  0.7750  |  0.3440  |
| D     |  0.5740  |  0.2490  |
| E     |  0.8050  |  0.3370  |
| H     |  0.7890  |  0.3110  |
| U     |  0.7860  |  0.3690  |
| V     |  0.7470  |  0.3290  |
| X     |  0.8210  |  0.3750  |
| Y     |  0.8110  |  0.3730  |
| d     |  0.5510  |  0.2240  |
| e     |  0.7790  |  0.3360  |
| h     |  0.7170  |  0.2900  |
| u     |  0.7380  |  0.3390  |
| v     |  0.7070  |  0.3120  |
| x     |  0.7840  |  0.3640  |
| y     |  0.7910 |  0.3560 |

