



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:19 PM UTC

PDB ID : 7P60 / pdb\_00007p60  
EMDB ID : EMD-13213  
Title : Structure of homomeric LRRC8A Volume-Regulated Anion Channel in complex with synthetic nanobody Sb4 at 1:0.5 ratio  
Authors : Deneka, D.; Rutz, S.; Sawicka, M.  
Deposited on : 2021-07-15  
Resolution : 3.80 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

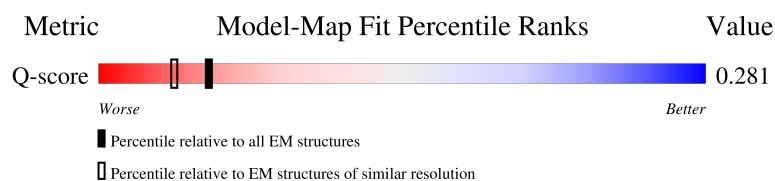
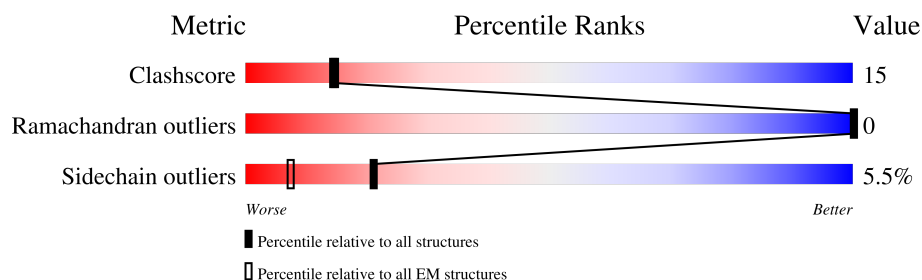
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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                       | 10198 ( 3.30 - 4.30 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 1   | A     | 810    | <div> <div>34%</div> <div>56%</div> <div>31%</div> <div>11%</div> </div> |
| 1   | B     | 810    | <div> <div>30%</div> <div>55%</div> <div>32%</div> <div>11%</div> </div> |
| 1   | C     | 810    | <div> <div>35%</div> <div>57%</div> <div>30%</div> <div>11%</div> </div> |
| 1   | D     | 810    | <div> <div>29%</div> <div>55%</div> <div>32%</div> <div>11%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                            |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 1   | E     | 810    | <div><div><div></div><div></div><div></div><div></div></div><div>35%53%34%•11%</div></div>  |
| 1   | F     | 810    | <div><div><div></div><div></div><div></div><div></div></div><div>29%55%32%•11%</div></div>  |
| 2   | G     | 154    | <div><div><div></div><div></div><div></div><div></div></div><div>53%47%29%5%19%</div></div> |
| 2   | H     | 154    | <div><div><div></div><div></div><div></div><div></div></div><div>52%47%31%•19%</div></div>  |
| 2   | I     | 154    | <div><div><div></div><div></div><div></div><div></div></div><div>51%45%33%•19%</div></div>  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38406 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 Volume-regulated anion channel subunit LRRC8A.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 1   | A     | 718      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997 | 1047 | 25 |         |       |
| 1   | B     | 718      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997 | 1047 | 25 |         |       |
| 1   | C     | 718      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997 | 1047 | 25 |         |       |
| 1   | D     | 718      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997 | 1047 | 25 |         |       |
| 1   | E     | 718      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997 | 1047 | 25 |         |       |
| 1   | F     | 718      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997 | 1047 | 25 |         |       |

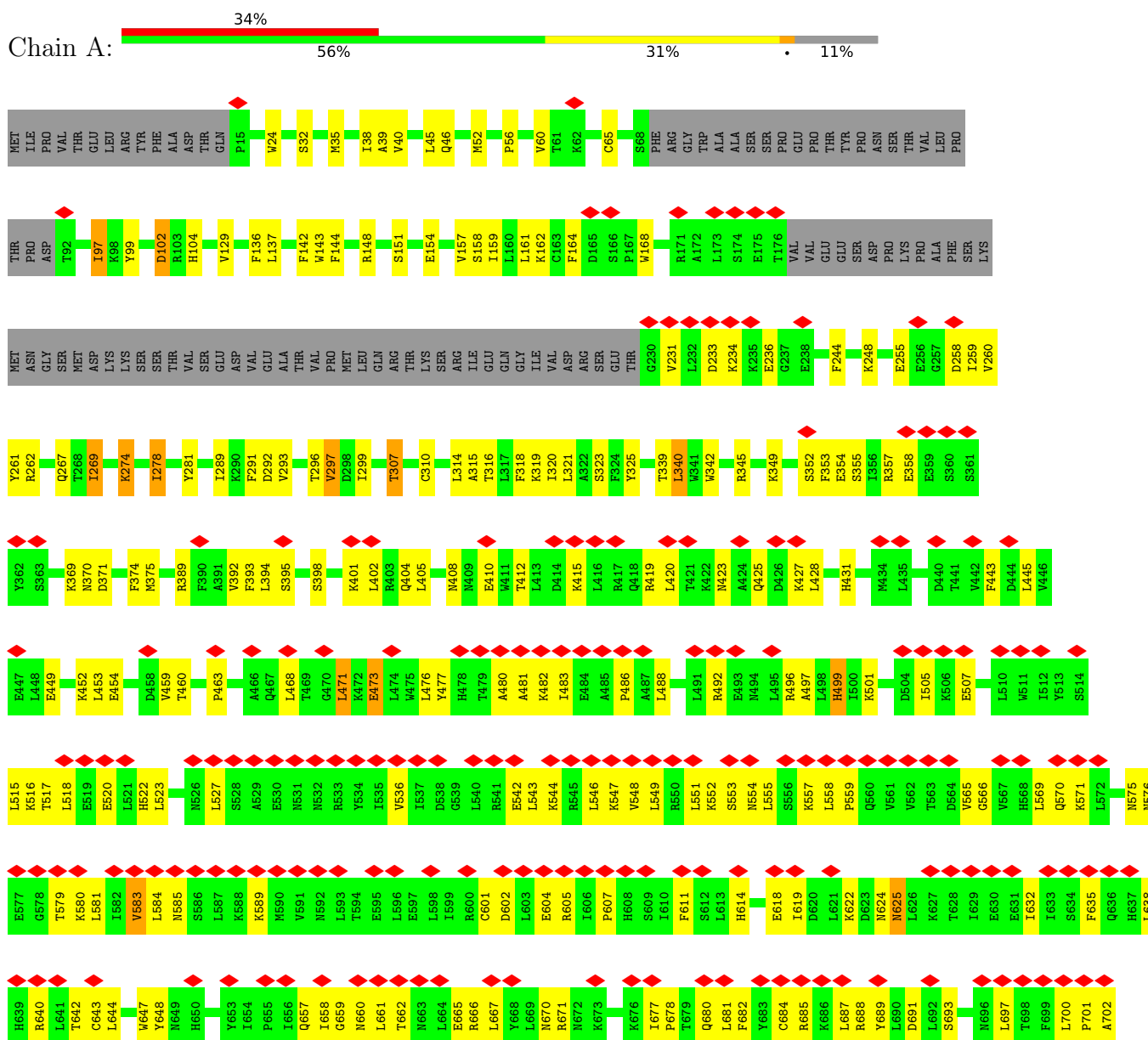
- Molecule 2 is a protein called synthetic nanobody Sb4.

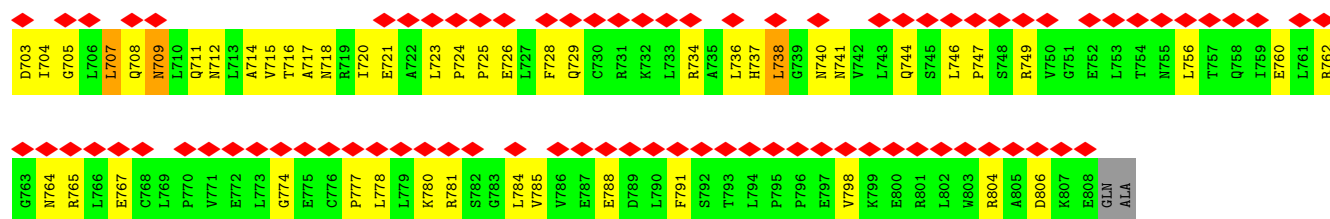
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | G     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 607 | 156 | 192 | 3 |         |       |
| 2   | I     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 607 | 156 | 192 | 3 |         |       |
| 2   | H     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 607 | 156 | 192 | 3 |         |       |

### 3 Residue-property plots

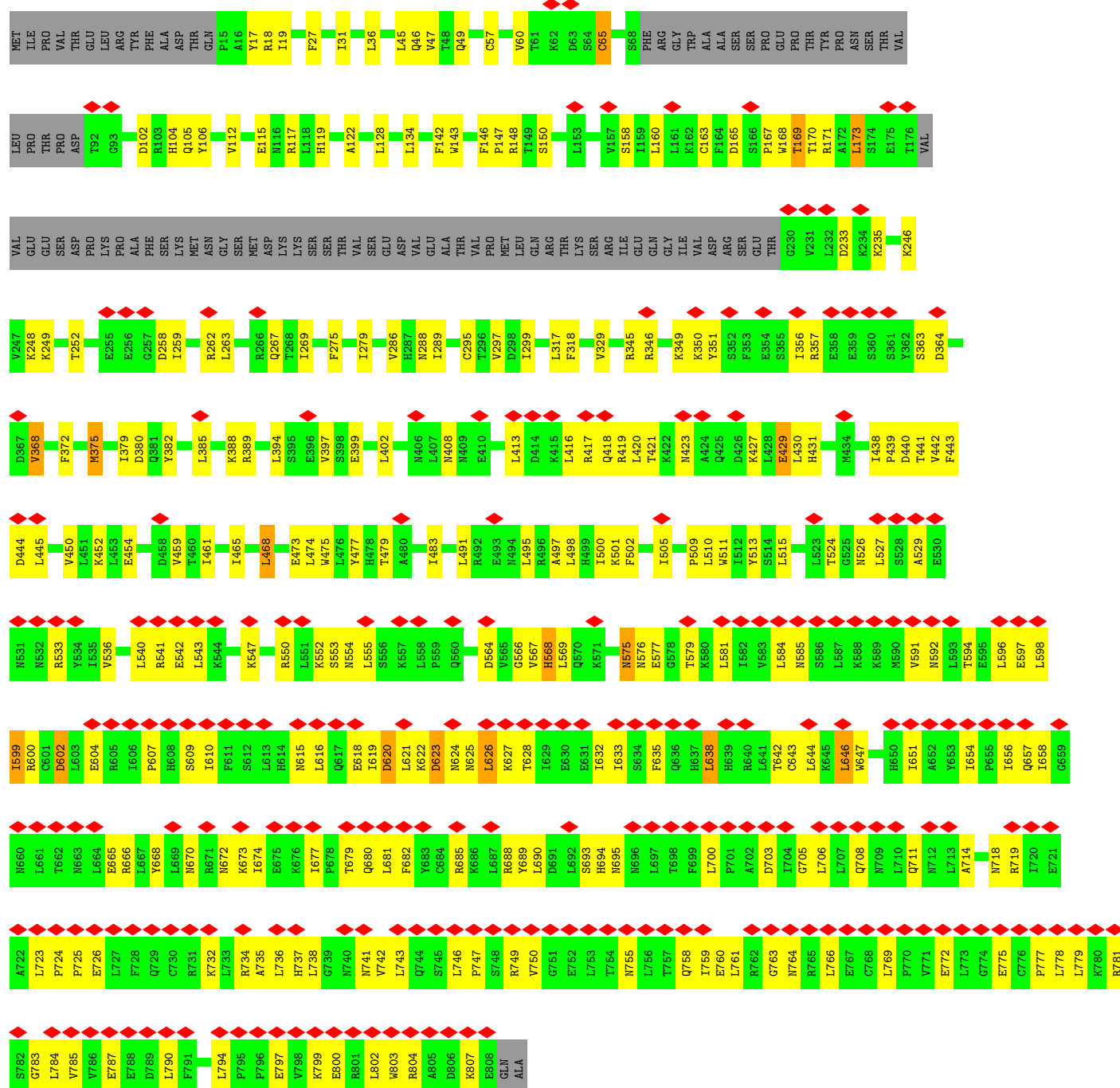
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Volume-regulated anion channel subunit LRRC8A

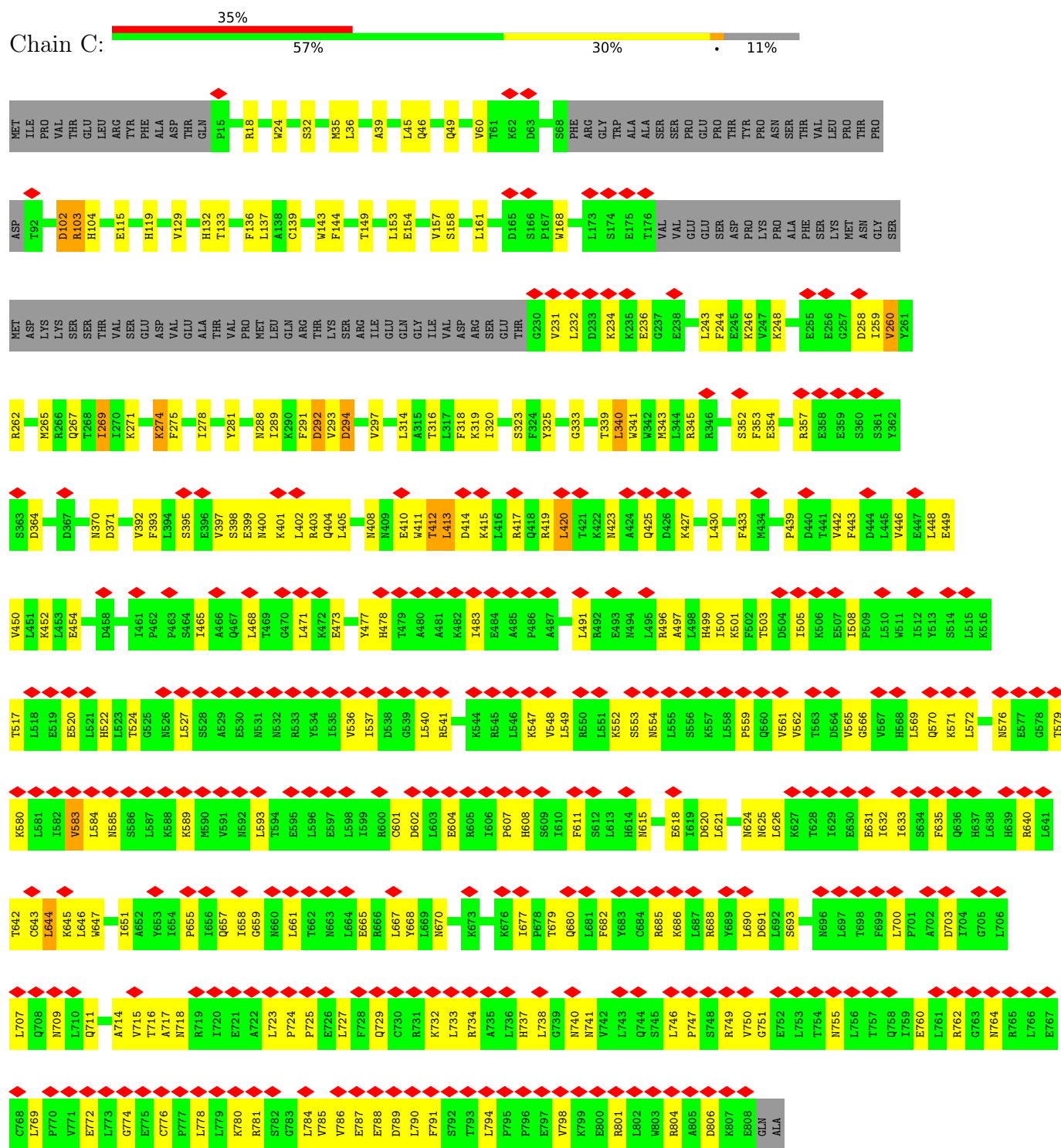




• Molecule 1: Volume-regulated anion channel subunit LRRC8A

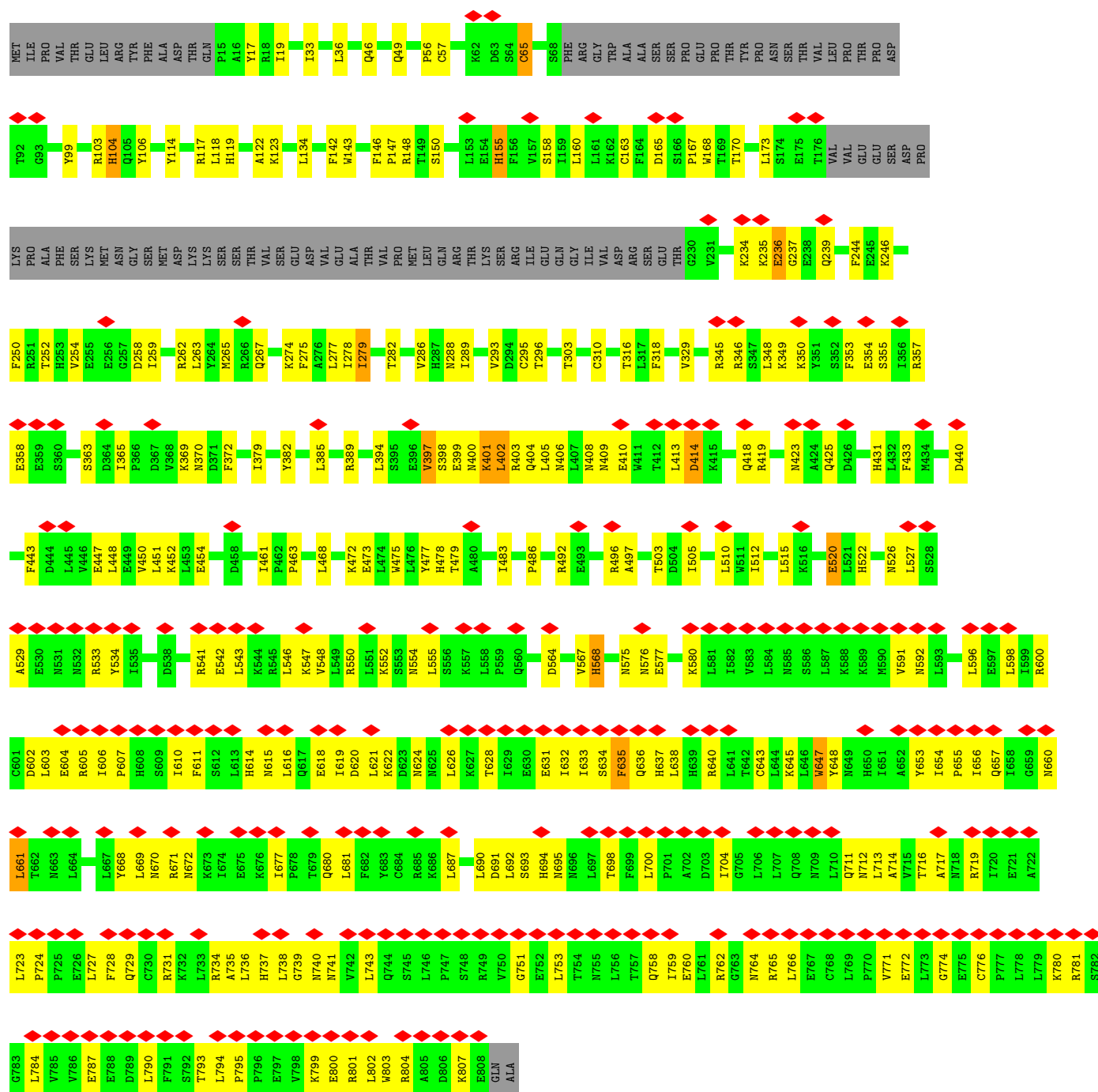


• Molecule 1: Volume-regulated anion channel subunit LRRC8A

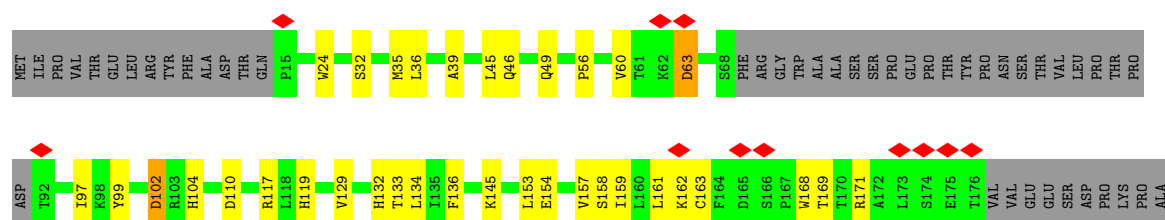


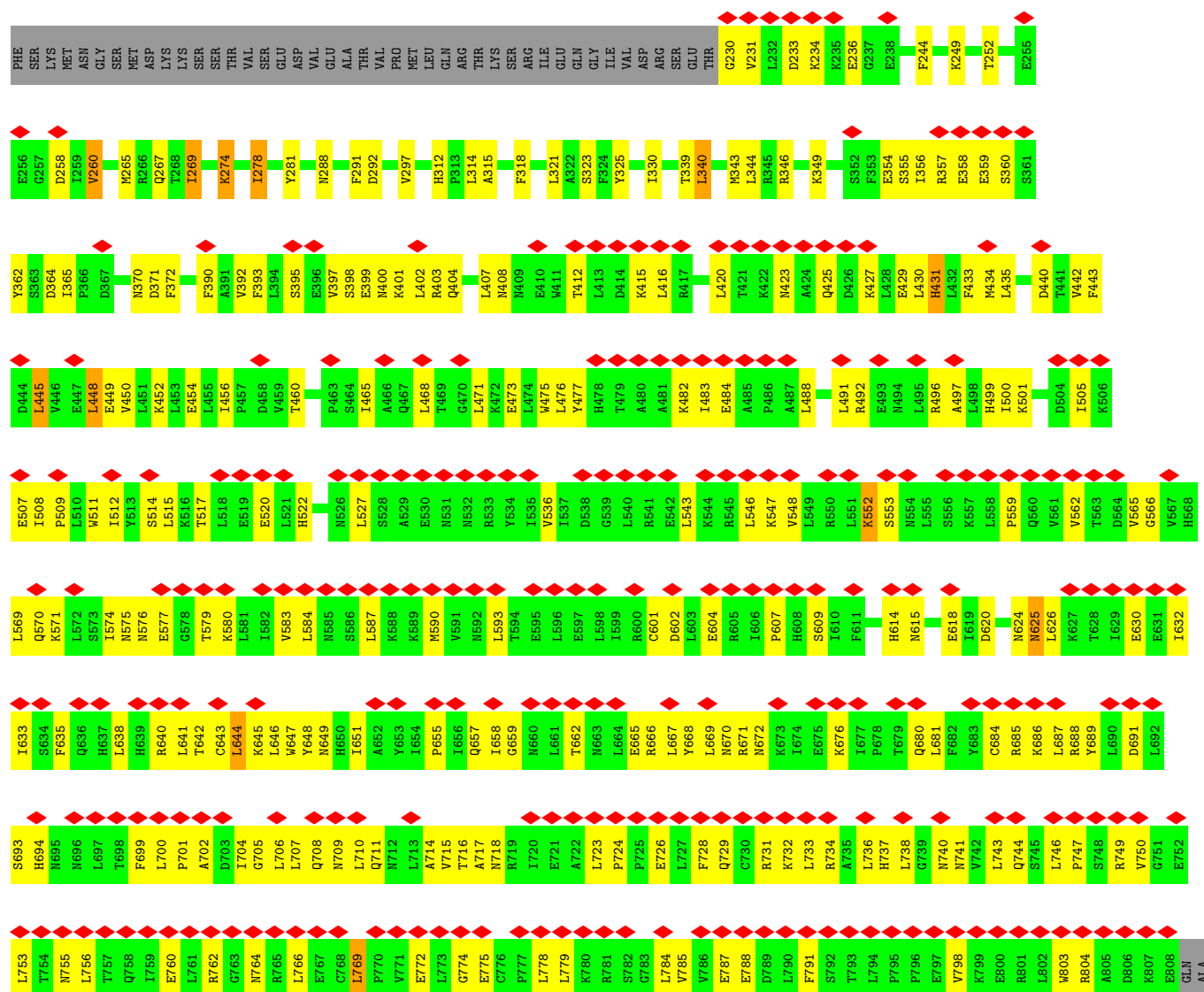
• Molecule 1: Volume-regulated anion channel subunit LRRC8A



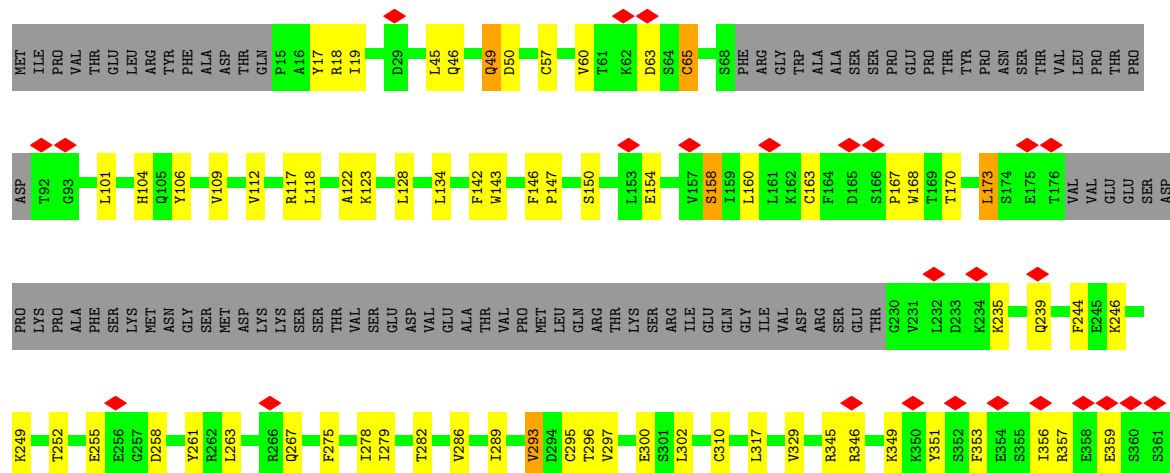


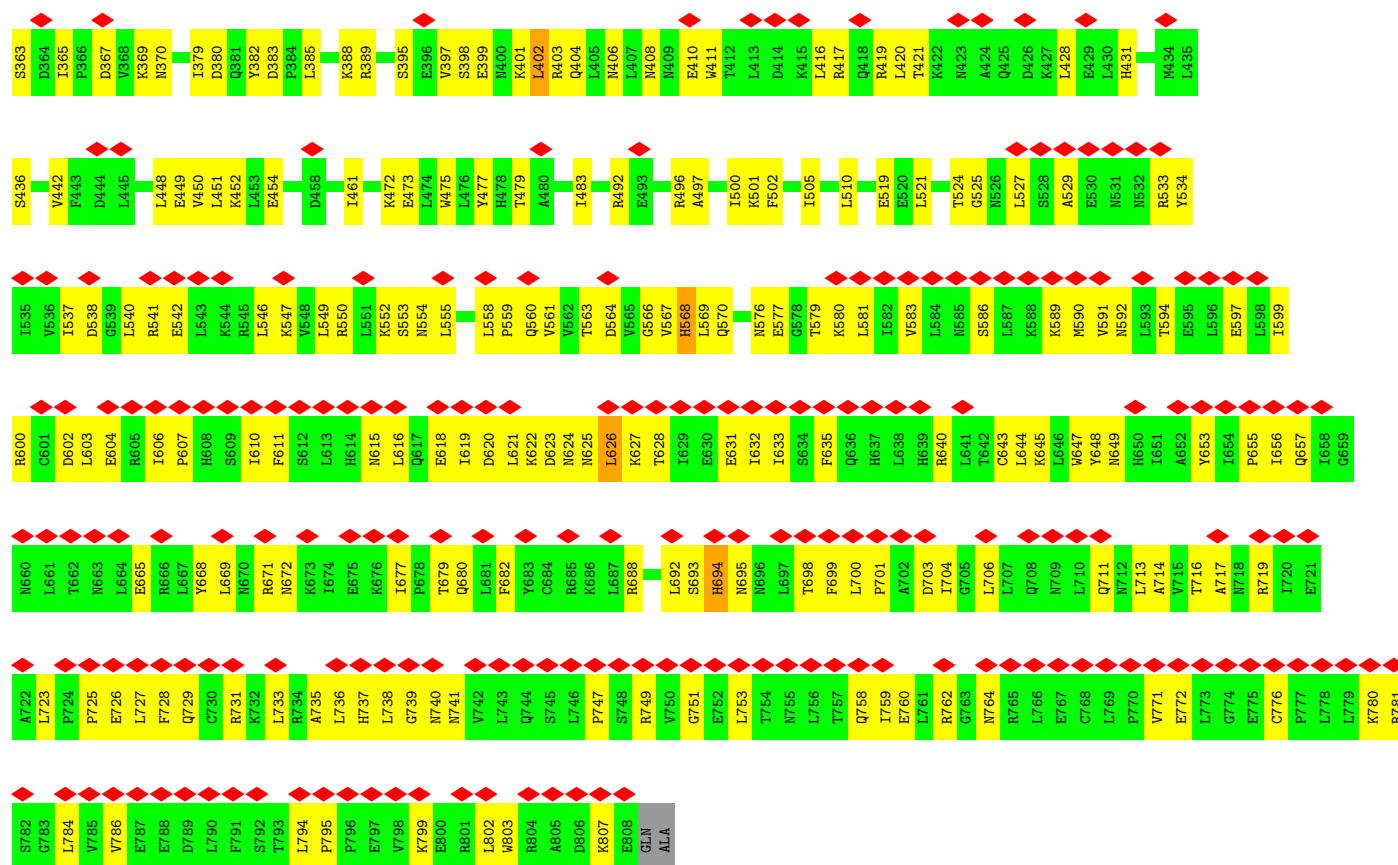
• Molecule 1: Volume-regulated anion channel subunit LRRC8A



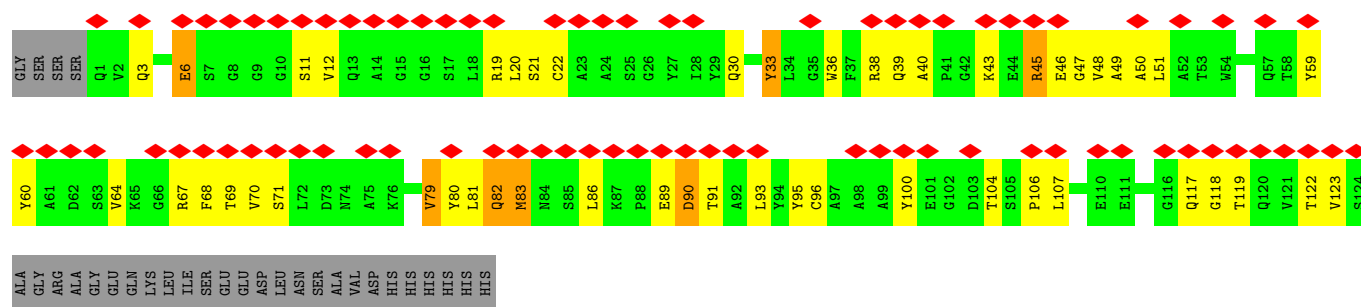


### • Molecule 1: Volume-regulated anion channel subunit LRRRC8A

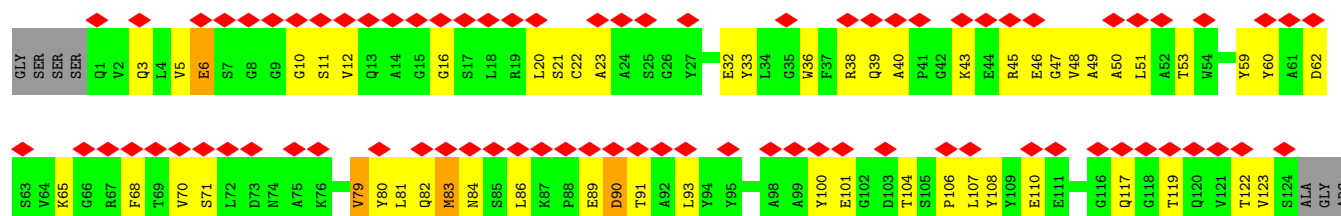




• Molecule 2: synthetic nanobody Sb4

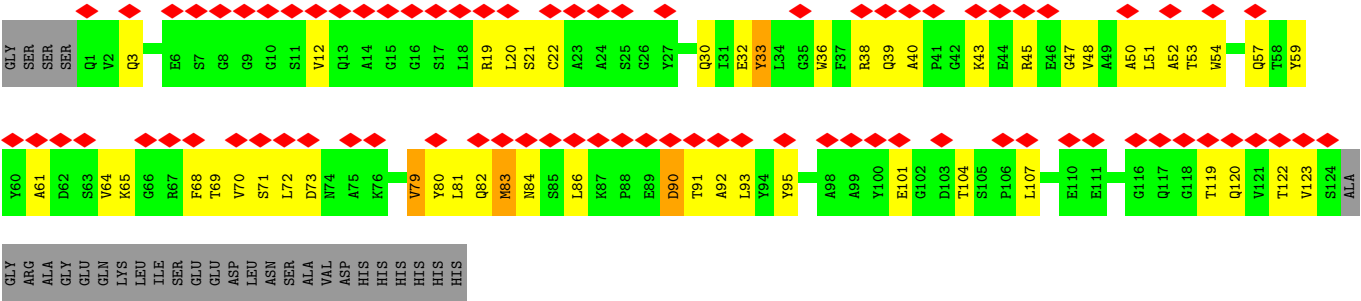


• Molecule 2: synthetic nanobody Sb4



ALA  
GLY  
GLU  
GLN  
SER  
LYS  
LEU  
ILE  
SER  
GLU  
GLU  
ASP  
LEU  
ASN  
SER  
ALA  
VAL  
ASP  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

● Molecule 2: synthetic nanobody Sb4



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

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 38121                                   | 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 ( $e^-/\text{\AA}^2$ ) | 67                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.140                                   | Depositor |
| Minimum map value                    | -0.060                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.003                                   | Depositor |
| Recommended contour level            | 0.027                                   | Depositor |
| Map size (Å)                         | 437.47202, 437.47202, 437.47202         | wwPDB     |
| Map dimensions                       | 336, 336, 336                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.302, 1.302, 1.302                     | Depositor |

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.19         | 0/6055      | 0.32        | 0/8207         |
| 1   | B     | 0.19         | 0/6055      | 0.32        | 0/8207         |
| 1   | C     | 0.19         | 0/6055      | 0.33        | 0/8207         |
| 1   | D     | 0.19         | 0/6055      | 0.32        | 0/8207         |
| 1   | E     | 0.19         | 0/6055      | 0.33        | 1/8207 (0.0%)  |
| 1   | F     | 0.19         | 0/6055      | 0.32        | 0/8207         |
| 2   | G     | 0.13         | 0/981       | 0.32        | 0/1334         |
| 2   | H     | 0.14         | 0/981       | 0.33        | 0/1334         |
| 2   | I     | 0.13         | 0/981       | 0.31        | 0/1334         |
| All | All   | 0.18         | 0/39273     | 0.32        | 1/53244 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1   | E     | 372 | PHE  | N-CA-C | -5.02 | 107.81                 | 114.04              |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5922  | 0        | 6081     | 176     | 0            |
| 1   | B     | 5922  | 0        | 6081     | 168     | 0            |
| 1   | C     | 5922  | 0        | 6081     | 185     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | D     | 5922  | 0        | 6081     | 174     | 0            |
| 1   | E     | 5922  | 0        | 6081     | 209     | 0            |
| 1   | F     | 5922  | 0        | 6081     | 166     | 0            |
| 2   | G     | 958   | 0        | 898      | 45      | 0            |
| 2   | H     | 958   | 0        | 898      | 35      | 0            |
| 2   | I     | 958   | 0        | 898      | 37      | 0            |
| All | All   | 38406 | 0        | 39180    | 1177    | 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 15.

All (1177) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 2:G:71:SER:HB2   | 2:G:80:TYR:HB2  | 1.54                     | 0.90              |
| 1:D:714:ALA:HA   | 1:D:737:HIS:HB2 | 1.61                     | 0.82              |
| 1:F:714:ALA:HA   | 1:F:737:HIS:HB2 | 1.62                     | 0.81              |
| 1:F:618:GLU:HG3  | 1:F:643:CYS:HB3 | 1.65                     | 0.79              |
| 1:B:737:HIS:HA   | 1:B:760:GLU:HB3 | 1.65                     | 0.79              |
| 2:G:50:ALA:HB3   | 2:G:59:TYR:HB2  | 1.63                     | 0.78              |
| 2:H:50:ALA:HB3   | 2:H:59:TYR:HB2  | 1.66                     | 0.78              |
| 1:B:577:GLU:HA   | 1:B:600:ARG:HE  | 1.48                     | 0.77              |
| 1:E:760:GLU:HA   | 1:E:785:VAL:HB  | 1.66                     | 0.77              |
| 2:I:50:ALA:HB3   | 2:I:59:TYR:HB2  | 1.67                     | 0.76              |
| 2:G:20:LEU:HB2   | 2:G:81:LEU:HB3  | 1.67                     | 0.76              |
| 2:I:12:VAL:HG11  | 2:I:86:LEU:HD12 | 1.68                     | 0.75              |
| 1:D:737:HIS:HA   | 1:D:760:GLU:HB3 | 1.68                     | 0.75              |
| 1:A:566:GLY:HA2  | 1:A:569:LEU:HG  | 1.67                     | 0.75              |
| 1:A:520:GLU:HG2  | 1:A:548:VAL:HB  | 1.69                     | 0.74              |
| 1:E:632:ILE:HD12 | 1:E:658:ILE:HB  | 1.67                     | 0.74              |
| 1:B:759:ILE:HD11 | 1:B:784:LEU:HG  | 1.70                     | 0.74              |
| 1:E:604:GLU:HG2  | 1:E:625:ASN:HB2 | 1.68                     | 0.74              |
| 1:F:737:HIS:HA   | 1:F:760:GLU:HB3 | 1.68                     | 0.74              |
| 1:A:714:ALA:HA   | 1:A:737:HIS:HB2 | 1.70                     | 0.73              |
| 1:C:520:GLU:HG2  | 1:C:548:VAL:HB  | 1.70                     | 0.73              |
| 1:D:618:GLU:HG3  | 1:D:643:CYS:HB3 | 1.70                     | 0.73              |
| 1:B:473:GLU:HG2  | 1:B:497:ALA:HB3 | 1.68                     | 0.73              |
| 1:C:292:ASP:OD1  | 1:C:292:ASP:N   | 2.21                     | 0.73              |
| 1:C:580:LYS:HA   | 1:C:602:ASP:HB3 | 1.71                     | 0.73              |
| 1:F:473:GLU:HG2  | 1:F:497:ALA:HB3 | 1.71                     | 0.73              |
| 1:F:711:GLN:HA   | 1:F:733:LEU:HA  | 1.70                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:566:GLY:HA2  | 1:E:569:LEU:HG   | 1.70                     | 0.72              |
| 1:C:611:PHE:HZ   | 1:C:631:GLU:HB3  | 1.54                     | 0.72              |
| 1:E:685:ARG:HD2  | 1:E:707:LEU:HD23 | 1.71                     | 0.72              |
| 1:F:577:GLU:HA   | 1:F:600:ARG:HE   | 1.53                     | 0.72              |
| 1:C:604:GLU:HG2  | 1:C:625:ASN:HB2  | 1.71                     | 0.72              |
| 1:C:760:GLU:HA   | 1:C:785:VAL:HB   | 1.72                     | 0.72              |
| 1:C:566:GLY:HA2  | 1:C:569:LEU:HG   | 1.71                     | 0.71              |
| 1:F:454:GLU:HA   | 1:F:477:TYR:HB2  | 1.71                     | 0.71              |
| 1:D:794:LEU:O    | 1:D:799:LYS:NZ   | 2.23                     | 0.71              |
| 2:G:12:VAL:HG11  | 2:G:86:LEU:HD12  | 1.73                     | 0.71              |
| 1:F:554:ASN:ND2  | 1:F:576:ASN:O    | 2.24                     | 0.70              |
| 1:F:563:THR:HB   | 1:F:589:LYS:HD2  | 1.72                     | 0.70              |
| 1:F:794:LEU:O    | 1:F:799:LYS:NZ   | 2.23                     | 0.70              |
| 1:B:452:LYS:HA   | 1:B:475:TRP:HB2  | 1.73                     | 0.70              |
| 1:E:473:GLU:HG3  | 1:E:497:ALA:HB3  | 1.72                     | 0.70              |
| 2:I:40:ALA:HB3   | 2:I:43:LYS:HB2   | 1.73                     | 0.70              |
| 1:E:670:ASN:O    | 1:E:672:ASN:ND2  | 2.24                     | 0.70              |
| 1:B:597:GLU:HA   | 1:B:620:ASP:HB3  | 1.74                     | 0.69              |
| 1:E:45:LEU:HG    | 1:E:314:LEU:HD21 | 1.74                     | 0.69              |
| 1:E:670:ASN:ND2  | 1:E:691:ASP:OD2  | 2.26                     | 0.69              |
| 1:C:45:LEU:HG    | 1:C:314:LEU:HD21 | 1.73                     | 0.69              |
| 1:A:580:LYS:HA   | 1:A:602:ASP:HB3  | 1.75                     | 0.69              |
| 1:A:700:LEU:HB2  | 1:A:724:PRO:HG3  | 1.75                     | 0.68              |
| 1:B:526:ASN:OD1  | 1:B:554:ASN:ND2  | 2.26                     | 0.68              |
| 2:G:40:ALA:HB3   | 2:G:43:LYS:HB2   | 1.74                     | 0.68              |
| 1:C:420:LEU:HD21 | 1:C:448:LEU:HD11 | 1.75                     | 0.68              |
| 1:E:431:HIS:HA   | 1:E:452:LYS:HB2  | 1.75                     | 0.68              |
| 1:F:567:VAL:O    | 1:F:592:ASN:ND2  | 2.27                     | 0.68              |
| 1:D:605:ARG:HH22 | 1:D:628:THR:H    | 1.39                     | 0.68              |
| 1:E:644:LEU:HB3  | 1:E:667:LEU:HD13 | 1.75                     | 0.68              |
| 1:A:583:VAL:HG21 | 1:A:607:PRO:HB3  | 1.74                     | 0.68              |
| 1:B:568:HIS:HA   | 1:B:592:ASN:HD22 | 1.58                     | 0.68              |
| 2:H:12:VAL:HG11  | 2:H:86:LEU:HD12  | 1.74                     | 0.68              |
| 1:E:420:LEU:HD11 | 1:E:448:LEU:HD11 | 1.76                     | 0.68              |
| 1:D:577:GLU:HA   | 1:D:600:ARG:HE   | 1.59                     | 0.67              |
| 1:E:520:GLU:HG2  | 1:E:548:VAL:HB   | 1.76                     | 0.67              |
| 1:E:686:LYS:HA   | 1:E:709:ASN:HD22 | 1.60                     | 0.67              |
| 1:F:541:ARG:NH2  | 1:F:564:ASP:OD2  | 2.28                     | 0.67              |
| 1:C:423:ASN:ND2  | 1:C:425:GLN:OE1  | 2.27                     | 0.67              |
| 1:A:736:LEU:HD22 | 1:A:738:LEU:HD21 | 1.76                     | 0.67              |
| 1:C:670:ASN:ND2  | 1:C:691:ASP:OD2  | 2.28                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:632:ILE:O    | 1:E:635:PHE:HB2  | 1.95                     | 0.67              |
| 2:G:39:GLN:OE1   | 2:G:95:TYR:OH    | 2.13                     | 0.67              |
| 1:F:580:LYS:NZ   | 1:F:602:ASP:OD2  | 2.27                     | 0.67              |
| 1:A:644:LEU:HB3  | 1:A:667:LEU:HD13 | 1.76                     | 0.67              |
| 1:B:454:GLU:HA   | 1:B:477:TYR:HB2  | 1.77                     | 0.66              |
| 1:E:804:ARG:O    | 1:E:804:ARG:NH1  | 2.29                     | 0.66              |
| 1:C:686:LYS:HA   | 1:C:709:ASN:HD22 | 1.60                     | 0.66              |
| 1:F:645:LYS:HA   | 1:F:668:TYR:HB2  | 1.78                     | 0.66              |
| 2:G:21:SER:HA    | 2:G:80:TYR:HA    | 1.77                     | 0.66              |
| 1:C:548:VAL:HG22 | 1:C:571:LYS:HB3  | 1.77                     | 0.66              |
| 1:B:794:LEU:O    | 1:B:799:LYS:NZ   | 2.23                     | 0.66              |
| 1:E:488:LEU:HG   | 1:E:492:ARG:HE   | 1.60                     | 0.66              |
| 1:E:404:GLN:O    | 1:E:408:ASN:ND2  | 2.29                     | 0.66              |
| 1:B:246:LYS:HD3  | 1:B:249:LYS:HD3  | 1.76                     | 0.66              |
| 1:C:601:CYS:N    | 1:C:624:ASN:OD1  | 2.28                     | 0.66              |
| 1:F:246:LYS:HD2  | 1:F:249:LYS:HD3  | 1.78                     | 0.66              |
| 2:I:11:SER:HA    | 2:I:122:THR:HB   | 1.78                     | 0.65              |
| 2:H:40:ALA:HB3   | 2:H:43:LYS:HB2   | 1.79                     | 0.65              |
| 1:D:448:LEU:HD21 | 1:D:451:LEU:HD13 | 1.77                     | 0.65              |
| 1:A:488:LEU:HG   | 1:A:492:ARG:HE   | 1.62                     | 0.65              |
| 1:D:399:GLU:HA   | 1:D:402:LEU:HD23 | 1.77                     | 0.65              |
| 1:F:448:LEU:HD21 | 1:F:451:LEU:HD13 | 1.78                     | 0.65              |
| 1:E:496:ARG:NH2  | 1:E:517:THR:OG1  | 2.30                     | 0.65              |
| 1:D:567:VAL:O    | 1:D:592:ASN:ND2  | 2.30                     | 0.65              |
| 1:D:611:PHE:HZ   | 1:D:631:GLU:HB3  | 1.61                     | 0.65              |
| 1:E:233:ASP:HB3  | 1:E:236:GLU:HG3  | 1.77                     | 0.65              |
| 1:E:431:HIS:HB3  | 1:E:452:LYS:HD2  | 1.78                     | 0.65              |
| 1:F:599:ILE:HG22 | 1:F:600:ARG:HG3  | 1.78                     | 0.65              |
| 1:E:708:GLN:HE22 | 1:E:729:GLN:HE21 | 1.44                     | 0.65              |
| 2:G:20:LEU:HD12  | 2:G:81:LEU:HD23  | 1.79                     | 0.65              |
| 1:B:18:ARG:NH1   | 1:B:382:TYR:OH   | 2.30                     | 0.64              |
| 1:A:404:GLN:O    | 1:A:408:ASN:ND2  | 2.30                     | 0.64              |
| 1:B:258:ASP:O    | 1:B:262:ARG:NH1  | 2.30                     | 0.64              |
| 1:C:269:ILE:HD12 | 1:C:340:LEU:HD21 | 1.78                     | 0.64              |
| 1:C:477:TYR:HA   | 1:C:501:LYS:HG2  | 1.78                     | 0.64              |
| 1:A:234:LYS:NZ   | 1:A:410:GLU:OE1  | 2.30                     | 0.64              |
| 1:D:555:LEU:O    | 1:D:576:ASN:ND2  | 2.31                     | 0.64              |
| 1:B:616:LEU:HD21 | 1:B:619:ILE:HD13 | 1.79                     | 0.64              |
| 1:A:601:CYS:N    | 1:A:624:ASN:OD1  | 2.29                     | 0.64              |
| 1:B:632:ILE:HA   | 1:B:635:PHE:HD2  | 1.61                     | 0.64              |
| 1:C:685:ARG:O    | 1:C:709:ASN:ND2  | 2.31                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:21:SER:HA    | 2:I:80:TYR:HA    | 1.79                     | 0.64              |
| 1:A:233:ASP:HB3  | 1:A:236:GLU:HG3  | 1.79                     | 0.64              |
| 1:E:477:TYR:HA   | 1:E:501:LYS:HB3  | 1.79                     | 0.64              |
| 1:E:711:GLN:HA   | 1:E:733:LEU:HA   | 1.80                     | 0.64              |
| 1:F:615:ASN:HA   | 1:F:640:ARG:HD3  | 1.79                     | 0.64              |
| 1:E:756:LEU:HG   | 1:E:779:LEU:HD21 | 1.79                     | 0.64              |
| 1:B:555:LEU:O    | 1:B:576:ASN:ND2  | 2.31                     | 0.63              |
| 1:B:760:GLU:HA   | 1:B:785:VAL:HB   | 1.79                     | 0.63              |
| 1:F:357:ARG:NH1  | 1:F:367:ASP:OD1  | 2.32                     | 0.63              |
| 1:C:496:ARG:NH2  | 1:C:517:THR:OG1  | 2.31                     | 0.63              |
| 1:E:499:HIS:HA   | 1:E:522:HIS:HB2  | 1.79                     | 0.63              |
| 1:E:615:ASN:OD1  | 1:E:640:ARG:NH1  | 2.32                     | 0.63              |
| 1:E:633:ILE:HG12 | 1:E:657:GLN:HG3  | 1.80                     | 0.63              |
| 1:A:480:ALA:HB2  | 1:A:507:GLU:HG2  | 1.81                     | 0.63              |
| 1:E:601:CYS:N    | 1:E:624:ASN:OD1  | 2.32                     | 0.63              |
| 1:A:269:ILE:HD12 | 1:A:340:LEU:HD21 | 1.81                     | 0.63              |
| 1:C:404:GLN:O    | 1:C:408:ASN:ND2  | 2.31                     | 0.63              |
| 1:D:693:SER:O    | 1:D:695:ASN:ND2  | 2.31                     | 0.63              |
| 1:A:516:LYS:NZ   | 1:A:542:GLU:O    | 2.31                     | 0.63              |
| 1:A:760:GLU:HA   | 1:A:785:VAL:HB   | 1.79                     | 0.63              |
| 1:E:258:ASP:OD1  | 1:E:349:LYS:NZ   | 2.31                     | 0.63              |
| 1:A:552:LYS:HG3  | 1:A:575:ASN:HB3  | 1.81                     | 0.62              |
| 1:C:554:ASN:OD1  | 1:C:579:THR:OG1  | 2.16                     | 0.62              |
| 1:D:723:LEU:HD21 | 1:D:727:LEU:HD23 | 1.81                     | 0.62              |
| 1:C:620:ASP:HA   | 1:C:645:LYS:HB2  | 1.81                     | 0.62              |
| 1:C:576:ASN:HB3  | 1:C:579:THR:HB   | 1.82                     | 0.62              |
| 1:E:548:VAL:HG22 | 1:E:571:LYS:HB3  | 1.82                     | 0.62              |
| 1:D:350:LYS:HZ1  | 1:D:369:LYS:HG3  | 1.64                     | 0.62              |
| 1:D:527:LEU:HD21 | 1:D:555:LEU:HD11 | 1.82                     | 0.62              |
| 1:B:741:ASN:N    | 1:B:764:ASN:OD1  | 2.29                     | 0.62              |
| 1:E:618:GLU:OE2  | 1:E:666:ARG:NH2  | 2.33                     | 0.62              |
| 1:A:45:LEU:HG    | 1:A:314:LEU:HD21 | 1.82                     | 0.62              |
| 1:A:292:ASP:OD1  | 1:A:292:ASP:N    | 2.33                     | 0.62              |
| 1:B:718:ASN:N    | 1:B:741:ASN:OD1  | 2.32                     | 0.62              |
| 1:B:746:LEU:HD23 | 1:B:766:LEU:HD22 | 1.82                     | 0.62              |
| 1:D:143:TRP:HB3  | 1:D:263:LEU:HD22 | 1.81                     | 0.62              |
| 1:F:611:PHE:HZ   | 1:F:631:GLU:HB3  | 1.63                     | 0.62              |
| 2:I:22:CYS:HB3   | 2:I:79:VAL:HG13  | 1.82                     | 0.62              |
| 1:A:702:ALA:HA   | 1:A:726:GLU:HG3  | 1.82                     | 0.61              |
| 1:C:633:ILE:HG12 | 1:C:657:GLN:HG3  | 1.82                     | 0.61              |
| 1:A:449:GLU:HA   | 1:A:471:LEU:HA   | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:643:CYS:SG   | 1:E:666:ARG:NH1  | 2.73                     | 0.61              |
| 1:D:694:HIS:N    | 1:D:716:THR:O    | 2.20                     | 0.61              |
| 1:F:590:MET:SD   | 1:F:590:MET:N    | 2.71                     | 0.61              |
| 1:A:604:GLU:HG2  | 1:A:625:ASN:HB2  | 1.83                     | 0.61              |
| 1:E:705:GLY:O    | 1:E:708:GLN:NE2  | 2.33                     | 0.61              |
| 1:F:143:TRP:HB3  | 1:F:263:LEU:HD22 | 1.82                     | 0.61              |
| 1:C:234:LYS:NZ   | 1:C:410:GLU:OE1  | 2.33                     | 0.61              |
| 1:E:102:ASP:OD2  | 1:F:106:TYR:OH   | 2.15                     | 0.61              |
| 1:F:505:ILE:HD11 | 1:F:527:LEU:HA   | 1.82                     | 0.61              |
| 1:F:693:SER:O    | 1:F:695:ASN:ND2  | 2.33                     | 0.61              |
| 1:A:804:ARG:O    | 1:A:804:ARG:NH1  | 2.33                     | 0.61              |
| 1:F:538:ASP:HA   | 1:F:561:VAL:HG11 | 1.80                     | 0.61              |
| 1:C:341:TRP:CD1  | 1:C:345:ARG:HE   | 2.18                     | 0.61              |
| 1:D:647:TRP:H    | 1:D:647:TRP:CD1  | 2.18                     | 0.61              |
| 1:B:693:SER:O    | 1:B:695:ASN:ND2  | 2.34                     | 0.61              |
| 1:E:580:LYS:HA   | 1:E:602:ASP:HB3  | 1.82                     | 0.61              |
| 1:C:473:GLU:HG3  | 1:C:497:ALA:HB3  | 1.83                     | 0.61              |
| 1:E:265:MET:HA   | 1:E:343:MET:HE1  | 1.82                     | 0.61              |
| 1:B:705:GLY:O    | 1:B:708:GLN:NE2  | 2.33                     | 0.60              |
| 1:F:692:LEU:N    | 1:F:714:ALA:O    | 2.30                     | 0.60              |
| 1:D:711:GLN:OE1  | 1:D:734:ARG:NH1  | 2.29                     | 0.60              |
| 1:F:399:GLU:HA   | 1:F:402:LEU:HD23 | 1.82                     | 0.60              |
| 1:B:647:TRP:HA   | 1:B:672:ASN:HD21 | 1.66                     | 0.60              |
| 2:G:38:ARG:NH1   | 2:G:89:GLU:O     | 2.35                     | 0.60              |
| 1:C:153:LEU:HD21 | 1:C:260:VAL:HG21 | 1.83                     | 0.60              |
| 1:E:711:GLN:O    | 1:E:734:ARG:N    | 2.33                     | 0.60              |
| 1:A:741:ASN:N    | 1:A:764:ASN:OD1  | 2.31                     | 0.60              |
| 1:B:714:ALA:HA   | 1:B:737:HIS:HB2  | 1.84                     | 0.60              |
| 1:C:136:PHE:O    | 1:C:271:LYS:NZ   | 2.35                     | 0.60              |
| 1:A:296:THR:HG22 | 1:A:307:THR:HB   | 1.84                     | 0.59              |
| 1:D:402:LEU:O    | 1:D:406:ASN:ND2  | 2.34                     | 0.59              |
| 1:E:602:ASP:OD1  | 1:E:625:ASN:ND2  | 2.35                     | 0.59              |
| 1:B:602:ASP:N    | 1:B:624:ASN:OD1  | 2.35                     | 0.59              |
| 1:D:400:ASN:OD1  | 1:D:403:ARG:NH2  | 2.27                     | 0.59              |
| 2:G:39:GLN:HE21  | 2:G:45:ARG:HH21  | 1.49                     | 0.59              |
| 1:D:526:ASN:ND2  | 1:D:554:ASN:OD1  | 2.34                     | 0.59              |
| 1:F:550:ARG:HH12 | 1:F:552:LYS:HD2  | 1.67                     | 0.59              |
| 2:H:36:TRP:O     | 2:H:48:VAL:N     | 2.28                     | 0.59              |
| 1:A:423:ASN:ND2  | 1:A:425:GLN:OE1  | 2.36                     | 0.59              |
| 1:E:483:ILE:HG21 | 1:E:488:LEU:HD13 | 1.84                     | 0.59              |
| 1:A:102:ASP:OD2  | 1:B:106:TYR:OH   | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:505:ILE:HD11 | 1:D:527:LEU:HA   | 1.84                     | 0.59              |
| 1:F:622:LYS:NZ   | 1:F:623:ASP:OD2  | 2.35                     | 0.59              |
| 1:A:774:GLY:HA3  | 1:A:798:VAL:HG13 | 1.84                     | 0.59              |
| 1:B:711:GLN:O    | 1:B:734:ARG:N    | 2.35                     | 0.59              |
| 1:C:36:LEU:HB2   | 1:C:133:THR:HG21 | 1.84                     | 0.59              |
| 1:D:615:ASN:HA   | 1:D:640:ARG:HD3  | 1.85                     | 0.59              |
| 1:A:499:HIS:HA   | 1:A:522:HIS:HB2  | 1.85                     | 0.59              |
| 1:B:738:LEU:O    | 1:B:764:ASN:ND2  | 2.34                     | 0.59              |
| 1:C:449:GLU:HA   | 1:C:471:LEU:HA   | 1.84                     | 0.59              |
| 1:B:618:GLU:HG3  | 1:B:643:CYS:HB3  | 1.84                     | 0.59              |
| 1:D:739:GLY:O    | 1:D:741:ASN:ND2  | 2.33                     | 0.59              |
| 1:E:666:ARG:HG2  | 1:E:689:TYR:HB2  | 1.85                     | 0.59              |
| 1:A:670:ASN:ND2  | 1:A:691:ASP:OD2  | 2.35                     | 0.59              |
| 1:E:292:ASP:OD1  | 1:E:292:ASP:N    | 2.36                     | 0.59              |
| 1:F:118:LEU:HD23 | 1:F:123:LYS:HG3  | 1.84                     | 0.59              |
| 1:A:547:LYS:HD2  | 1:A:570:GLN:HG3  | 1.83                     | 0.58              |
| 1:B:732:LYS:HA   | 1:B:755:ASN:HB2  | 1.84                     | 0.58              |
| 1:B:763:GLY:N    | 1:B:787:GLU:OE2  | 2.25                     | 0.58              |
| 1:D:670:ASN:ND2  | 1:D:691:ASP:OD2  | 2.36                     | 0.58              |
| 1:D:692:LEU:N    | 1:D:714:ALA:O    | 2.34                     | 0.58              |
| 1:E:401:LYS:HG3  | 1:E:402:LEU:HD12 | 1.85                     | 0.58              |
| 1:F:555:LEU:O    | 1:F:576:ASN:ND2  | 2.36                     | 0.58              |
| 1:A:496:ARG:NH2  | 1:A:517:THR:OG1  | 2.36                     | 0.58              |
| 1:B:759:ILE:HG12 | 1:B:779:LEU:HD11 | 1.84                     | 0.58              |
| 1:E:423:ASN:ND2  | 1:E:425:GLN:OE1  | 2.36                     | 0.58              |
| 1:C:499:HIS:HA   | 1:C:522:HIS:HB2  | 1.85                     | 0.58              |
| 1:C:615:ASN:HA   | 1:C:640:ARG:HD3  | 1.85                     | 0.58              |
| 1:C:711:GLN:HB3  | 1:C:734:ARG:HG2  | 1.85                     | 0.58              |
| 1:B:607:PRO:HG2  | 1:B:610:ILE:HG13 | 1.84                     | 0.58              |
| 1:B:620:ASP:OD1  | 1:B:622:LYS:HG2  | 2.03                     | 0.58              |
| 1:C:527:LEU:HG   | 1:C:553:SER:HB3  | 1.86                     | 0.58              |
| 1:D:577:GLU:OE2  | 2:H:33:TYR:OH    | 2.20                     | 0.58              |
| 1:F:759:ILE:HD11 | 1:F:784:LEU:HG   | 1.85                     | 0.58              |
| 1:A:548:VAL:HG22 | 1:A:571:LYS:HB3  | 1.85                     | 0.58              |
| 1:B:505:ILE:HD11 | 1:B:527:LEU:HA   | 1.85                     | 0.58              |
| 1:C:265:MET:HA   | 1:C:343:MET:HE1  | 1.85                     | 0.58              |
| 1:C:647:TRP:CE3  | 1:C:668:TYR:HB2  | 2.39                     | 0.58              |
| 1:D:713:LEU:O    | 1:D:737:HIS:N    | 2.36                     | 0.58              |
| 1:E:753:LEU:HB3  | 1:E:756:LEU:HB2  | 1.85                     | 0.58              |
| 1:C:716:THR:O    | 1:C:718:ASN:ND2  | 2.36                     | 0.58              |
| 1:C:804:ARG:O    | 1:C:804:ARG:NH1  | 2.37                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:38:ARG:NH1   | 2:I:89:GLU:O     | 2.36                     | 0.58              |
| 1:C:32:SER:HA    | 1:C:35:MET:HE2   | 1.84                     | 0.58              |
| 1:E:618:GLU:HG2  | 1:E:643:CYS:HB3  | 1.85                     | 0.58              |
| 1:E:668:TYR:HB3  | 1:E:691:ASP:HB3  | 1.85                     | 0.58              |
| 2:H:21:SER:HA    | 2:H:80:TYR:HA    | 1.86                     | 0.58              |
| 1:B:621:LEU:HD12 | 1:B:646:LEU:HD21 | 1.86                     | 0.58              |
| 1:C:787:GLU:O    | 1:C:791:PHE:N    | 2.35                     | 0.58              |
| 1:D:461:ILE:HB   | 1:D:483:ILE:HG13 | 1.86                     | 0.58              |
| 1:D:554:ASN:ND2  | 1:D:576:ASN:O    | 2.37                     | 0.58              |
| 1:A:781:ARG:NH1  | 1:A:784:LEU:O    | 2.36                     | 0.57              |
| 1:C:401:LYS:HG3  | 1:C:402:LEU:HD12 | 1.85                     | 0.57              |
| 1:D:669:LEU:O    | 1:D:672:ASN:ND2  | 2.36                     | 0.57              |
| 1:A:392:VAL:HG23 | 1:A:393:PHE:HD1  | 1.69                     | 0.57              |
| 1:E:153:LEU:HD21 | 1:E:260:VAL:HG21 | 1.87                     | 0.57              |
| 1:F:525:GLY:O    | 1:F:553:SER:OG   | 2.18                     | 0.57              |
| 2:I:5:VAL:O      | 2:I:23:ALA:N     | 2.36                     | 0.57              |
| 2:I:82:GLN:NE2   | 2:I:84:ASN:OD1   | 2.36                     | 0.57              |
| 1:C:392:VAL:HG23 | 1:C:393:PHE:HD1  | 1.68                     | 0.57              |
| 1:A:349:LYS:HD2  | 1:A:370:ASN:HB3  | 1.86                     | 0.57              |
| 1:B:461:ILE:HB   | 1:B:483:ILE:HG13 | 1.87                     | 0.57              |
| 2:H:39:GLN:OE1   | 2:H:95:TYR:OH    | 2.22                     | 0.57              |
| 1:F:633:ILE:HA   | 1:F:657:GLN:HG2  | 1.86                     | 0.57              |
| 1:A:614:HIS:HB2  | 1:A:640:ARG:HH21 | 1.70                     | 0.57              |
| 1:C:450:VAL:HG22 | 1:C:473:GLU:HB2  | 1.87                     | 0.57              |
| 1:C:665:GLU:O    | 1:C:688:ARG:N    | 2.32                     | 0.57              |
| 1:D:606:ILE:HD13 | 1:D:631:GLU:HB2  | 1.86                     | 0.57              |
| 1:E:647:TRP:CE3  | 1:E:668:TYR:HB2  | 2.39                     | 0.57              |
| 1:C:741:ASN:N    | 1:C:764:ASN:OD1  | 2.33                     | 0.57              |
| 2:I:6:GLU:HA     | 2:I:22:CYS:HA    | 1.87                     | 0.57              |
| 2:H:50:ALA:O     | 2:H:59:TYR:N     | 2.33                     | 0.57              |
| 1:C:794:LEU:HD22 | 1:C:798:VAL:HG11 | 1.87                     | 0.56              |
| 1:F:647:TRP:O    | 1:F:649:ASN:ND2  | 2.38                     | 0.56              |
| 2:H:20:LEU:HB2   | 2:H:81:LEU:HB3   | 1.86                     | 0.56              |
| 1:A:648:TYR:HE1  | 1:A:671:ARG:HG3  | 1.70                     | 0.56              |
| 1:A:697:LEU:HB2  | 1:A:720:ILE:HD11 | 1.85                     | 0.56              |
| 1:B:421:THR:OG1  | 1:B:429:GLU:OE1  | 2.23                     | 0.56              |
| 1:E:547:LYS:HD2  | 1:E:570:GLN:HG3  | 1.87                     | 0.56              |
| 1:A:688:ARG:NH1  | 1:A:709:ASN:HB2  | 2.21                     | 0.56              |
| 1:B:143:TRP:HB3  | 1:B:263:LEU:HD22 | 1.87                     | 0.56              |
| 1:C:353:PHE:O    | 1:C:357:ARG:NH1  | 2.39                     | 0.56              |
| 2:H:120:GLN:OE1  | 2:H:122:THR:OG1  | 2.21                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:11:SER:HA    | 2:G:122:THR:HB   | 1.86                     | 0.56              |
| 1:C:632:ILE:O    | 1:C:635:PHE:HB2  | 2.05                     | 0.56              |
| 2:I:36:TRP:O     | 2:I:48:VAL:N     | 2.34                     | 0.56              |
| 1:E:102:ASP:OD1  | 1:E:102:ASP:N    | 2.37                     | 0.56              |
| 1:B:431:HIS:HA   | 1:B:452:LYS:HB2  | 1.88                     | 0.56              |
| 1:C:755:ASN:HA   | 1:C:778:LEU:HD12 | 1.87                     | 0.56              |
| 1:D:602:ASP:N    | 1:D:624:ASN:OD1  | 2.38                     | 0.56              |
| 1:F:351:TYR:OH   | 1:F:380:ASP:OD2  | 2.21                     | 0.56              |
| 1:F:656:ILE:HB   | 1:F:680:GLN:HG3  | 1.87                     | 0.56              |
| 2:G:91:THR:HG23  | 2:G:122:THR:HA   | 1.87                     | 0.56              |
| 1:A:734:ARG:HA   | 1:A:756:LEU:HA   | 1.88                     | 0.56              |
| 1:C:547:LYS:HD2  | 1:C:570:GLN:HG3  | 1.87                     | 0.56              |
| 2:H:82:GLN:NE2   | 2:H:84:ASN:OD1   | 2.39                     | 0.56              |
| 1:A:492:ARG:HG2  | 1:A:515:LEU:HA   | 1.88                     | 0.56              |
| 1:A:554:ASN:OD1  | 1:A:579:THR:OG1  | 2.22                     | 0.55              |
| 1:C:115:GLU:OE2  | 1:D:316:THR:OG1  | 2.24                     | 0.55              |
| 1:C:700:LEU:HB2  | 1:C:724:PRO:HG3  | 1.88                     | 0.55              |
| 1:F:461:ILE:HB   | 1:F:483:ILE:HG13 | 1.86                     | 0.55              |
| 2:H:22:CYS:HB3   | 2:H:79:VAL:HG13  | 1.86                     | 0.55              |
| 1:D:473:GLU:HG2  | 1:D:497:ALA:HB3  | 1.88                     | 0.55              |
| 1:A:483:ILE:HG21 | 1:A:488:LEU:HD13 | 1.88                     | 0.55              |
| 1:B:452:LYS:HG2  | 1:B:475:TRP:CG   | 2.42                     | 0.55              |
| 1:B:633:ILE:HA   | 1:B:657:GLN:HG2  | 1.89                     | 0.55              |
| 1:C:585:ASN:O    | 1:C:589:LYS:NZ   | 2.39                     | 0.55              |
| 1:E:755:ASN:HA   | 1:E:778:LEU:HD12 | 1.89                     | 0.55              |
| 1:F:603:LEU:O    | 1:F:604:GLU:HG3  | 2.07                     | 0.55              |
| 1:C:693:SER:HA   | 1:C:718:ASN:HD21 | 1.71                     | 0.55              |
| 1:E:443:PHE:HA   | 1:E:468:LEU:HD21 | 1.88                     | 0.55              |
| 1:F:622:LYS:HD3  | 1:F:647:TRP:HD1  | 1.71                     | 0.55              |
| 1:A:555:LEU:HD21 | 1:A:558:LEU:HA   | 1.87                     | 0.55              |
| 1:B:351:TYR:OH   | 1:B:380:ASP:OD2  | 2.16                     | 0.55              |
| 1:C:412:THR:OG1  | 1:C:414:ASP:OD1  | 2.21                     | 0.55              |
| 1:C:632:ILE:HD11 | 1:C:655:PRO:HB2  | 1.88                     | 0.55              |
| 1:D:357:ARG:NH2  | 1:D:363:SER:O    | 2.40                     | 0.55              |
| 1:E:685:ARG:O    | 1:E:709:ASN:ND2  | 2.40                     | 0.55              |
| 1:E:709:ASN:HA   | 1:E:732:LYS:HE2  | 1.88                     | 0.55              |
| 2:G:50:ALA:O     | 2:G:59:TYR:N     | 2.35                     | 0.55              |
| 1:D:522:HIS:HA   | 1:D:550:ARG:HB3  | 1.88                     | 0.55              |
| 1:E:32:SER:HA    | 1:E:35:MET:HE2   | 1.89                     | 0.55              |
| 1:A:419:ARG:NH2  | 1:A:431:HIS:HB3  | 2.22                     | 0.55              |
| 1:A:693:SER:HA   | 1:A:718:ASN:HD21 | 1.72                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:345:ARG:HG3  | 1:D:346:ARG:HE   | 1.72                     | 0.55              |
| 1:D:700:LEU:HD21 | 1:D:704:ILE:HG21 | 1.88                     | 0.55              |
| 1:E:46:GLN:HB2   | 1:E:318:PHE:HZ   | 1.71                     | 0.55              |
| 2:H:91:THR:HG23  | 2:H:122:THR:HA   | 1.89                     | 0.55              |
| 1:D:512:ILE:HA   | 1:D:515:LEU:HD23 | 1.89                     | 0.55              |
| 1:D:605:ARG:NH1  | 1:D:628:THR:OG1  | 2.38                     | 0.54              |
| 1:A:102:ASP:N    | 1:A:102:ASP:OD1  | 2.38                     | 0.54              |
| 1:B:345:ARG:O    | 1:B:346:ARG:NE   | 2.38                     | 0.54              |
| 1:C:39:ALA:HB2   | 1:C:129:VAL:HG12 | 1.89                     | 0.54              |
| 1:C:565:VAL:HG13 | 1:C:569:LEU:HD11 | 1.88                     | 0.54              |
| 1:E:171:ARG:NH2  | 1:E:230:GLY:O    | 2.40                     | 0.54              |
| 1:E:642:THR:O    | 1:E:665:GLU:N    | 2.32                     | 0.54              |
| 1:D:607:PRO:HG2  | 1:D:610:ILE:HG13 | 1.88                     | 0.54              |
| 1:D:723:LEU:HD12 | 1:D:724:PRO:HD2  | 1.89                     | 0.54              |
| 1:E:429:GLU:HB3  | 1:E:450:VAL:HB   | 1.90                     | 0.54              |
| 1:E:484:GLU:O    | 1:E:488:LEU:N    | 2.32                     | 0.54              |
| 1:E:577:GLU:OE1  | 1:F:492:ARG:NH2  | 2.38                     | 0.54              |
| 2:G:38:ARG:NE    | 2:G:46:GLU:OE1   | 2.40                     | 0.54              |
| 1:D:616:LEU:HD21 | 1:D:619:ILE:HB   | 1.88                     | 0.54              |
| 1:E:505:ILE:HG23 | 1:E:536:VAL:HG11 | 1.90                     | 0.54              |
| 1:E:576:ASN:HB3  | 1:E:579:THR:HB   | 1.89                     | 0.54              |
| 2:I:32:GLU:HG3   | 2:I:33:TYR:HD1   | 1.73                     | 0.54              |
| 1:A:678:PRO:HG2  | 1:A:681:LEU:HB2  | 1.88                     | 0.54              |
| 1:B:591:VAL:O    | 1:B:615:ASN:ND2  | 2.39                     | 0.54              |
| 1:B:711:GLN:OE1  | 1:B:734:ARG:NE   | 2.40                     | 0.54              |
| 1:C:103:ARG:HH22 | 1:D:103:ARG:HE   | 1.55                     | 0.54              |
| 1:D:414:ASP:OD1  | 1:D:418:GLN:NE2  | 2.41                     | 0.54              |
| 1:E:450:VAL:HG22 | 1:E:473:GLU:HB2  | 1.88                     | 0.54              |
| 1:F:597:GLU:OE2  | 1:F:645:LYS:NZ   | 2.38                     | 0.54              |
| 1:B:566:GLY:HA2  | 1:B:569:LEU:HB2  | 1.89                     | 0.54              |
| 1:C:714:ALA:HA   | 1:C:737:HIS:HB2  | 1.89                     | 0.54              |
| 1:A:473:GLU:HB3  | 1:A:497:ALA:HB3  | 1.90                     | 0.54              |
| 1:A:648:TYR:CE1  | 1:A:671:ARG:HG3  | 2.43                     | 0.54              |
| 1:D:454:GLU:HA   | 1:D:477:TYR:HB2  | 1.90                     | 0.54              |
| 1:E:779:LEU:HB3  | 1:E:784:LEU:HD21 | 1.90                     | 0.54              |
| 1:F:547:LYS:NZ   | 1:F:568:HIS:O    | 2.32                     | 0.54              |
| 2:H:33:TYR:HE2   | 2:H:104:THR:HA   | 1.73                     | 0.54              |
| 1:A:721:GLU:OE1  | 1:A:744:GLN:NE2  | 2.41                     | 0.54              |
| 1:B:554:ASN:ND2  | 1:B:577:GLU:OE2  | 2.41                     | 0.54              |
| 1:F:154:GLU:O    | 1:F:158:SER:OG   | 2.26                     | 0.54              |
| 1:C:411:TRP:HA   | 1:C:415:LYS:HD3  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:454:GLU:OE1  | 1:C:454:GLU:N    | 2.41                     | 0.53              |
| 2:I:50:ALA:O     | 2:I:59:TYR:N     | 2.38                     | 0.53              |
| 1:C:781:ARG:NH1  | 1:C:784:LEU:O    | 2.41                     | 0.53              |
| 1:D:759:ILE:HD11 | 1:D:784:LEU:HG   | 1.91                     | 0.53              |
| 1:A:353:PHE:O    | 1:A:357:ARG:NH1  | 2.40                     | 0.53              |
| 1:B:117:ARG:HG3  | 1:B:295:CYS:HA   | 1.91                     | 0.53              |
| 1:C:611:PHE:CZ   | 1:C:631:GLU:HB3  | 2.40                     | 0.53              |
| 1:B:541:ARG:NH1  | 1:B:564:ASP:OD2  | 2.41                     | 0.53              |
| 1:A:401:LYS:HG3  | 1:A:402:LEU:HD12 | 1.90                     | 0.53              |
| 1:A:723:LEU:HD12 | 1:A:724:PRO:HD2  | 1.90                     | 0.53              |
| 1:B:529:ALA:H    | 1:B:533:ARG:HB3  | 1.74                     | 0.53              |
| 2:G:22:CYS:N     | 2:G:79:VAL:O     | 2.41                     | 0.53              |
| 1:A:622:LYS:HD2  | 1:A:647:TRP:HE1  | 1.73                     | 0.53              |
| 1:C:549:LEU:HB3  | 1:C:572:LEU:HD12 | 1.91                     | 0.53              |
| 1:C:668:TYR:HB3  | 1:C:691:ASP:HB3  | 1.90                     | 0.53              |
| 1:E:244:PHE:CE1  | 1:E:399:GLU:HB2  | 2.44                     | 0.53              |
| 1:E:449:GLU:HA   | 1:E:471:LEU:HA   | 1.89                     | 0.53              |
| 1:F:606:ILE:HD12 | 1:F:631:GLU:HB2  | 1.90                     | 0.53              |
| 2:H:69:THR:OG1   | 2:H:82:GLN:OE1   | 2.20                     | 0.53              |
| 1:A:255:GLU:OE2  | 1:A:369:LYS:N    | 2.34                     | 0.53              |
| 1:B:766:LEU:HD23 | 1:B:790:LEU:HD13 | 1.91                     | 0.53              |
| 1:E:715:VAL:O    | 1:E:718:ASN:ND2  | 2.42                     | 0.53              |
| 1:C:644:LEU:HB3  | 1:C:667:LEU:HD13 | 1.91                     | 0.52              |
| 1:E:36:LEU:HB2   | 1:E:133:THR:HG21 | 1.92                     | 0.52              |
| 2:H:39:GLN:HE21  | 2:H:45:ARG:HH21  | 1.58                     | 0.52              |
| 1:E:355:SER:O    | 1:E:359:GLU:HG3  | 2.09                     | 0.52              |
| 1:E:423:ASN:HB3  | 1:E:429:GLU:HG2  | 1.92                     | 0.52              |
| 1:E:638:LEU:HD23 | 1:E:641:LEU:HD22 | 1.91                     | 0.52              |
| 1:C:478:HIS:CE1  | 1:C:503:THR:HG23 | 2.45                     | 0.52              |
| 1:E:662:THR:HA   | 1:E:684:CYS:HA   | 1.91                     | 0.52              |
| 1:E:788:GLU:HA   | 1:E:791:PHE:HB3  | 1.91                     | 0.52              |
| 1:F:146:PHE:HD2  | 1:F:263:LEU:HD11 | 1.74                     | 0.52              |
| 1:F:365:ILE:HG12 | 1:F:395:SER:HA   | 1.92                     | 0.52              |
| 2:I:89:GLU:OE1   | 2:I:89:GLU:N     | 2.42                     | 0.52              |
| 1:D:117:ARG:HG3  | 1:D:295:CYS:HA   | 1.90                     | 0.52              |
| 1:E:492:ARG:HG2  | 1:E:515:LEU:HA   | 1.91                     | 0.52              |
| 1:E:583:VAL:HG23 | 1:E:584:LEU:H    | 1.75                     | 0.52              |
| 1:A:32:SER:HA    | 1:A:35:MET:HE2   | 1.91                     | 0.52              |
| 1:B:399:GLU:OE1  | 1:B:399:GLU:N    | 2.39                     | 0.52              |
| 1:C:682:PHE:CD2  | 1:C:703:ASP:HB3  | 2.45                     | 0.52              |
| 1:E:425:GLN:HB2  | 1:E:427:LYS:HE2  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:22:CYS:HB3   | 2:G:79:VAL:HG13  | 1.90                     | 0.52              |
| 1:C:583:VAL:HG23 | 1:C:584:LEU:H    | 1.75                     | 0.52              |
| 1:C:709:ASN:HA   | 1:C:732:LYS:HE3  | 1.91                     | 0.52              |
| 1:C:723:LEU:HD12 | 1:C:724:PRO:HD2  | 1.91                     | 0.52              |
| 1:E:615:ASN:HA   | 1:E:640:ARG:HD2  | 1.91                     | 0.52              |
| 1:E:723:LEU:HD12 | 1:E:724:PRO:HD2  | 1.92                     | 0.52              |
| 1:B:723:LEU:HD23 | 1:B:747:PRO:HD2  | 1.91                     | 0.52              |
| 1:D:656:ILE:HB   | 1:D:680:GLN:HG3  | 1.90                     | 0.52              |
| 1:E:740:ASN:N    | 1:E:762:ARG:O    | 2.37                     | 0.52              |
| 2:H:39:GLN:N     | 2:H:93:LEU:O     | 2.43                     | 0.52              |
| 1:B:803:TRP:O    | 1:B:807:LYS:HG2  | 2.10                     | 0.52              |
| 1:E:714:ALA:HA   | 1:E:737:HIS:HB2  | 1.91                     | 0.52              |
| 1:F:739:GLY:O    | 1:F:741:ASN:ND2  | 2.37                     | 0.52              |
| 1:A:342:TRP:HA   | 1:A:345:ARG:HE   | 1.74                     | 0.52              |
| 1:D:781:ARG:HB2  | 1:D:802:LEU:HB3  | 1.92                     | 0.52              |
| 1:A:52:MET:HG2   | 1:A:310:CYS:HB3  | 1.92                     | 0.51              |
| 1:A:643:CYS:SG   | 1:A:644:LEU:N    | 2.83                     | 0.51              |
| 1:A:691:ASP:HA   | 1:A:714:ALA:HB3  | 1.91                     | 0.51              |
| 1:D:687:LEU:HD21 | 1:D:690:LEU:HD13 | 1.92                     | 0.51              |
| 1:F:452:LYS:HA   | 1:F:475:TRP:HB2  | 1.91                     | 0.51              |
| 1:E:132:HIS:CD2  | 1:E:278:ILE:HG13 | 2.45                     | 0.51              |
| 1:E:632:ILE:HD11 | 1:E:655:PRO:HB2  | 1.90                     | 0.51              |
| 1:A:527:LEU:HG   | 1:A:553:SER:HB3  | 1.91                     | 0.51              |
| 1:F:803:TRP:O    | 1:F:807:LYS:HG2  | 2.10                     | 0.51              |
| 1:C:626:LEU:HB3  | 1:C:651:ILE:HD11 | 1.93                     | 0.51              |
| 1:E:24:TRP:CD1   | 1:E:339:THR:HG1  | 2.28                     | 0.51              |
| 1:E:741:ASN:N    | 1:E:764:ASN:OD1  | 2.41                     | 0.51              |
| 1:A:404:GLN:OE1  | 1:A:408:ASN:ND2  | 2.44                     | 0.51              |
| 1:C:24:TRP:CD1   | 1:C:339:THR:HG1  | 2.27                     | 0.51              |
| 1:C:168:TRP:CE2  | 1:C:244:PHE:HZ   | 2.28                     | 0.51              |
| 1:C:352:SER:HB3  | 1:C:354:GLU:HG2  | 1.91                     | 0.51              |
| 1:C:420:LEU:HD11 | 1:C:448:LEU:HD21 | 1.92                     | 0.51              |
| 1:D:647:TRP:H    | 1:D:647:TRP:HD1  | 1.59                     | 0.51              |
| 1:E:527:LEU:HG   | 1:E:553:SER:HB3  | 1.92                     | 0.51              |
| 2:G:89:GLU:N     | 2:G:89:GLU:OE1   | 2.38                     | 0.51              |
| 2:H:32:GLU:HB2   | 2:H:101:GLU:HG2  | 1.91                     | 0.51              |
| 1:B:604:GLU:HG3  | 1:B:625:ASN:HB2  | 1.93                     | 0.51              |
| 1:D:49:GLN:N     | 1:D:49:GLN:OE1   | 2.44                     | 0.51              |
| 1:D:520:GLU:HB3  | 1:D:548:VAL:HB   | 1.93                     | 0.51              |
| 1:D:645:LYS:HA   | 1:D:668:TYR:HB2  | 1.92                     | 0.51              |
| 1:E:736:LEU:HD22 | 1:E:738:LEU:HD21 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:787:GLU:O    | 1:E:791:PHE:N    | 2.41                     | 0.51              |
| 1:B:725:PRO:HB3  | 1:B:749:ARG:HD3  | 1.92                     | 0.51              |
| 1:D:408:ASN:ND2  | 1:D:440:ASP:OD2  | 2.44                     | 0.51              |
| 1:E:492:ARG:HA   | 1:E:515:LEU:HG   | 1.92                     | 0.51              |
| 1:E:565:VAL:HG13 | 1:E:569:LEU:HD11 | 1.93                     | 0.51              |
| 1:E:685:ARG:HH21 | 1:E:706:LEU:HB3  | 1.76                     | 0.51              |
| 1:F:369:LYS:NZ   | 1:F:370:ASN:OD1  | 2.42                     | 0.51              |
| 1:F:688:ARG:HB3  | 1:F:711:GLN:HE22 | 1.75                     | 0.51              |
| 1:A:665:GLU:O    | 1:A:688:ARG:N    | 2.22                     | 0.51              |
| 1:A:459:VAL:HG23 | 1:A:481:ALA:HA   | 1.93                     | 0.51              |
| 2:I:90:ASP:OD1   | 2:I:90:ASP:N     | 2.43                     | 0.51              |
| 1:B:550:ARG:NH2  | 1:B:575:ASN:OD1  | 2.44                     | 0.50              |
| 1:B:736:LEU:O    | 1:B:760:GLU:N    | 2.43                     | 0.50              |
| 1:F:558:LEU:HD13 | 1:F:581:LEU:HD21 | 1.93                     | 0.50              |
| 1:A:711:GLN:HB3  | 1:A:734:ARG:HE   | 1.76                     | 0.50              |
| 1:B:148:ARG:HD2  | 1:B:259:ILE:HG12 | 1.93                     | 0.50              |
| 1:B:160:LEU:HD21 | 1:B:379:ILE:HG21 | 1.92                     | 0.50              |
| 1:C:505:ILE:O    | 1:C:508:ILE:HG22 | 2.12                     | 0.50              |
| 1:D:472:LYS:O    | 1:D:497:ALA:N    | 2.36                     | 0.50              |
| 1:A:39:ALA:HB2   | 1:A:129:VAL:HG12 | 1.92                     | 0.50              |
| 1:C:682:PHE:HA   | 1:C:707:LEU:HD11 | 1.93                     | 0.50              |
| 1:E:700:LEU:HD21 | 1:E:704:ILE:HG21 | 1.92                     | 0.50              |
| 2:I:47:GLY:HA3   | 2:I:107:LEU:HB3  | 1.94                     | 0.50              |
| 1:B:735:ALA:HA   | 1:B:758:GLN:O    | 2.11                     | 0.50              |
| 1:C:433:PHE:HA   | 1:C:454:GLU:HG2  | 1.93                     | 0.50              |
| 1:C:740:ASN:N    | 1:C:762:ARG:O    | 2.40                     | 0.50              |
| 1:E:435:LEU:HB2  | 1:E:456:ILE:HD12 | 1.93                     | 0.50              |
| 1:F:541:ARG:HH22 | 1:F:561:VAL:HA   | 1.77                     | 0.50              |
| 2:I:38:ARG:NE    | 2:I:46:GLU:OE1   | 2.43                     | 0.50              |
| 1:A:632:ILE:O    | 1:A:635:PHE:HB2  | 2.11                     | 0.50              |
| 1:A:687:LEU:O    | 1:A:688:ARG:NH1  | 2.43                     | 0.50              |
| 1:C:635:PHE:HB3  | 1:C:661:LEU:HD21 | 1.93                     | 0.50              |
| 1:D:146:PHE:HD2  | 1:D:263:LEU:HD11 | 1.76                     | 0.50              |
| 1:F:632:ILE:HG23 | 1:F:657:GLN:HB3  | 1.94                     | 0.50              |
| 1:A:777:PRO:HB2  | 1:A:778:LEU:HD12 | 1.93                     | 0.50              |
| 1:C:410:GLU:OE2  | 1:C:415:LYS:NZ   | 2.44                     | 0.50              |
| 1:D:803:TRP:O    | 1:D:807:LYS:HG2  | 2.12                     | 0.50              |
| 1:E:700:LEU:HB3  | 1:E:724:PRO:HG3  | 1.93                     | 0.50              |
| 1:A:168:TRP:CE2  | 1:A:244:PHE:HZ   | 2.30                     | 0.50              |
| 1:A:505:ILE:HG23 | 1:A:536:VAL:HG11 | 1.93                     | 0.50              |
| 1:C:679:THR:HA   | 1:C:682:PHE:HD2  | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:541:ARG:H    | 1:F:541:ARG:HD2  | 1.76                     | 0.50              |
| 2:I:20:LEU:HB2   | 2:I:81:LEU:HB3   | 1.94                     | 0.50              |
| 2:I:39:GLN:N     | 2:I:93:LEU:O     | 2.44                     | 0.50              |
| 1:B:777:PRO:HB2  | 1:B:778:LEU:HD12 | 1.93                     | 0.50              |
| 2:I:62:ASP:HA    | 2:I:65:LYS:HD2   | 1.94                     | 0.50              |
| 1:C:154:GLU:HA   | 1:C:157:VAL:HG12 | 1.94                     | 0.50              |
| 1:D:274:LYS:HD2  | 1:D:277:LEU:HD21 | 1.94                     | 0.50              |
| 1:D:633:ILE:HA   | 1:D:657:GLN:HG2  | 1.93                     | 0.50              |
| 1:F:117:ARG:HG3  | 1:F:295:CYS:HA   | 1.94                     | 0.50              |
| 1:F:529:ALA:H    | 1:F:533:ARG:HB3  | 1.77                     | 0.50              |
| 2:G:6:GLU:HB3    | 2:G:22:CYS:HB2   | 1.93                     | 0.50              |
| 2:G:19:ARG:HH11  | 2:G:82:GLN:HG3   | 1.77                     | 0.50              |
| 1:A:516:LYS:HZ1  | 1:A:544:LYS:HG2  | 1.77                     | 0.49              |
| 1:A:716:THR:O    | 1:A:718:ASN:ND2  | 2.45                     | 0.49              |
| 1:C:119:HIS:CD2  | 1:C:288:ASN:HD22 | 2.30                     | 0.49              |
| 1:D:433:PHE:HA   | 1:D:454:GLU:HB3  | 1.93                     | 0.49              |
| 1:D:647:TRP:CD1  | 1:D:647:TRP:N    | 2.79                     | 0.49              |
| 2:H:53:THR:HG22  | 2:H:54:TRP:HE3   | 1.77                     | 0.49              |
| 1:A:392:VAL:HG23 | 1:A:393:PHE:CD1  | 2.47                     | 0.49              |
| 1:A:740:ASN:N    | 1:A:762:ARG:O    | 2.42                     | 0.49              |
| 1:B:632:ILE:HG23 | 1:B:657:GLN:HB3  | 1.94                     | 0.49              |
| 1:A:688:ARG:HD2  | 1:A:711:GLN:HE22 | 1.78                     | 0.49              |
| 1:A:746:LEU:HD12 | 1:A:747:PRO:HD2  | 1.94                     | 0.49              |
| 1:C:154:GLU:OE2  | 1:D:382:TYR:OH   | 2.29                     | 0.49              |
| 1:D:399:GLU:OE1  | 1:D:399:GLU:N    | 2.44                     | 0.49              |
| 1:D:602:ASP:HA   | 1:D:624:ASN:HA   | 1.95                     | 0.49              |
| 1:E:766:LEU:HD21 | 1:E:769:LEU:HB3  | 1.93                     | 0.49              |
| 1:F:357:ARG:HB3  | 1:F:365:ILE:HB   | 1.94                     | 0.49              |
| 1:F:519:GLU:HA   | 1:F:546:LEU:HA   | 1.93                     | 0.49              |
| 1:F:738:LEU:O    | 1:F:764:ASN:ND2  | 2.45                     | 0.49              |
| 1:B:623:ASP:N    | 1:B:623:ASP:OD1  | 2.46                     | 0.49              |
| 1:C:631:GLU:OE1  | 1:C:631:GLU:N    | 2.43                     | 0.49              |
| 1:D:716:THR:HA   | 1:D:739:GLY:O    | 2.11                     | 0.49              |
| 1:E:39:ALA:HB2   | 1:E:129:VAL:HG12 | 1.95                     | 0.49              |
| 2:G:6:GLU:OE2    | 2:G:118:GLY:N    | 2.30                     | 0.49              |
| 1:B:510:LEU:HD23 | 1:B:510:LEU:H    | 1.76                     | 0.49              |
| 1:E:746:LEU:HD21 | 1:E:750:VAL:HG11 | 1.95                     | 0.49              |
| 1:A:488:LEU:HG   | 1:A:492:ARG:NE   | 2.25                     | 0.49              |
| 1:D:622:LYS:HD2  | 1:D:648:TYR:HB2  | 1.93                     | 0.49              |
| 1:E:505:ILE:O    | 1:E:508:ILE:HG22 | 2.12                     | 0.49              |
| 2:I:22:CYS:N     | 2:I:79:VAL:O     | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:259:ILE:HD12 | 1:A:262:ARG:HD3  | 1.93                     | 0.49              |
| 1:C:243:LEU:HA   | 1:C:246:LYS:HG2  | 1.95                     | 0.49              |
| 1:D:510:LEU:HD23 | 1:D:510:LEU:H    | 1.78                     | 0.49              |
| 1:F:700:LEU:HB3  | 1:F:704:ILE:HD13 | 1.94                     | 0.49              |
| 1:E:488:LEU:HG   | 1:E:492:ARG:NE   | 2.26                     | 0.49              |
| 1:F:771:VAL:HG23 | 1:F:795:PRO:HG2  | 1.95                     | 0.49              |
| 2:I:6:GLU:OE2    | 2:I:117:GLN:N    | 2.46                     | 0.49              |
| 1:B:443:PHE:HA   | 1:B:468:LEU:HD21 | 1.95                     | 0.49              |
| 1:E:370:ASN:OD1  | 1:E:370:ASN:N    | 2.46                     | 0.49              |
| 1:F:255:GLU:O    | 1:F:369:LYS:NZ   | 2.42                     | 0.49              |
| 1:F:534:TYR:HE2  | 1:F:559:PRO:HG3  | 1.78                     | 0.49              |
| 2:G:39:GLN:N     | 2:G:93:LEU:O     | 2.46                     | 0.49              |
| 1:C:632:ILE:HD12 | 1:C:658:ILE:HB   | 1.95                     | 0.48              |
| 1:E:354:GLU:HA   | 1:E:357:ARG:NH1  | 2.29                     | 0.48              |
| 1:D:534:TYR:HE1  | 1:D:555:LEU:HD13 | 1.78                     | 0.48              |
| 1:E:620:ASP:HA   | 1:E:645:LYS:HB2  | 1.95                     | 0.48              |
| 1:F:357:ARG:HD2  | 1:F:363:SER:O    | 2.13                     | 0.48              |
| 1:C:341:TRP:CG   | 1:C:345:ARG:HH21 | 2.31                     | 0.48              |
| 1:C:746:LEU:HD12 | 1:C:747:PRO:HD2  | 1.95                     | 0.48              |
| 1:D:117:ARG:NH1  | 1:D:296:THR:O    | 2.46                     | 0.48              |
| 1:D:234:LYS:HE3  | 1:D:410:GLU:HA   | 1.95                     | 0.48              |
| 1:E:709:ASN:O    | 1:E:711:GLN:NE2  | 2.47                     | 0.48              |
| 1:B:146:PHE:HD1  | 1:B:147:PRO:HD2  | 1.78                     | 0.48              |
| 1:C:520:GLU:HA   | 1:C:548:VAL:O    | 2.14                     | 0.48              |
| 1:D:527:LEU:HG   | 1:D:555:LEU:HD21 | 1.94                     | 0.48              |
| 1:F:472:LYS:HD2  | 1:F:496:ARG:HG2  | 1.94                     | 0.48              |
| 1:A:555:LEU:HD21 | 1:A:559:PRO:HD3  | 1.95                     | 0.48              |
| 1:E:398:SER:HA   | 1:E:401:LYS:HG2  | 1.94                     | 0.48              |
| 1:E:583:VAL:HG21 | 1:E:607:PRO:HB3  | 1.96                     | 0.48              |
| 1:E:626:LEU:HB3  | 1:E:651:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:781:ARG:HB2  | 1:B:802:LEU:HB3  | 1.95                     | 0.48              |
| 1:E:452:LYS:HE3  | 1:E:475:TRP:HZ3  | 1.78                     | 0.48              |
| 1:F:510:LEU:H    | 1:F:510:LEU:HD23 | 1.78                     | 0.48              |
| 1:D:452:LYS:HA   | 1:D:475:TRP:HB2  | 1.95                     | 0.48              |
| 1:F:616:LEU:HD21 | 1:F:619:ILE:HB   | 1.94                     | 0.48              |
| 2:I:91:THR:HG23  | 2:I:122:THR:HA   | 1.95                     | 0.48              |
| 1:A:158:SER:O    | 1:A:161:LEU:HG   | 2.14                     | 0.48              |
| 1:C:158:SER:O    | 1:C:161:LEU:HG   | 2.13                     | 0.48              |
| 1:C:478:HIS:CD2  | 1:C:501:LYS:HZ3  | 2.31                     | 0.48              |
| 1:D:293:VAL:HG13 | 1:D:310:CYS:HB2  | 1.96                     | 0.48              |
| 1:D:616:LEU:HB3  | 1:D:638:LEU:HD21 | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:433:PHE:HA   | 1:E:454:GLU:HG2  | 1.95                     | 0.48              |
| 1:F:428:LEU:HB2  | 1:F:449:GLU:HG3  | 1.96                     | 0.48              |
| 2:H:90:ASP:N     | 2:H:90:ASP:OD1   | 2.46                     | 0.48              |
| 1:A:129:VAL:HG13 | 1:A:325:TYR:CE1  | 2.49                     | 0.48              |
| 1:B:602:ASP:HA   | 1:B:624:ASN:HA   | 1.95                     | 0.48              |
| 1:C:129:VAL:HG13 | 1:C:325:TYR:CE1  | 2.49                     | 0.48              |
| 1:C:769:LEU:HD11 | 1:C:790:LEU:HG   | 1.96                     | 0.48              |
| 1:C:788:GLU:HA   | 1:C:791:PHE:HB3  | 1.94                     | 0.48              |
| 1:E:408:ASN:OD1  | 1:E:440:ASP:N    | 2.45                     | 0.48              |
| 1:E:552:LYS:HD3  | 1:E:575:ASN:HB3  | 1.95                     | 0.48              |
| 1:A:737:HIS:HA   | 1:A:760:GLU:CD   | 2.39                     | 0.48              |
| 1:D:423:ASN:HD21 | 1:D:425:GLN:HB2  | 1.77                     | 0.48              |
| 1:E:154:GLU:OE2  | 1:F:382:TYR:OH   | 2.29                     | 0.48              |
| 1:F:682:PHE:CD2  | 1:F:703:ASP:HB2  | 2.48                     | 0.48              |
| 1:B:122:ALA:HB2  | 1:B:289:ILE:HG22 | 1.96                     | 0.47              |
| 1:B:167:PRO:O    | 1:B:170:THR:OG1  | 2.30                     | 0.47              |
| 1:B:550:ARG:NH1  | 1:B:552:LYS:HB2  | 2.29                     | 0.47              |
| 1:C:751:GLY:HA3  | 1:C:772:GLU:HB3  | 1.95                     | 0.47              |
| 1:E:364:ASP:OD1  | 1:E:364:ASP:N    | 2.34                     | 0.47              |
| 2:G:36:TRP:O     | 2:G:48:VAL:N     | 2.36                     | 0.47              |
| 2:I:12:VAL:HG22  | 2:I:16:GLY:HA3   | 1.96                     | 0.47              |
| 1:A:154:GLU:HA   | 1:A:157:VAL:HG12 | 1.95                     | 0.47              |
| 1:F:235:LYS:NZ   | 1:F:239:GLN:OE1  | 2.47                     | 0.47              |
| 1:A:289:ILE:O    | 1:A:319:LYS:NZ   | 2.43                     | 0.47              |
| 1:A:443:PHE:HA   | 1:A:468:LEU:HD21 | 1.96                     | 0.47              |
| 1:B:142:PHE:HB3  | 1:B:267:GLN:OE1  | 2.14                     | 0.47              |
| 1:B:420:LEU:HD23 | 1:B:430:LEU:HB2  | 1.95                     | 0.47              |
| 1:C:46:GLN:HB2   | 1:C:318:PHE:HZ   | 1.78                     | 0.47              |
| 1:C:289:ILE:O    | 1:C:319:LYS:NZ   | 2.47                     | 0.47              |
| 1:E:718:ASN:N    | 1:E:741:ASN:OD1  | 2.44                     | 0.47              |
| 1:F:419:ARG:NH1  | 1:F:431:HIS:O    | 2.36                     | 0.47              |
| 2:H:36:TRP:NE1   | 2:H:81:LEU:HB2   | 2.29                     | 0.47              |
| 1:A:700:LEU:HD12 | 1:A:724:PRO:HD2  | 1.97                     | 0.47              |
| 1:D:634:SER:O    | 1:D:637:HIS:ND1  | 2.42                     | 0.47              |
| 1:E:688:ARG:HA   | 1:E:710:LEU:HA   | 1.97                     | 0.47              |
| 1:A:136:PHE:CE1  | 1:A:274:LYS:HG2  | 2.50                     | 0.47              |
| 1:A:354:GLU:HA   | 1:A:357:ARG:HH11 | 1.78                     | 0.47              |
| 1:A:463:PRO:HB3  | 1:A:486:PRO:HB2  | 1.96                     | 0.47              |
| 1:B:618:GLU:OE2  | 1:B:642:THR:OG1  | 2.32                     | 0.47              |
| 1:C:370:ASN:OD1  | 1:C:370:ASN:N    | 2.48                     | 0.47              |
| 1:C:774:GLY:HA3  | 1:C:798:VAL:HG13 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:568:HIS:HA   | 1:D:592:ASN:HD22 | 1.79                     | 0.47              |
| 1:D:729:GLN:HA   | 1:D:731:ARG:HE   | 1.80                     | 0.47              |
| 1:A:56:PRO:HG2   | 1:A:99:TYR:CD2   | 2.49                     | 0.47              |
| 1:B:46:GLN:HB2   | 1:B:318:PHE:HZ   | 1.78                     | 0.47              |
| 1:D:635:PHE:HB3  | 1:D:661:LEU:HD21 | 1.97                     | 0.47              |
| 1:F:45:LEU:HD21  | 1:F:317:LEU:HD23 | 1.96                     | 0.47              |
| 1:F:537:ILE:HG22 | 1:F:540:LEU:HG   | 1.96                     | 0.47              |
| 1:B:258:ASP:OD1  | 1:B:349:LYS:HE2  | 2.15                     | 0.47              |
| 1:C:505:ILE:HG23 | 1:C:536:VAL:HG11 | 1.96                     | 0.47              |
| 1:D:443:PHE:HA   | 1:D:468:LEU:HD21 | 1.95                     | 0.47              |
| 1:D:552:LYS:HG3  | 1:D:575:ASN:HB3  | 1.96                     | 0.47              |
| 1:E:119:HIS:CD2  | 1:E:288:ASN:HD22 | 2.31                     | 0.47              |
| 1:E:269:ILE:HD12 | 1:E:340:LEU:HD21 | 1.96                     | 0.47              |
| 1:E:659:GLY:HA3  | 1:E:680:GLN:O    | 2.14                     | 0.47              |
| 1:E:693:SER:HA   | 1:E:718:ASN:HD21 | 1.79                     | 0.47              |
| 2:H:12:VAL:HG12  | 2:H:123:VAL:HG22 | 1.96                     | 0.47              |
| 2:H:22:CYS:N     | 2:H:79:VAL:O     | 2.46                     | 0.47              |
| 1:A:583:VAL:HG23 | 1:A:584:LEU:H    | 1.80                     | 0.47              |
| 1:D:605:ARG:HH12 | 1:D:628:THR:HG1  | 1.59                     | 0.47              |
| 1:D:771:VAL:HG23 | 1:D:795:PRO:HG2  | 1.96                     | 0.47              |
| 1:E:154:GLU:HA   | 1:E:157:VAL:HG12 | 1.96                     | 0.47              |
| 1:E:168:TRP:CE2  | 1:E:402:LEU:HD22 | 2.50                     | 0.47              |
| 1:E:509:PRO:HB2  | 1:E:512:ILE:HG23 | 1.97                     | 0.47              |
| 1:F:403:ARG:HH21 | 1:F:436:SER:HB3  | 1.79                     | 0.47              |
| 1:A:658:ILE:HG21 | 1:A:681:LEU:HD12 | 1.97                     | 0.47              |
| 1:C:420:LEU:HA   | 1:C:430:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:119:HIS:CG   | 1:E:288:ASN:HD22 | 2.33                     | 0.47              |
| 1:E:364:ASP:OD2  | 1:E:397:VAL:HB   | 2.15                     | 0.47              |
| 1:F:669:LEU:O    | 1:F:672:ASN:ND2  | 2.48                     | 0.47              |
| 2:H:68:PHE:CD2   | 2:H:83:MET:HG2   | 2.50                     | 0.47              |
| 1:A:154:GLU:OE2  | 1:B:382:TYR:OH   | 2.30                     | 0.47              |
| 1:A:565:VAL:HG13 | 1:A:569:LEU:HD11 | 1.96                     | 0.47              |
| 1:B:651:ILE:O    | 1:B:673:LYS:HG3  | 2.14                     | 0.47              |
| 1:E:340:LEU:HD22 | 1:E:340:LEU:HA   | 1.73                     | 0.47              |
| 1:E:648:TYR:HE1  | 1:E:671:ARG:HG3  | 1.80                     | 0.47              |
| 1:E:694:HIS:CE1  | 1:E:717:ALA:HB3  | 2.50                     | 0.47              |
| 1:F:359:GLU:OE2  | 1:F:388:LYS:NZ   | 2.35                     | 0.47              |
| 1:F:554:ASN:HD21 | 1:F:577:GLU:HB2  | 1.79                     | 0.47              |
| 1:F:632:ILE:HD12 | 1:F:635:PHE:HD2  | 1.79                     | 0.47              |
| 2:G:33:TYR:HE2   | 2:G:104:THR:HA   | 1.79                     | 0.47              |
| 2:H:38:ARG:HG2   | 2:H:48:VAL:HG22  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:518:LEU:HB3  | 1:A:543:LEU:HD22 | 1.97                     | 0.46              |
| 1:D:766:LEU:HD23 | 1:D:790:LEU:HD13 | 1.96                     | 0.46              |
| 1:F:122:ALA:HB2  | 1:F:289:ILE:HG22 | 1.98                     | 0.46              |
| 1:A:765:ARG:HH12 | 1:A:767:GLU:HB2  | 1.80                     | 0.46              |
| 1:B:679:THR:HA   | 1:B:682:PHE:HD1  | 1.79                     | 0.46              |
| 1:D:258:ASP:O    | 1:D:262:ARG:NE   | 2.49                     | 0.46              |
| 1:F:18:ARG:NH1   | 1:F:382:TYR:OH   | 2.45                     | 0.46              |
| 1:F:411:TRP:HB3  | 1:F:416:LEU:HD21 | 1.97                     | 0.46              |
| 2:H:33:TYR:CE2   | 2:H:104:THR:HA   | 2.50                     | 0.46              |
| 1:A:297:VAL:HB   | 1:A:299:ILE:HG12 | 1.97                     | 0.46              |
| 1:B:416:LEU:HD11 | 1:B:441:THR:HG23 | 1.97                     | 0.46              |
| 1:B:567:VAL:O    | 1:B:592:ASN:ND2  | 2.49                     | 0.46              |
| 1:C:417:ARG:HA   | 1:C:420:LEU:HB2  | 1.97                     | 0.46              |
| 1:D:632:ILE:HG12 | 1:D:661:LEU:HD13 | 1.96                     | 0.46              |
| 1:D:653:TYR:CZ   | 1:D:655:PRO:HG3  | 2.50                     | 0.46              |
| 1:F:665:GLU:O    | 1:F:688:ARG:N    | 2.43                     | 0.46              |
| 1:A:46:GLN:HB2   | 1:A:318:PHE:HZ   | 1.80                     | 0.46              |
| 1:A:765:ARG:HD3  | 1:B:688:ARG:NH2  | 2.30                     | 0.46              |
| 1:A:164:PHE:HA   | 1:A:389:ARG:HH12 | 1.80                     | 0.46              |
| 1:A:682:PHE:CD2  | 1:A:703:ASP:HB2  | 2.51                     | 0.46              |
| 1:C:132:HIS:CG   | 1:C:278:ILE:HD12 | 2.51                     | 0.46              |
| 1:D:622:LYS:HE3  | 1:D:622:LYS:HB3  | 1.76                     | 0.46              |
| 1:D:691:ASP:OD1  | 1:D:691:ASP:N    | 2.47                     | 0.46              |
| 1:E:460:THR:HA   | 1:E:482:LYS:O    | 2.16                     | 0.46              |
| 1:F:542:GLU:N    | 1:F:542:GLU:OE1  | 2.49                     | 0.46              |
| 1:F:602:ASP:N    | 1:F:624:ASN:OD1  | 2.48                     | 0.46              |
| 1:C:659:GLY:HA3  | 1:C:680:GLN:O    | 2.15                     | 0.46              |
| 1:C:762:ARG:NH1  | 1:C:787:GLU:HG3  | 2.31                     | 0.46              |
| 1:C:781:ARG:H    | 1:C:806:ASP:HB2  | 1.79                     | 0.46              |
| 1:D:57:CYS:HB3   | 1:D:65:CYS:HB3   | 1.77                     | 0.46              |
| 1:D:357:ARG:HB2  | 1:D:365:ILE:HB   | 1.98                     | 0.46              |
| 1:D:463:PRO:HB3  | 1:D:486:PRO:HG2  | 1.97                     | 0.46              |
| 1:E:665:GLU:HA   | 1:E:687:LEU:HA   | 1.97                     | 0.46              |
| 1:E:716:THR:O    | 1:E:718:ASN:ND2  | 2.49                     | 0.46              |
| 1:E:762:ARG:HH11 | 1:E:787:GLU:HG3  | 1.81                     | 0.46              |
| 1:F:726:GLU:HG3  | 1:F:729:GLN:CD   | 2.41                     | 0.46              |
| 1:B:800:GLU:HG2  | 1:B:804:ARG:NE   | 2.31                     | 0.46              |
| 1:C:136:PHE:CE1  | 1:C:274:LYS:HG2  | 2.50                     | 0.46              |
| 1:D:104:HIS:NE2  | 1:E:110:ASP:OD2  | 2.47                     | 0.46              |
| 1:D:603:LEU:HB2  | 1:D:624:ASN:ND2  | 2.31                     | 0.46              |
| 1:F:725:PRO:HB3  | 1:F:749:ARG:HD3  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:735:ALA:HA   | 1:F:758:GLN:O    | 2.15                     | 0.46              |
| 1:A:677:ILE:HD13 | 1:A:701:PRO:HD3  | 1.98                     | 0.46              |
| 1:B:356:ILE:HD13 | 1:B:388:LYS:HA   | 1.97                     | 0.46              |
| 1:B:656:ILE:HB   | 1:B:680:GLN:HG3  | 1.97                     | 0.46              |
| 1:E:136:PHE:CE1  | 1:E:274:LYS:HG2  | 2.50                     | 0.46              |
| 1:B:585:ASN:OD1  | 1:B:609:SER:OG   | 2.34                     | 0.46              |
| 1:E:454:GLU:HB3  | 1:E:477:TYR:HB2  | 1.98                     | 0.46              |
| 1:E:511:TRP:O    | 1:E:514:SER:OG   | 2.26                     | 0.46              |
| 1:E:731:ARG:NH1  | 1:E:731:ARG:HA   | 2.31                     | 0.46              |
| 1:F:19:ILE:HG23  | 1:F:382:TYR:CD2  | 2.51                     | 0.46              |
| 1:F:160:LEU:HD21 | 1:F:379:ILE:HG21 | 1.98                     | 0.46              |
| 2:G:33:TYR:CE2   | 2:G:104:THR:HA   | 2.51                     | 0.46              |
| 1:B:575:ASN:HD21 | 1:B:599:ILE:HG13 | 1.80                     | 0.46              |
| 1:B:658:ILE:HD13 | 1:B:681:LEU:HD13 | 1.98                     | 0.46              |
| 1:C:524:THR:HG22 | 1:C:552:LYS:HB3  | 1.99                     | 0.46              |
| 1:E:49:GLN:OE1   | 1:E:49:GLN:N     | 2.48                     | 0.46              |
| 1:E:452:LYS:HE3  | 1:E:475:TRP:CZ3  | 2.51                     | 0.46              |
| 2:G:68:PHE:CD2   | 2:G:83:MET:HG2   | 2.51                     | 0.46              |
| 1:A:780:LYS:HD2  | 1:A:806:ASP:HA   | 1.97                     | 0.45              |
| 1:B:439:PRO:HB2  | 1:B:442:VAL:HG13 | 1.97                     | 0.45              |
| 1:E:129:VAL:HG13 | 1:E:325:TYR:CE1  | 2.51                     | 0.45              |
| 1:F:261:TYR:CD2  | 1:F:349:LYS:HD3  | 2.50                     | 0.45              |
| 2:H:71:SER:OG    | 2:H:80:TYR:HB2   | 2.15                     | 0.45              |
| 1:A:148:ARG:O    | 1:A:151:SER:OG   | 2.33                     | 0.45              |
| 1:A:736:LEU:HD13 | 1:A:738:LEU:HD11 | 1.97                     | 0.45              |
| 1:B:600:ARG:HD2  | 2:G:104:THR:HB   | 1.98                     | 0.45              |
| 1:D:419:ARG:NH2  | 1:D:431:HIS:O    | 2.49                     | 0.45              |
| 1:E:360:SER:HB3  | 1:E:362:TYR:CD2  | 2.51                     | 0.45              |
| 1:E:416:LEU:HD23 | 1:E:445:LEU:HD11 | 1.98                     | 0.45              |
| 1:F:57:CYS:HB3   | 1:F:65:CYS:HB3   | 1.79                     | 0.45              |
| 2:G:47:GLY:HA3   | 2:G:107:LEU:HB3  | 1.98                     | 0.45              |
| 1:B:772:GLU:O    | 1:B:775:GLU:HG2  | 2.16                     | 0.45              |
| 1:C:642:THR:O    | 1:C:665:GLU:N    | 2.31                     | 0.45              |
| 1:F:167:PRO:O    | 1:F:170:THR:OG1  | 2.33                     | 0.45              |
| 1:F:576:ASN:HB3  | 1:F:579:THR:HB   | 1.98                     | 0.45              |
| 1:B:419:ARG:NH1  | 1:B:431:HIS:O    | 2.39                     | 0.45              |
| 1:D:160:LEU:HD21 | 1:D:379:ILE:HG21 | 1.99                     | 0.45              |
| 1:D:731:ARG:HD3  | 1:D:753:LEU:HD23 | 1.99                     | 0.45              |
| 1:E:700:LEU:HD12 | 1:E:701:PRO:HD2  | 1.97                     | 0.45              |
| 1:F:731:ARG:HD3  | 1:F:753:LEU:HD23 | 1.98                     | 0.45              |
| 2:G:45:ARG:CZ    | 2:G:45:ARG:H     | 2.29                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:69:THR:OG1   | 2:G:82:GLN:NE2   | 2.48                     | 0.45              |
| 2:G:104:THR:O    | 2:G:106:PRO:HD3  | 2.17                     | 0.45              |
| 2:I:49:ALA:HA    | 2:I:60:TYR:HA    | 1.98                     | 0.45              |
| 2:H:64:VAL:HB    | 2:H:68:PHE:CG    | 2.51                     | 0.45              |
| 1:D:167:PRO:O    | 1:D:170:THR:OG1  | 2.32                     | 0.45              |
| 2:G:6:GLU:HG2    | 2:G:96:CYS:HB2   | 1.98                     | 0.45              |
| 2:I:38:ARG:NH1   | 2:I:90:ASP:HA    | 2.32                     | 0.45              |
| 1:A:24:TRP:CD1   | 1:A:339:THR:HG1  | 2.33                     | 0.45              |
| 1:B:357:ARG:NH2  | 1:B:363:SER:O    | 2.49                     | 0.45              |
| 1:D:668:TYR:HA   | 1:D:691:ASP:OD1  | 2.17                     | 0.45              |
| 1:D:671:ARG:HD2  | 1:D:694:HIS:HB3  | 1.99                     | 0.45              |
| 1:D:698:THR:HG22 | 1:D:719:ARG:HB2  | 1.99                     | 0.45              |
| 1:E:258:ASP:HB2  | 1:E:370:ASN:ND2  | 2.31                     | 0.45              |
| 1:F:406:ASN:O    | 1:F:410:GLU:HG2  | 2.17                     | 0.45              |
| 1:F:607:PRO:HG2  | 1:F:610:ILE:HG13 | 1.99                     | 0.45              |
| 1:F:671:ARG:HA   | 1:F:671:ARG:HD2  | 1.79                     | 0.45              |
| 1:A:142:PHE:HE1  | 1:B:27:PHE:HZ    | 1.65                     | 0.45              |
| 1:A:523:LEU:HD12 | 1:A:551:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:704:ILE:HD12 | 1:A:707:LEU:HD12 | 1.98                     | 0.45              |
| 1:B:45:LEU:HD21  | 1:B:317:LEU:HD23 | 1.98                     | 0.45              |
| 1:B:576:ASN:HB3  | 1:B:579:THR:HB   | 1.98                     | 0.45              |
| 1:D:123:LYS:HB2  | 1:D:123:LYS:HE3  | 1.79                     | 0.45              |
| 1:F:143:TRP:H    | 1:F:143:TRP:CD1  | 2.35                     | 0.45              |
| 1:A:717:ALA:HA   | 1:A:740:ASN:O    | 2.16                     | 0.45              |
| 1:E:676:LYS:NZ   | 1:E:699:PHE:H    | 2.15                     | 0.45              |
| 2:G:39:GLN:NE2   | 2:G:45:ARG:HH21  | 2.14                     | 0.45              |
| 2:G:49:ALA:HA    | 2:G:60:TYR:HA    | 1.98                     | 0.45              |
| 2:G:71:SER:O     | 2:G:80:TYR:N     | 2.29                     | 0.45              |
| 2:H:19:ARG:HH11  | 2:H:82:GLN:HG3   | 1.81                     | 0.45              |
| 1:C:780:LYS:HD2  | 1:C:806:ASP:HA   | 1.98                     | 0.45              |
| 1:D:146:PHE:HD1  | 1:D:147:PRO:HD2  | 1.82                     | 0.45              |
| 1:D:148:ARG:HD2  | 1:D:259:ILE:HG12 | 1.98                     | 0.45              |
| 1:D:529:ALA:H    | 1:D:533:ARG:HB3  | 1.81                     | 0.45              |
| 1:E:278:ILE:HD11 | 1:E:325:TYR:CE2  | 2.51                     | 0.45              |
| 1:F:385:LEU:O    | 1:F:389:ARG:HG2  | 2.17                     | 0.45              |
| 1:F:620:ASP:OD1  | 1:F:621:LEU:N    | 2.50                     | 0.45              |
| 1:F:716:THR:HG23 | 1:F:740:ASN:HB2  | 1.99                     | 0.45              |
| 2:G:64:VAL:HG12  | 2:G:67:ARG:HH21  | 1.82                     | 0.45              |
| 1:B:553:SER:HB2  | 1:B:555:LEU:HG   | 1.98                     | 0.45              |
| 1:C:632:ILE:HG22 | 1:C:635:PHE:CE2  | 2.52                     | 0.45              |
| 1:E:552:LYS:HZ1  | 1:E:574:ILE:C    | 2.25                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:501:LYS:HA   | 1:F:524:THR:HB   | 1.98                     | 0.45              |
| 1:F:679:THR:HA   | 1:F:682:PHE:CD2  | 2.52                     | 0.45              |
| 1:F:703:ASP:HA   | 1:F:706:LEU:HG   | 1.99                     | 0.45              |
| 1:F:751:GLY:HA2  | 1:F:776:CYS:SG   | 2.57                     | 0.45              |
| 1:A:576:ASN:HB3  | 1:A:579:THR:HB   | 1.98                     | 0.44              |
| 1:A:715:VAL:O    | 1:A:718:ASN:ND2  | 2.50                     | 0.44              |
| 1:C:168:TRP:CE2  | 1:C:402:LEU:HD22 | 2.52                     | 0.44              |
| 1:D:246:LYS:HD3  | 1:D:246:LYS:HA   | 1.76                     | 0.44              |
| 1:E:168:TRP:HH2  | 1:E:398:SER:HB3  | 1.81                     | 0.44              |
| 1:E:646:LEU:O    | 1:E:649:ASN:ND2  | 2.43                     | 0.44              |
| 1:F:399:GLU:HA   | 1:F:402:LEU:CD2  | 2.47                     | 0.44              |
| 1:F:550:ARG:HH22 | 1:F:552:LYS:HE3  | 1.82                     | 0.44              |
| 1:A:291:PHE:HA   | 1:A:315:ALA:HB3  | 1.99                     | 0.44              |
| 1:A:705:GLY:O    | 1:A:708:GLN:NE2  | 2.50                     | 0.44              |
| 1:B:647:TRP:HB2  | 1:B:670:ASN:O    | 2.16                     | 0.44              |
| 1:C:559:PRO:HB2  | 1:C:562:VAL:HG23 | 1.98                     | 0.44              |
| 1:C:691:ASP:HA   | 1:C:714:ALA:HB3  | 1.98                     | 0.44              |
| 1:F:293:VAL:HG13 | 1:F:310:CYS:HB2  | 1.99                     | 0.44              |
| 1:A:419:ARG:HH22 | 1:A:431:HIS:HB3  | 1.82                     | 0.44              |
| 1:D:234:LYS:HD3  | 1:D:409:ASN:HB3  | 2.00                     | 0.44              |
| 1:D:580:LYS:HG2  | 1:D:602:ASP:O    | 2.18                     | 0.44              |
| 1:D:235:LYS:NZ   | 1:D:239:GLN:OE1  | 2.50                     | 0.44              |
| 1:D:645:LYS:HG2  | 1:D:668:TYR:CD1  | 2.52                     | 0.44              |
| 1:F:142:PHE:HB3  | 1:F:267:GLN:OE1  | 2.18                     | 0.44              |
| 1:F:168:TRP:CZ3  | 1:F:398:SER:HB3  | 2.53                     | 0.44              |
| 1:F:369:LYS:HG2  | 1:F:370:ASN:H    | 1.82                     | 0.44              |
| 1:F:723:LEU:HD21 | 1:F:727:LEU:HB3  | 1.99                     | 0.44              |
| 1:A:662:THR:HA   | 1:A:684:CYS:HA   | 2.00                     | 0.44              |
| 1:B:438:ILE:HG13 | 1:B:459:VAL:HG21 | 2.00                     | 0.44              |
| 1:B:759:ILE:N    | 1:B:783:GLY:O    | 2.43                     | 0.44              |
| 1:D:244:PHE:CD2  | 1:D:402:LEU:HD22 | 2.52                     | 0.44              |
| 1:D:591:VAL:O    | 1:D:615:ASN:ND2  | 2.50                     | 0.44              |
| 1:D:780:LYS:O    | 1:D:784:LEU:N    | 2.51                     | 0.44              |
| 1:F:417:ARG:HA   | 1:F:420:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:159:ILE:HA   | 1:A:162:LYS:NZ   | 2.33                     | 0.44              |
| 1:A:520:GLU:HA   | 1:A:548:VAL:O    | 2.18                     | 0.44              |
| 1:B:350:LYS:HE3  | 1:B:350:LYS:HB3  | 1.68                     | 0.44              |
| 1:D:738:LEU:O    | 1:D:764:ASN:ND2  | 2.51                     | 0.44              |
| 1:E:647:TRP:HA   | 1:E:672:ASN:HD21 | 1.81                     | 0.44              |
| 2:G:38:ARG:NH1   | 2:G:90:ASP:HA    | 2.33                     | 0.44              |
| 2:I:68:PHE:CG    | 2:I:83:MET:HG2   | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:427:LYS:NZ   | 1:B:473:GLU:OE2  | 2.34                     | 0.44              |
| 1:B:644:LEU:HD21 | 1:B:646:LEU:HD23 | 1.99                     | 0.44              |
| 1:C:404:GLN:OE1  | 1:C:408:ASN:ND2  | 2.49                     | 0.44              |
| 1:C:621:LEU:HD22 | 1:C:624:ASN:HD22 | 1.82                     | 0.44              |
| 1:C:682:PHE:O    | 1:C:707:LEU:HD21 | 2.18                     | 0.44              |
| 1:D:385:LEU:O    | 1:D:389:ARG:HG2  | 2.18                     | 0.44              |
| 1:D:677:ILE:HG23 | 1:D:681:LEU:HD23 | 2.00                     | 0.44              |
| 1:E:791:PHE:HZ   | 1:E:803:TRP:HE1  | 1.66                     | 0.44              |
| 1:C:425:GLN:HB2  | 1:C:427:LYS:HD2  | 2.00                     | 0.44              |
| 1:C:729:GLN:OE1  | 1:C:749:ARG:NH2  | 2.51                     | 0.44              |
| 1:C:746:LEU:HD21 | 1:C:750:VAL:HG11 | 1.99                     | 0.44              |
| 1:D:762:ARG:HG3  | 1:D:787:GLU:HG3  | 1.99                     | 0.44              |
| 1:E:159:ILE:HA   | 1:E:162:LYS:HZ3  | 1.82                     | 0.44              |
| 1:E:346:ARG:H    | 1:E:346:ARG:HG2  | 1.65                     | 0.44              |
| 1:F:46:GLN:HA    | 1:F:50:ASP:HB2   | 2.00                     | 0.44              |
| 2:I:106:PRO:HD2  | 2:I:108:TYR:CE2  | 2.53                     | 0.44              |
| 1:A:97:ILE:HD11  | 1:F:302:LEU:C    | 2.43                     | 0.44              |
| 1:A:258:ASP:N    | 1:A:371:ASP:OD2  | 2.51                     | 0.44              |
| 1:B:724:PRO:HB2  | 1:B:726:GLU:OE1  | 2.18                     | 0.44              |
| 1:C:679:THR:HA   | 1:C:682:PHE:CD2  | 2.53                     | 0.44              |
| 1:D:147:PRO:HA   | 1:D:150:SER:OG   | 2.18                     | 0.44              |
| 1:E:543:LEU:HB3  | 1:E:546:LEU:HB2  | 1.99                     | 0.44              |
| 1:F:244:PHE:CD2  | 1:F:402:LEU:HD22 | 2.53                     | 0.44              |
| 1:F:626:LEU:HA   | 1:F:626:LEU:HD13 | 1.82                     | 0.44              |
| 2:G:20:LEU:N     | 2:G:81:LEU:O     | 2.50                     | 0.44              |
| 1:A:136:PHE:HE1  | 1:A:274:LYS:HG2  | 1.83                     | 0.43              |
| 1:A:725:PRO:HA   | 1:A:728:PHE:CD2  | 2.52                     | 0.43              |
| 1:B:19:ILE:HG23  | 1:B:382:TYR:CD2  | 2.53                     | 0.43              |
| 1:B:399:GLU:HA   | 1:B:402:LEU:CD2  | 2.49                     | 0.43              |
| 1:B:513:TYR:OH   | 1:B:536:VAL:O    | 2.25                     | 0.43              |
| 1:C:18:ARG:HD3   | 1:C:18:ARG:H     | 1.83                     | 0.43              |
| 1:C:688:ARG:HB3  | 1:C:711:GLN:OE1  | 2.18                     | 0.43              |
| 1:E:559:PRO:HB2  | 1:E:562:VAL:HG23 | 1.99                     | 0.43              |
| 1:F:694:HIS:N    | 1:F:716:THR:O    | 2.40                     | 0.43              |
| 1:C:354:GLU:HA   | 1:C:357:ARG:HH11 | 1.82                     | 0.43              |
| 1:C:398:SER:HA   | 1:C:401:LYS:HG2  | 2.01                     | 0.43              |
| 1:D:620:ASP:OD1  | 1:D:621:LEU:N    | 2.51                     | 0.43              |
| 1:D:751:GLY:HA2  | 1:D:776:CYS:SG   | 2.58                     | 0.43              |
| 1:E:258:ASP:HB2  | 1:E:370:ASN:HD22 | 1.83                     | 0.43              |
| 1:E:278:ILE:HA   | 1:E:281:TYR:CD1  | 2.53                     | 0.43              |
| 1:E:520:GLU:HA   | 1:E:548:VAL:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:746:LEU:HD12 | 1:E:747:PRO:HD2  | 2.00                     | 0.43              |
| 1:F:128:LEU:HD23 | 1:F:128:LEU:HA   | 1.87                     | 0.43              |
| 1:F:622:LYS:HD3  | 1:F:647:TRP:CD1  | 2.51                     | 0.43              |
| 1:A:410:GLU:OE2  | 1:A:415:LYS:NZ   | 2.51                     | 0.43              |
| 1:A:453:LEU:HB2  | 1:A:476:LEU:HD23 | 1.99                     | 0.43              |
| 1:A:460:THR:HG22 | 1:A:482:LYS:HE2  | 2.01                     | 0.43              |
| 1:B:627:LYS:HG3  | 1:B:628:THR:HG23 | 2.00                     | 0.43              |
| 1:C:400:ASN:O    | 1:C:403:ARG:NH2  | 2.52                     | 0.43              |
| 1:D:654:ILE:HD13 | 1:D:681:LEU:HD22 | 2.00                     | 0.43              |
| 1:F:398:SER:HA   | 1:F:401:LYS:HD2  | 2.00                     | 0.43              |
| 1:A:244:PHE:HB3  | 1:A:248:LYS:NZ   | 2.34                     | 0.43              |
| 1:A:278:ILE:HA   | 1:A:281:TYR:CD1  | 2.53                     | 0.43              |
| 1:B:647:TRP:CE3  | 1:B:668:TYR:HB2  | 2.54                     | 0.43              |
| 1:C:413:LEU:HD21 | 1:C:417:ARG:HH12 | 1.84                     | 0.43              |
| 1:D:543:LEU:HB3  | 1:D:546:LEU:HB2  | 2.00                     | 0.43              |
| 1:D:735:ALA:HA   | 1:D:758:GLN:O    | 2.17                     | 0.43              |
| 1:F:173:LEU:HD13 | 1:F:173:LEU:HA   | 1.89                     | 0.43              |
| 2:I:12:VAL:O     | 2:I:123:VAL:HA   | 2.18                     | 0.43              |
| 2:H:52:ALA:HB3   | 2:H:57:GLN:H     | 1.84                     | 0.43              |
| 1:A:137:LEU:HD23 | 1:A:137:LEU:HA   | 1.82                     | 0.43              |
| 1:A:477:TYR:HA   | 1:A:501:LYS:HB3  | 2.00                     | 0.43              |
| 1:B:690:LEU:HD12 | 1:B:690:LEU:HA   | 1.88                     | 0.43              |
| 1:B:761:LEU:HD22 | 1:B:769:LEU:HD21 | 1.99                     | 0.43              |
| 1:C:711:GLN:HE21 | 1:C:732:LYS:HD2  | 1.83                     | 0.43              |
| 1:D:596:LEU:HD11 | 1:D:598:LEU:HD21 | 2.01                     | 0.43              |
| 1:E:702:ALA:HA   | 1:E:726:GLU:CD   | 2.43                     | 0.43              |
| 1:F:527:LEU:HG   | 1:F:553:SER:HB3  | 2.00                     | 0.43              |
| 1:A:657:GLN:O    | 1:A:660:ASN:ND2  | 2.50                     | 0.43              |
| 1:B:616:LEU:HB3  | 1:B:638:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:608:HIS:CD2  | 1:C:611:PHE:HD2  | 2.36                     | 0.43              |
| 1:C:711:GLN:HA   | 1:C:733:LEU:HA   | 2.00                     | 0.43              |
| 1:D:19:ILE:HG23  | 1:D:382:TYR:CD2  | 2.53                     | 0.43              |
| 1:D:772:GLU:CD   | 1:D:772:GLU:H    | 2.27                     | 0.43              |
| 1:F:147:PRO:HA   | 1:F:150:SER:OG   | 2.18                     | 0.43              |
| 2:G:90:ASP:OD1   | 2:G:90:ASP:N     | 2.51                     | 0.43              |
| 2:I:32:GLU:HB2   | 2:I:101:GLU:CD   | 2.44                     | 0.43              |
| 1:A:619:ILE:HB   | 1:A:644:LEU:HD12 | 2.01                     | 0.43              |
| 1:B:146:PHE:HD2  | 1:B:263:LEU:HD11 | 1.84                     | 0.43              |
| 1:B:168:TRP:O    | 1:B:171:ARG:HG2  | 2.19                     | 0.43              |
| 1:B:297:VAL:HG23 | 1:B:299:ILE:HG12 | 2.00                     | 0.43              |
| 1:B:626:LEU:HD13 | 1:B:626:LEU:HA   | 1.87                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:401:LYS:O    | 1:D:404:GLN:HG3  | 2.18                     | 0.43              |
| 1:D:774:GLY:O    | 1:D:801:ARG:NH2  | 2.52                     | 0.43              |
| 1:F:599:ILE:HD12 | 1:F:622:LYS:HB3  | 2.01                     | 0.43              |
| 1:A:576:ASN:ND2  | 1:A:581:LEU:HB2  | 2.33                     | 0.43              |
| 1:B:102:ASP:N    | 1:B:105:GLN:OE1  | 2.46                     | 0.43              |
| 1:B:248:LYS:HD2  | 1:B:248:LYS:HA   | 1.81                     | 0.43              |
| 1:C:294:ASP:OD1  | 1:C:294:ASP:N    | 2.51                     | 0.43              |
| 1:D:168:TRP:CH2  | 1:D:398:SER:HB3  | 2.54                     | 0.43              |
| 1:D:279:ILE:HD13 | 1:D:279:ILE:HA   | 1.81                     | 0.43              |
| 1:E:158:SER:O    | 1:E:161:LEU:HG   | 2.18                     | 0.43              |
| 1:E:159:ILE:HA   | 1:E:162:LYS:NZ   | 2.34                     | 0.43              |
| 2:H:38:ARG:HH21  | 2:H:92:ALA:HB2   | 1.83                     | 0.43              |
| 1:B:233:ASP:OD2  | 1:B:235:LYS:HG2  | 2.19                     | 0.43              |
| 1:B:501:LYS:HG2  | 1:B:524:THR:HB   | 2.01                     | 0.43              |
| 1:C:364:ASP:OD1  | 1:C:364:ASP:N    | 2.36                     | 0.43              |
| 1:C:572:LEU:HB2  | 1:C:593:LEU:HD11 | 2.00                     | 0.43              |
| 1:D:370:ASN:C    | 1:D:372:PHE:H    | 2.27                     | 0.43              |
| 1:E:420:LEU:HA   | 1:E:430:LEU:HD13 | 2.00                     | 0.43              |
| 1:F:278:ILE:O    | 1:F:282:THR:OG1  | 2.34                     | 0.43              |
| 2:H:47:GLY:HA3   | 2:H:107:LEU:HB3  | 2.01                     | 0.43              |
| 1:B:147:PRO:HA   | 1:B:150:SER:OG   | 2.19                     | 0.43              |
| 1:C:395:SER:O    | 1:C:399:GLU:HG3  | 2.19                     | 0.43              |
| 1:C:618:GLU:HG2  | 1:C:643:CYS:HB3  | 2.01                     | 0.43              |
| 1:E:728:PHE:CD2  | 1:E:749:ARG:HB2  | 2.53                     | 0.43              |
| 1:F:49:GLN:N     | 1:F:49:GLN:OE1   | 2.51                     | 0.43              |
| 1:F:602:ASP:HA   | 1:F:624:ASN:HA   | 2.01                     | 0.43              |
| 1:C:168:TRP:HZ3  | 1:C:392:VAL:HB   | 1.84                     | 0.42              |
| 1:C:724:PRO:HA   | 1:C:725:PRO:HD3  | 1.93                     | 0.42              |
| 1:D:142:PHE:HB3  | 1:D:267:GLN:OE1  | 2.19                     | 0.42              |
| 1:D:717:ALA:H    | 1:D:740:ASN:HB2  | 1.83                     | 0.42              |
| 1:D:790:LEU:O    | 1:D:793:THR:OG1  | 2.36                     | 0.42              |
| 1:F:648:TYR:OH   | 2:I:110:GLU:OE1  | 2.29                     | 0.42              |
| 2:G:12:VAL:O     | 2:G:123:VAL:HA   | 2.19                     | 0.42              |
| 2:G:36:TRP:NE1   | 2:G:81:LEU:HB2   | 2.34                     | 0.42              |
| 1:A:431:HIS:CD2  | 1:A:452:LYS:HB2  | 2.54                     | 0.42              |
| 1:B:542:GLU:N    | 1:B:542:GLU:OE1  | 2.52                     | 0.42              |
| 1:C:583:VAL:HG21 | 1:C:607:PRO:HB3  | 2.00                     | 0.42              |
| 1:E:56:PRO:HG2   | 1:E:99:TYR:CD1   | 2.53                     | 0.42              |
| 1:E:274:LYS:O    | 1:E:278:ILE:HG22 | 2.19                     | 0.42              |
| 1:E:644:LEU:HD12 | 1:E:644:LEU:HA   | 1.78                     | 0.42              |
| 1:F:117:ARG:NH1  | 1:F:296:THR:O    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:717:ALA:HA   | 1:F:740:ASN:O    | 2.18                     | 0.42              |
| 1:A:659:GLY:HA3  | 1:A:680:GLN:O    | 2.19                     | 0.42              |
| 1:A:682:PHE:HE1  | 1:A:704:ILE:HD13 | 1.84                     | 0.42              |
| 1:B:368:VAL:HG11 | 1:B:372:PHE:CD1  | 2.55                     | 0.42              |
| 1:B:540:LEU:HD22 | 1:B:543:LEU:HD12 | 2.00                     | 0.42              |
| 1:C:439:PRO:HB2  | 1:C:442:VAL:HG13 | 2.02                     | 0.42              |
| 1:D:547:LYS:NZ   | 1:D:568:HIS:O    | 2.42                     | 0.42              |
| 2:I:36:TRP:NE1   | 2:I:81:LEU:HB2   | 2.35                     | 0.42              |
| 1:A:685:ARG:HA   | 1:A:707:LEU:HD23 | 2.00                     | 0.42              |
| 1:B:27:PHE:O     | 1:B:31:ILE:HG12  | 2.20                     | 0.42              |
| 1:B:385:LEU:O    | 1:B:389:ARG:HG2  | 2.19                     | 0.42              |
| 1:B:654:ILE:HD13 | 1:B:681:LEU:HD22 | 2.01                     | 0.42              |
| 1:C:258:ASP:N    | 1:C:371:ASP:OD2  | 2.53                     | 0.42              |
| 1:C:446:VAL:HA   | 1:C:468:LEU:HD22 | 2.02                     | 0.42              |
| 1:C:776:CYS:O    | 1:C:801:ARG:NH2  | 2.46                     | 0.42              |
| 1:D:691:ASP:O    | 1:D:692:LEU:HD23 | 2.19                     | 0.42              |
| 1:E:258:ASP:N    | 1:E:371:ASP:OD2  | 2.52                     | 0.42              |
| 1:E:356:ILE:HG21 | 1:E:365:ILE:HD12 | 2.00                     | 0.42              |
| 1:F:611:PHE:CZ   | 1:F:631:GLU:HB3  | 2.50                     | 0.42              |
| 1:A:168:TRP:CE2  | 1:A:402:LEU:HD22 | 2.54                     | 0.42              |
| 1:A:736:LEU:HD23 | 1:A:736:LEU:HA   | 1.82                     | 0.42              |
| 1:D:355:SER:O    | 1:D:358:GLU:HG3  | 2.19                     | 0.42              |
| 2:H:61:ALA:O     | 2:H:65:LYS:HG3   | 2.19                     | 0.42              |
| 1:A:340:LEU:HD22 | 1:A:340:LEU:HA   | 1.80                     | 0.42              |
| 1:B:112:VAL:HG12 | 1:B:297:VAL:HG11 | 2.02                     | 0.42              |
| 1:B:700:LEU:O    | 1:B:724:PRO:HG3  | 2.19                     | 0.42              |
| 1:D:122:ALA:HB2  | 1:D:289:ILE:HG22 | 2.01                     | 0.42              |
| 1:D:354:GLU:O    | 1:D:357:ARG:HG2  | 2.19                     | 0.42              |
| 1:E:762:ARG:NH1  | 1:E:787:GLU:HG3  | 2.35                     | 0.42              |
| 1:E:772:GLU:O    | 1:E:775:GLU:HG2  | 2.19                     | 0.42              |
| 1:F:627:LYS:HG3  | 1:F:628:THR:HG23 | 2.01                     | 0.42              |
| 1:F:698:THR:HG22 | 1:F:719:ARG:HB2  | 2.02                     | 0.42              |
| 1:A:428:LEU:HD12 | 1:A:428:LEU:HA   | 1.94                     | 0.42              |
| 1:A:618:GLU:HG2  | 1:A:643:CYS:HB3  | 2.01                     | 0.42              |
| 1:E:291:PHE:O    | 1:E:312:HIS:N    | 2.38                     | 0.42              |
| 1:E:291:PHE:HA   | 1:E:315:ALA:HB3  | 2.02                     | 0.42              |
| 1:E:416:LEU:HD21 | 1:E:442:VAL:HG12 | 2.01                     | 0.42              |
| 1:A:394:LEU:HD13 | 1:A:394:LEU:HA   | 1.90                     | 0.42              |
| 1:C:258:ASP:H    | 1:C:371:ASP:HB2  | 1.84                     | 0.42              |
| 1:C:364:ASP:OD2  | 1:C:397:VAL:HB   | 2.19                     | 0.42              |
| 1:C:737:HIS:CD2  | 1:C:737:HIS:N    | 2.88                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:169:THR:HG22 | 1:E:392:VAL:HG21 | 2.01                     | 0.42              |
| 1:E:647:TRP:CZ3  | 1:E:668:TYR:HB2  | 2.55                     | 0.42              |
| 1:A:585:ASN:O    | 1:A:589:LYS:NZ   | 2.53                     | 0.42              |
| 1:A:611:PHE:HA   | 1:A:638:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:417:ARG:HA   | 1:B:420:LEU:HD12 | 2.02                     | 0.42              |
| 1:B:677:ILE:HG23 | 1:B:681:LEU:HD23 | 2.02                     | 0.42              |
| 1:B:685:ARG:HH21 | 1:B:706:LEU:HD13 | 1.83                     | 0.42              |
| 1:C:139:CYS:HB2  | 1:C:271:LYS:HZ1  | 1.85                     | 0.42              |
| 1:C:232:LEU:HB3  | 1:C:236:GLU:OE1  | 2.20                     | 0.42              |
| 1:C:714:ALA:HB2  | 1:C:737:HIS:ND1  | 2.35                     | 0.42              |
| 1:D:345:ARG:HG3  | 1:D:346:ARG:NE   | 2.33                     | 0.42              |
| 1:D:496:ARG:HA   | 1:D:496:ARG:HD3  | 1.84                     | 0.42              |
| 1:E:587:LEU:HB2  | 1:E:609:SER:CB   | 2.50                     | 0.42              |
| 1:F:258:ASP:HB2  | 1:F:370:ASN:ND2  | 2.35                     | 0.42              |
| 1:F:583:VAL:O    | 1:F:586:SER:OG   | 2.30                     | 0.42              |
| 1:F:762:ARG:NH2  | 1:F:786:VAL:O    | 2.53                     | 0.42              |
| 2:G:83:MET:HB2   | 2:G:86:LEU:HD21  | 2.02                     | 0.42              |
| 1:A:143:TRP:NE1  | 1:A:144:PHE:HD1  | 2.18                     | 0.42              |
| 1:A:321:LEU:HD23 | 1:A:321:LEU:HA   | 1.88                     | 0.42              |
| 1:A:643:CYS:SG   | 1:A:666:ARG:HG3  | 2.59                     | 0.42              |
| 1:A:689:TYR:CD2  | 1:A:712:ASN:HB2  | 2.54                     | 0.42              |
| 1:B:408:ASN:ND2  | 1:B:440:ASP:OD2  | 2.53                     | 0.42              |
| 1:B:596:LEU:HD11 | 1:B:598:LEU:HD21 | 2.02                     | 0.42              |
| 1:D:119:HIS:CD2  | 1:D:288:ASN:HB3  | 2.54                     | 0.42              |
| 1:D:690:LEU:HD12 | 1:D:690:LEU:HA   | 1.93                     | 0.42              |
| 1:E:443:PHE:CE1  | 1:E:465:ILE:HG22 | 2.54                     | 0.42              |
| 1:E:638:LEU:HG   | 1:E:641:LEU:HB2  | 2.01                     | 0.42              |
| 1:F:63:ASP:OD1   | 1:F:63:ASP:N     | 2.53                     | 0.42              |
| 1:A:354:GLU:HA   | 1:A:357:ARG:NH1  | 2.34                     | 0.41              |
| 1:A:724:PRO:HB2  | 1:A:726:GLU:CD   | 2.45                     | 0.41              |
| 1:B:452:LYS:HE3  | 1:B:475:TRP:CD2  | 2.55                     | 0.41              |
| 1:B:495:LEU:HD23 | 1:B:515:LEU:HD13 | 2.01                     | 0.41              |
| 1:B:500:ILE:HG22 | 1:B:502:PHE:HD1  | 1.84                     | 0.41              |
| 1:C:642:THR:O    | 1:C:665:GLU:HG2  | 2.21                     | 0.41              |
| 1:D:604:GLU:O    | 1:D:605:ARG:NE   | 2.41                     | 0.41              |
| 1:E:321:LEU:HD23 | 1:E:321:LEU:HA   | 1.88                     | 0.41              |
| 1:E:330:ILE:HD13 | 1:E:330:ILE:HA   | 1.93                     | 0.41              |
| 1:E:590:MET:HB3  | 1:E:593:LEU:HB2  | 2.01                     | 0.41              |
| 1:E:630:GLU:O    | 1:E:633:ILE:HG13 | 2.20                     | 0.41              |
| 1:E:648:TYR:CE1  | 1:E:671:ARG:HG3  | 2.55                     | 0.41              |
| 1:B:429:GLU:HA   | 1:B:450:VAL:HB   | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:666:ARG:HG2  | 1:B:689:TYR:HB2  | 2.02                     | 0.41              |
| 1:B:726:GLU:OE1  | 1:B:726:GLU:N    | 2.47                     | 0.41              |
| 1:D:46:GLN:HB2   | 1:D:318:PHE:HZ   | 1.84                     | 0.41              |
| 1:D:250:PHE:CZ   | 1:D:254:VAL:HG21 | 2.55                     | 0.41              |
| 1:D:278:ILE:O    | 1:D:282:THR:OG1  | 2.33                     | 0.41              |
| 1:D:603:LEU:HB2  | 1:D:624:ASN:HD22 | 1.85                     | 0.41              |
| 1:D:632:ILE:HG13 | 1:D:635:PHE:HD2  | 1.85                     | 0.41              |
| 1:E:635:PHE:CE2  | 1:E:644:LEU:HD21 | 2.54                     | 0.41              |
| 1:E:669:LEU:HD23 | 1:E:669:LEU:HA   | 1.90                     | 0.41              |
| 1:F:566:GLY:HA2  | 1:F:569:LEU:HD23 | 2.01                     | 0.41              |
| 1:F:699:PHE:HE2  | 1:F:701:PRO:HG3  | 1.85                     | 0.41              |
| 1:F:759:ILE:HG12 | 1:F:784:LEU:HA   | 2.01                     | 0.41              |
| 2:G:6:GLU:OE2    | 2:G:117:GLN:N    | 2.52                     | 0.41              |
| 2:I:60:TYR:OH    | 2:I:70:VAL:HG12  | 2.20                     | 0.41              |
| 2:H:12:VAL:O     | 2:H:123:VAL:HA   | 2.20                     | 0.41              |
| 1:A:760:GLU:N    | 1:A:760:GLU:OE1  | 2.53                     | 0.41              |
| 1:B:57:CYS:HB3   | 1:B:65:CYS:HB3   | 1.90                     | 0.41              |
| 1:B:576:ASN:ND2  | 1:B:581:LEU:HB2  | 2.35                     | 0.41              |
| 1:B:679:THR:HA   | 1:B:682:PHE:CD1  | 2.56                     | 0.41              |
| 1:C:258:ASP:HB2  | 1:C:370:ASN:ND2  | 2.35                     | 0.41              |
| 1:C:316:THR:O    | 1:C:320:ILE:HG23 | 2.21                     | 0.41              |
| 1:C:443:PHE:CE1  | 1:C:465:ILE:HG22 | 2.56                     | 0.41              |
| 1:C:762:ARG:HH11 | 1:C:787:GLU:HG3  | 1.85                     | 0.41              |
| 1:D:614:HIS:CE1  | 1:D:637:HIS:HB3  | 2.56                     | 0.41              |
| 1:D:723:LEU:HD23 | 1:D:728:PHE:CZ   | 2.55                     | 0.41              |
| 1:E:476:LEU:HB2  | 1:E:500:ILE:HD13 | 2.02                     | 0.41              |
| 1:E:647:TRP:HB2  | 1:E:670:ASN:O    | 2.21                     | 0.41              |
| 2:G:68:PHE:CG    | 2:G:83:MET:HG2   | 2.55                     | 0.41              |
| 1:A:278:ILE:HD11 | 1:A:325:TYR:CE2  | 2.55                     | 0.41              |
| 1:A:548:VAL:HG13 | 1:A:571:LYS:HD3  | 2.03                     | 0.41              |
| 1:A:576:ASN:HD21 | 1:A:581:LEU:HB2  | 1.85                     | 0.41              |
| 1:A:728:PHE:CD2  | 1:A:749:ARG:HB2  | 2.56                     | 0.41              |
| 1:C:244:PHE:HB3  | 1:C:248:LYS:NZ   | 2.36                     | 0.41              |
| 1:C:443:PHE:HA   | 1:C:468:LEU:HD21 | 2.02                     | 0.41              |
| 1:C:541:ARG:HG3  | 1:C:561:VAL:HG23 | 2.03                     | 0.41              |
| 1:C:789:ASP:OD1  | 1:C:789:ASP:N    | 2.52                     | 0.41              |
| 1:D:56:PRO:HG2   | 1:D:99:TYR:CD1   | 2.56                     | 0.41              |
| 1:E:400:ASN:O    | 1:E:403:ARG:NH2  | 2.53                     | 0.41              |
| 1:F:101:LEU:HD23 | 1:F:101:LEU:HA   | 1.90                     | 0.41              |
| 1:F:653:TYR:CZ   | 1:F:655:PRO:HG3  | 2.55                     | 0.41              |
| 1:F:781:ARG:HB2  | 1:F:802:LEU:HB3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:316:THR:O    | 1:A:320:ILE:HG23 | 2.20                     | 0.41              |
| 1:A:355:SER:O    | 1:A:358:GLU:HG2  | 2.20                     | 0.41              |
| 1:C:727:LEU:HD23 | 1:C:727:LEU:HA   | 1.91                     | 0.41              |
| 1:D:33:ILE:HD13  | 1:D:33:ILE:HA    | 1.94                     | 0.41              |
| 1:D:712:ASN:HA   | 1:D:735:ALA:O    | 2.21                     | 0.41              |
| 1:F:500:ILE:HG22 | 1:F:502:PHE:HD1  | 1.85                     | 0.41              |
| 2:G:6:GLU:HA     | 2:G:22:CYS:HA    | 2.02                     | 0.41              |
| 1:A:546:LEU:HD21 | 1:A:549:LEU:HD13 | 2.03                     | 0.41              |
| 1:B:427:LYS:HE3  | 1:B:427:LYS:HB2  | 1.87                     | 0.41              |
| 1:B:599:ILE:CD1  | 1:B:622:LYS:HB2  | 2.51                     | 0.41              |
| 1:C:102:ASP:OD1  | 1:C:102:ASP:N    | 2.53                     | 0.41              |
| 1:C:340:LEU:HA   | 1:C:340:LEU:HD22 | 1.79                     | 0.41              |
| 1:C:667:LEU:O    | 1:C:690:LEU:HA   | 2.21                     | 0.41              |
| 1:D:716:THR:HG23 | 1:D:740:ASN:HB2  | 2.03                     | 0.41              |
| 1:F:46:GLN:NE2   | 1:F:123:LYS:O    | 2.45                     | 0.41              |
| 1:F:772:GLU:CD   | 1:F:772:GLU:H    | 2.28                     | 0.41              |
| 1:A:425:GLN:HB2  | 1:A:427:LYS:HE2  | 2.02                     | 0.41              |
| 1:B:128:LEU:HD23 | 1:B:128:LEU:HA   | 1.90                     | 0.41              |
| 1:B:134:LEU:HD23 | 1:B:134:LEU:HA   | 1.93                     | 0.41              |
| 1:B:719:ARG:HD2  | 1:B:719:ARG:HA   | 1.89                     | 0.41              |
| 1:C:278:ILE:HA   | 1:C:281:TYR:CD1  | 2.55                     | 0.41              |
| 1:C:537:ILE:HG22 | 1:C:540:LEU:HB2  | 2.03                     | 0.41              |
| 1:C:715:VAL:O    | 1:C:718:ASN:ND2  | 2.54                     | 0.41              |
| 1:C:717:ALA:HA   | 1:C:740:ASN:O    | 2.20                     | 0.41              |
| 1:D:541:ARG:NH1  | 1:D:564:ASP:OD2  | 2.54                     | 0.41              |
| 1:E:117:ARG:HD3  | 1:E:117:ARG:HA   | 1.81                     | 0.41              |
| 1:E:134:LEU:HD23 | 1:E:134:LEU:HA   | 1.84                     | 0.41              |
| 1:E:233:ASP:OD1  | 1:E:234:LYS:N    | 2.54                     | 0.41              |
| 1:E:431:HIS:O    | 1:E:431:HIS:ND1  | 2.52                     | 0.41              |
| 1:E:717:ALA:HA   | 1:E:740:ASN:O    | 2.20                     | 0.41              |
| 1:E:774:GLY:HA3  | 1:E:798:VAL:HG13 | 2.02                     | 0.41              |
| 1:F:600:ARG:HD2  | 2:I:104:THR:HB   | 2.02                     | 0.41              |
| 1:F:728:PHE:CE2  | 1:F:747:PRO:HB2  | 2.55                     | 0.41              |
| 1:A:261:TYR:HD1  | 1:A:374:PHE:CD1  | 2.39                     | 0.41              |
| 1:A:557:LYS:HE3  | 1:A:557:LYS:HB2  | 1.87                     | 0.41              |
| 1:A:788:GLU:HA   | 1:A:791:PHE:HB3  | 2.02                     | 0.41              |
| 1:B:173:LEU:HD13 | 1:B:173:LEU:HA   | 1.91                     | 0.41              |
| 1:B:509:PRO:HB3  | 1:B:511:TRP:NE1  | 2.36                     | 0.41              |
| 1:B:719:ARG:NH1  | 1:B:742:VAL:HG11 | 2.35                     | 0.41              |
| 1:D:236:GLU:HG3  | 1:D:237:GLY:N    | 2.36                     | 0.41              |
| 1:E:163:CYS:SG   | 1:E:390:PHE:HA   | 2.61                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:10:GLY:O     | 2:I:122:THR:N    | 2.38                     | 0.41              |
| 1:A:392:VAL:O    | 1:A:395:SER:OG   | 2.27                     | 0.41              |
| 1:A:454:GLU:HA   | 1:A:477:TYR:HB2  | 2.03                     | 0.41              |
| 1:A:724:PRO:HA   | 1:A:725:PRO:HD3  | 1.99                     | 0.41              |
| 1:B:119:HIS:CD2  | 1:B:288:ASN:HD22 | 2.39                     | 0.41              |
| 1:B:163:CYS:O    | 1:B:169:THR:HG21 | 2.21                     | 0.41              |
| 1:B:375:MET:HB2  | 1:B:375:MET:HE3  | 1.73                     | 0.41              |
| 1:B:399:GLU:O    | 1:B:402:LEU:HG   | 2.21                     | 0.41              |
| 1:B:474:LEU:O    | 1:B:498:LEU:HD12 | 2.21                     | 0.41              |
| 1:C:341:TRP:NE1  | 1:C:345:ARG:HE   | 2.19                     | 0.41              |
| 1:D:492:ARG:HA   | 1:D:515:LEU:HD13 | 2.02                     | 0.41              |
| 1:E:587:LEU:HB2  | 1:E:609:SER:HB3  | 2.02                     | 0.41              |
| 1:F:428:LEU:H    | 1:F:449:GLU:CD   | 2.29                     | 0.41              |
| 1:A:352:SER:HB3  | 1:A:354:GLU:HG2  | 2.03                     | 0.41              |
| 1:A:642:THR:HB   | 1:A:665:GLU:OE2  | 2.21                     | 0.41              |
| 1:B:413:LEU:HG   | 1:B:417:ARG:HH12 | 1.85                     | 0.41              |
| 1:B:465:ILE:HD13 | 1:B:491:LEU:HD21 | 2.03                     | 0.41              |
| 1:C:168:TRP:CZ2  | 1:C:402:LEU:HD13 | 2.56                     | 0.41              |
| 1:C:786:VAL:HG13 | 1:C:791:PHE:HB2  | 2.03                     | 0.41              |
| 1:D:114:TYR:CE1  | 1:D:118:LEU:HD22 | 2.56                     | 0.41              |
| 1:D:258:ASP:OD1  | 1:D:349:LYS:HE2  | 2.21                     | 0.41              |
| 1:D:447:GLU:OE1  | 1:D:447:GLU:N    | 2.46                     | 0.41              |
| 1:E:145:LYS:HA   | 1:E:145:LYS:HD3  | 1.91                     | 0.41              |
| 1:E:244:PHE:CE1  | 1:E:393:PHE:HA   | 2.56                     | 0.41              |
| 1:E:249:LYS:O    | 1:E:252:THR:OG1  | 2.34                     | 0.41              |
| 1:E:404:GLN:HE22 | 1:E:407:LEU:HD23 | 1.85                     | 0.41              |
| 1:E:415:LYS:HA   | 1:E:415:LYS:HD3  | 1.84                     | 0.41              |
| 1:E:632:ILE:HG22 | 1:E:635:PHE:CE2  | 2.56                     | 0.41              |
| 1:E:688:ARG:C    | 1:E:710:LEU:HD12 | 2.46                     | 0.41              |
| 1:F:356:ILE:HG23 | 1:F:388:LYS:NZ   | 2.36                     | 0.41              |
| 1:F:591:VAL:O    | 1:F:615:ASN:ND2  | 2.53                     | 0.41              |
| 1:F:780:LYS:O    | 1:F:784:LEU:N    | 2.54                     | 0.41              |
| 1:A:398:SER:HA   | 1:A:401:LYS:HG2  | 2.03                     | 0.40              |
| 1:D:780:LYS:HE3  | 1:D:780:LYS:HB2  | 1.89                     | 0.40              |
| 1:E:364:ASP:O    | 1:E:395:SER:HA   | 2.21                     | 0.40              |
| 1:E:420:LEU:HD12 | 1:E:430:LEU:HD13 | 2.03                     | 0.40              |
| 1:F:112:VAL:HG12 | 1:F:297:VAL:HG11 | 2.03                     | 0.40              |
| 1:F:258:ASP:HB2  | 1:F:370:ASN:HD22 | 1.86                     | 0.40              |
| 1:F:345:ARG:HG2  | 1:F:346:ARG:HD3  | 2.03                     | 0.40              |
| 1:F:521:LEU:O    | 1:F:549:LEU:HA   | 2.21                     | 0.40              |
| 2:H:72:LEU:HD23  | 2:H:73:ASP:N     | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:423:ASN:OD1  | 1:B:427:LYS:N    | 2.38                     | 0.40              |
| 1:B:547:LYS:HA   | 1:B:547:LYS:HD3  | 1.85                     | 0.40              |
| 1:C:452:LYS:HE2  | 1:C:454:GLU:CD   | 2.47                     | 0.40              |
| 1:D:155:HIS:HB3  | 1:D:250:PHE:CE2  | 2.56                     | 0.40              |
| 1:D:265:MET:HE3  | 1:D:265:MET:HB3  | 2.00                     | 0.40              |
| 1:D:645:LYS:HG2  | 1:D:668:TYR:HD1  | 1.86                     | 0.40              |
| 1:E:349:LYS:HE3  | 1:E:370:ASN:HB3  | 2.02                     | 0.40              |
| 1:F:379:ILE:O    | 1:F:383:ASP:N    | 2.44                     | 0.40              |
| 1:F:713:LEU:O    | 1:F:737:HIS:N    | 2.54                     | 0.40              |
| 1:A:635:PHE:HB2  | 1:A:661:LEU:HD21 | 2.02                     | 0.40              |
| 1:B:682:PHE:CG   | 1:B:703:ASP:HB3  | 2.56                     | 0.40              |
| 1:C:45:LEU:HD12  | 1:C:45:LEU:HA    | 1.88                     | 0.40              |
| 1:C:137:LEU:HD23 | 1:C:137:LEU:HA   | 1.84                     | 0.40              |
| 1:C:415:LYS:HG3  | 1:C:419:ARG:NH1  | 2.36                     | 0.40              |
| 1:C:454:GLU:HB3  | 1:C:477:TYR:HB2  | 2.03                     | 0.40              |
| 1:D:397:VAL:HA   | 1:D:400:ASN:ND2  | 2.36                     | 0.40              |
| 1:E:63:ASP:N     | 1:E:63:ASP:OD1   | 2.53                     | 0.40              |
| 1:E:483:ILE:HD11 | 1:E:491:LEU:HD12 | 2.03                     | 0.40              |
| 1:F:404:GLN:OE1  | 1:F:408:ASN:ND2  | 2.53                     | 0.40              |
| 2:G:36:TRP:CD1   | 2:G:81:LEU:HD22  | 2.55                     | 0.40              |
| 2:I:6:GLU:HB3    | 2:I:22:CYS:HB2   | 2.03                     | 0.40              |
| 2:I:12:VAL:HG12  | 2:I:123:VAL:HG22 | 2.03                     | 0.40              |
| 1:A:516:LYS:NZ   | 1:A:544:LYS:HG2  | 2.36                     | 0.40              |
| 1:B:364:ASP:OD1  | 1:B:364:ASP:N    | 2.52                     | 0.40              |
| 1:C:102:ASP:OD2  | 1:D:106:TYR:OH   | 2.24                     | 0.40              |
| 1:C:143:TRP:NE1  | 1:C:144:PHE:HD1  | 2.20                     | 0.40              |
| 1:C:483:ILE:HD11 | 1:C:491:LEU:HD12 | 2.02                     | 0.40              |
| 1:C:621:LEU:HD12 | 1:C:646:LEU:HD22 | 2.03                     | 0.40              |
| 1:D:636:GLN:NE2  | 1:D:660:ASN:HB3  | 2.37                     | 0.40              |
| 1:D:800:GLU:HG2  | 1:D:804:ARG:NE   | 2.36                     | 0.40              |
| 1:A:38:ILE:HG13  | 1:A:39:ALA:N     | 2.37                     | 0.40              |
| 1:A:542:GLU:OE1  | 1:A:542:GLU:N    | 2.55                     | 0.40              |
| 1:B:115:GLU:HG3  | 1:C:291:PHE:CD1  | 2.56                     | 0.40              |
| 1:B:143:TRP:CD1  | 1:B:143:TRP:H    | 2.40                     | 0.40              |
| 1:B:444:ASP:OD1  | 1:B:445:LEU:HD22 | 2.21                     | 0.40              |
| 1:B:665:GLU:OE1  | 1:B:666:ARG:HG3  | 2.21                     | 0.40              |
| 1:C:259:ILE:HD12 | 1:C:262:ARG:HD3  | 2.03                     | 0.40              |
| 1:C:275:PHE:CD1  | 1:C:333:GLY:HA3  | 2.56                     | 0.40              |
| 1:C:505:ILE:HD12 | 1:C:536:VAL:HG11 | 2.04                     | 0.40              |
| 1:D:636:GLN:HE21 | 1:D:660:ASN:HB3  | 1.86                     | 0.40              |
| 1:E:614:HIS:O    | 1:E:640:ARG:NE   | 2.54                     | 0.40              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:F:560:GLN:H | 1:F:560:GLN:HG3 | 1.74                     | 0.40              |
| 1:F:603:LEU:H | 1:F:624:ASN:CG  | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 712/810 (88%)   | 679 (95%)  | 33 (5%)  | 0        | 100         | 100 |
| 1   | B     | 712/810 (88%)   | 683 (96%)  | 29 (4%)  | 0        | 100         | 100 |
| 1   | C     | 712/810 (88%)   | 685 (96%)  | 27 (4%)  | 0        | 100         | 100 |
| 1   | D     | 712/810 (88%)   | 686 (96%)  | 26 (4%)  | 0        | 100         | 100 |
| 1   | E     | 712/810 (88%)   | 680 (96%)  | 32 (4%)  | 0        | 100         | 100 |
| 1   | F     | 712/810 (88%)   | 682 (96%)  | 30 (4%)  | 0        | 100         | 100 |
| 2   | G     | 122/154 (79%)   | 121 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 2   | H     | 122/154 (79%)   | 119 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 2   | I     | 122/154 (79%)   | 120 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 4638/5322 (87%) | 4455 (96%) | 183 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

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

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 666/749 (89%)   | 634 (95%)  | 32 (5%)  | 23          | 47 |
| 1   | B     | 666/749 (89%)   | 625 (94%)  | 41 (6%)  | 16          | 42 |
| 1   | C     | 666/749 (89%)   | 640 (96%)  | 26 (4%)  | 28          | 52 |
| 1   | D     | 666/749 (89%)   | 626 (94%)  | 40 (6%)  | 17          | 43 |
| 1   | E     | 666/749 (89%)   | 637 (96%)  | 29 (4%)  | 25          | 49 |
| 1   | F     | 666/749 (89%)   | 633 (95%)  | 33 (5%)  | 22          | 47 |
| 2   | G     | 96/120 (80%)    | 83 (86%)   | 13 (14%) | 4           | 19 |
| 2   | H     | 96/120 (80%)    | 87 (91%)   | 9 (9%)   | 8           | 30 |
| 2   | I     | 96/120 (80%)    | 85 (88%)   | 11 (12%) | 5           | 23 |
| All | All   | 4284/4854 (88%) | 4050 (94%) | 234 (6%) | 21          | 45 |

All (234) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | VAL  |
| 1   | A     | 60  | VAL  |
| 1   | A     | 65  | CYS  |
| 1   | A     | 97  | ILE  |
| 1   | A     | 102 | ASP  |
| 1   | A     | 104 | HIS  |
| 1   | A     | 231 | VAL  |
| 1   | A     | 260 | VAL  |
| 1   | A     | 267 | GLN  |
| 1   | A     | 269 | ILE  |
| 1   | A     | 274 | LYS  |
| 1   | A     | 278 | ILE  |
| 1   | A     | 293 | VAL  |
| 1   | A     | 297 | VAL  |
| 1   | A     | 307 | THR  |
| 1   | A     | 323 | SER  |
| 1   | A     | 340 | LEU  |
| 1   | A     | 375 | MET  |
| 1   | A     | 405 | LEU  |
| 1   | A     | 412 | THR  |
| 1   | A     | 420 | LEU  |
| 1   | A     | 445 | LEU  |
| 1   | A     | 471 | LEU  |
| 1   | A     | 473 | GLU  |
| 1   | A     | 499 | HIS  |
| 1   | A     | 583 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 605 | ARG  |
| 1   | A     | 625 | ASN  |
| 1   | A     | 707 | LEU  |
| 1   | A     | 709 | ASN  |
| 1   | A     | 729 | GLN  |
| 1   | A     | 738 | LEU  |
| 1   | B     | 17  | TYR  |
| 1   | B     | 36  | LEU  |
| 1   | B     | 47  | VAL  |
| 1   | B     | 49  | GLN  |
| 1   | B     | 60  | VAL  |
| 1   | B     | 65  | CYS  |
| 1   | B     | 104 | HIS  |
| 1   | B     | 158 | SER  |
| 1   | B     | 165 | ASP  |
| 1   | B     | 169 | THR  |
| 1   | B     | 173 | LEU  |
| 1   | B     | 252 | THR  |
| 1   | B     | 269 | ILE  |
| 1   | B     | 275 | PHE  |
| 1   | B     | 279 | ILE  |
| 1   | B     | 286 | VAL  |
| 1   | B     | 329 | VAL  |
| 1   | B     | 368 | VAL  |
| 1   | B     | 375 | MET  |
| 1   | B     | 394 | LEU  |
| 1   | B     | 397 | VAL  |
| 1   | B     | 418 | GLN  |
| 1   | B     | 429 | GLU  |
| 1   | B     | 468 | LEU  |
| 1   | B     | 479 | THR  |
| 1   | B     | 568 | HIS  |
| 1   | B     | 575 | ASN  |
| 1   | B     | 584 | LEU  |
| 1   | B     | 594 | THR  |
| 1   | B     | 599 | ILE  |
| 1   | B     | 602 | ASP  |
| 1   | B     | 620 | ASP  |
| 1   | B     | 623 | ASP  |
| 1   | B     | 626 | LEU  |
| 1   | B     | 638 | LEU  |
| 1   | B     | 646 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 674 | ILE  |
| 1   | B     | 694 | HIS  |
| 1   | B     | 743 | LEU  |
| 1   | B     | 750 | VAL  |
| 1   | B     | 797 | GLU  |
| 1   | C     | 49  | GLN  |
| 1   | C     | 60  | VAL  |
| 1   | C     | 102 | ASP  |
| 1   | C     | 103 | ARG  |
| 1   | C     | 104 | HIS  |
| 1   | C     | 149 | THR  |
| 1   | C     | 231 | VAL  |
| 1   | C     | 260 | VAL  |
| 1   | C     | 267 | GLN  |
| 1   | C     | 269 | ILE  |
| 1   | C     | 274 | LYS  |
| 1   | C     | 292 | ASP  |
| 1   | C     | 293 | VAL  |
| 1   | C     | 294 | ASP  |
| 1   | C     | 297 | VAL  |
| 1   | C     | 323 | SER  |
| 1   | C     | 340 | LEU  |
| 1   | C     | 405 | LEU  |
| 1   | C     | 412 | THR  |
| 1   | C     | 413 | LEU  |
| 1   | C     | 420 | LEU  |
| 1   | C     | 500 | ILE  |
| 1   | C     | 583 | VAL  |
| 1   | C     | 644 | LEU  |
| 1   | C     | 677 | ILE  |
| 1   | C     | 738 | LEU  |
| 1   | D     | 17  | TYR  |
| 1   | D     | 36  | LEU  |
| 1   | D     | 65  | CYS  |
| 1   | D     | 104 | HIS  |
| 1   | D     | 134 | LEU  |
| 1   | D     | 155 | HIS  |
| 1   | D     | 158 | SER  |
| 1   | D     | 163 | CYS  |
| 1   | D     | 165 | ASP  |
| 1   | D     | 173 | LEU  |
| 1   | D     | 236 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 252 | THR  |
| 1   | D     | 275 | PHE  |
| 1   | D     | 279 | ILE  |
| 1   | D     | 286 | VAL  |
| 1   | D     | 303 | THR  |
| 1   | D     | 329 | VAL  |
| 1   | D     | 348 | LEU  |
| 1   | D     | 353 | PHE  |
| 1   | D     | 394 | LEU  |
| 1   | D     | 397 | VAL  |
| 1   | D     | 401 | LYS  |
| 1   | D     | 402 | LEU  |
| 1   | D     | 405 | LEU  |
| 1   | D     | 413 | LEU  |
| 1   | D     | 414 | ASP  |
| 1   | D     | 450 | VAL  |
| 1   | D     | 478 | HIS  |
| 1   | D     | 479 | THR  |
| 1   | D     | 503 | THR  |
| 1   | D     | 520 | GLU  |
| 1   | D     | 542 | GLU  |
| 1   | D     | 568 | HIS  |
| 1   | D     | 626 | LEU  |
| 1   | D     | 635 | PHE  |
| 1   | D     | 647 | TRP  |
| 1   | D     | 661 | LEU  |
| 1   | D     | 736 | LEU  |
| 1   | D     | 743 | LEU  |
| 1   | D     | 765 | ARG  |
| 1   | E     | 60  | VAL  |
| 1   | E     | 63  | ASP  |
| 1   | E     | 97  | ILE  |
| 1   | E     | 102 | ASP  |
| 1   | E     | 104 | HIS  |
| 1   | E     | 231 | VAL  |
| 1   | E     | 260 | VAL  |
| 1   | E     | 267 | GLN  |
| 1   | E     | 269 | ILE  |
| 1   | E     | 274 | LYS  |
| 1   | E     | 278 | ILE  |
| 1   | E     | 297 | VAL  |
| 1   | E     | 323 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 340 | LEU  |
| 1   | E     | 344 | LEU  |
| 1   | E     | 358 | GLU  |
| 1   | E     | 412 | THR  |
| 1   | E     | 431 | HIS  |
| 1   | E     | 434 | MET  |
| 1   | E     | 445 | LEU  |
| 1   | E     | 448 | LEU  |
| 1   | E     | 507 | GLU  |
| 1   | E     | 552 | LYS  |
| 1   | E     | 625 | ASN  |
| 1   | E     | 644 | LEU  |
| 1   | E     | 681 | LEU  |
| 1   | E     | 743 | LEU  |
| 1   | E     | 744 | GLN  |
| 1   | E     | 769 | LEU  |
| 1   | F     | 17  | TYR  |
| 1   | F     | 49  | GLN  |
| 1   | F     | 60  | VAL  |
| 1   | F     | 65  | CYS  |
| 1   | F     | 104 | HIS  |
| 1   | F     | 109 | VAL  |
| 1   | F     | 134 | LEU  |
| 1   | F     | 158 | SER  |
| 1   | F     | 163 | CYS  |
| 1   | F     | 173 | LEU  |
| 1   | F     | 252 | THR  |
| 1   | F     | 275 | PHE  |
| 1   | F     | 279 | ILE  |
| 1   | F     | 286 | VAL  |
| 1   | F     | 293 | VAL  |
| 1   | F     | 300 | GLU  |
| 1   | F     | 329 | VAL  |
| 1   | F     | 353 | PHE  |
| 1   | F     | 397 | VAL  |
| 1   | F     | 402 | LEU  |
| 1   | F     | 421 | THR  |
| 1   | F     | 442 | VAL  |
| 1   | F     | 450 | VAL  |
| 1   | F     | 479 | THR  |
| 1   | F     | 568 | HIS  |
| 1   | F     | 570 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 594 | THR  |
| 1   | F     | 625 | ASN  |
| 1   | F     | 626 | LEU  |
| 1   | F     | 644 | LEU  |
| 1   | F     | 677 | ILE  |
| 1   | F     | 694 | HIS  |
| 1   | F     | 736 | LEU  |
| 2   | G     | 3   | GLN  |
| 2   | G     | 6   | GLU  |
| 2   | G     | 30  | GLN  |
| 2   | G     | 33  | TYR  |
| 2   | G     | 45  | ARG  |
| 2   | G     | 51  | LEU  |
| 2   | G     | 70  | VAL  |
| 2   | G     | 79  | VAL  |
| 2   | G     | 82  | GLN  |
| 2   | G     | 83  | MET  |
| 2   | G     | 90  | ASP  |
| 2   | G     | 100 | TYR  |
| 2   | G     | 119 | THR  |
| 2   | I     | 3   | GLN  |
| 2   | I     | 6   | GLU  |
| 2   | I     | 45  | ARG  |
| 2   | I     | 51  | LEU  |
| 2   | I     | 53  | THR  |
| 2   | I     | 71  | SER  |
| 2   | I     | 79  | VAL  |
| 2   | I     | 83  | MET  |
| 2   | I     | 90  | ASP  |
| 2   | I     | 100 | TYR  |
| 2   | I     | 119 | THR  |
| 2   | H     | 3   | GLN  |
| 2   | H     | 30  | GLN  |
| 2   | H     | 33  | TYR  |
| 2   | H     | 51  | LEU  |
| 2   | H     | 70  | VAL  |
| 2   | H     | 79  | VAL  |
| 2   | H     | 83  | MET  |
| 2   | H     | 90  | ASP  |
| 2   | H     | 119 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 49  | GLN  |
| 1   | A     | 409 | ASN  |
| 1   | A     | 718 | ASN  |
| 1   | B     | 288 | ASN  |
| 1   | B     | 522 | HIS  |
| 1   | B     | 576 | ASN  |
| 1   | B     | 592 | ASN  |
| 1   | B     | 755 | ASN  |
| 1   | C     | 49  | GLN  |
| 1   | C     | 288 | ASN  |
| 1   | C     | 409 | ASN  |
| 1   | C     | 660 | ASN  |
| 1   | C     | 694 | HIS  |
| 1   | C     | 709 | ASN  |
| 1   | C     | 718 | ASN  |
| 1   | D     | 377 | HIS  |
| 1   | D     | 499 | HIS  |
| 1   | D     | 592 | ASN  |
| 1   | D     | 639 | HIS  |
| 1   | D     | 708 | GLN  |
| 1   | E     | 105 | GLN  |
| 1   | E     | 288 | ASN  |
| 1   | E     | 409 | ASN  |
| 1   | E     | 672 | ASN  |
| 1   | E     | 708 | GLN  |
| 1   | E     | 709 | ASN  |
| 1   | E     | 718 | ASN  |
| 1   | F     | 575 | ASN  |
| 1   | F     | 576 | ASN  |
| 1   | F     | 592 | ASN  |
| 1   | F     | 708 | GLN  |
| 1   | F     | 755 | ASN  |
| 2   | I     | 82  | GLN  |
| 2   | I     | 84  | ASN  |
| 2   | H     | 82  | GLN  |
| 2   | H     | 84  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

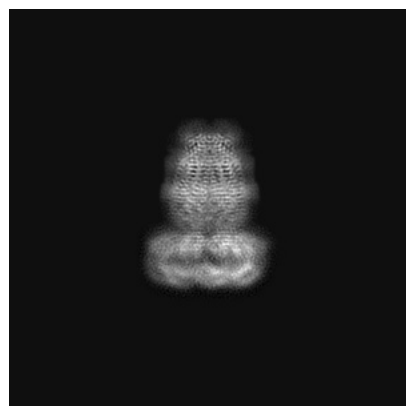
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13213. These allow visual inspection of the internal detail of the map and identification of artifacts.

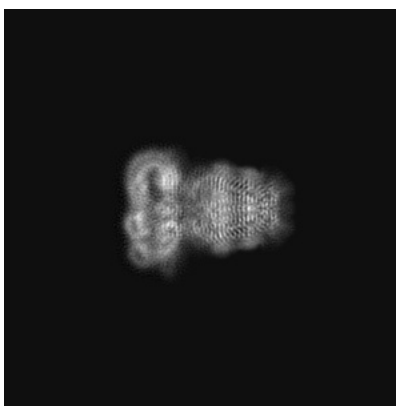
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

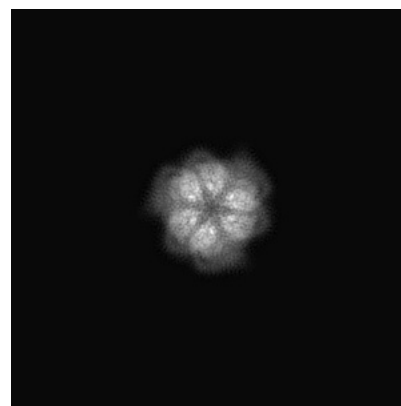
#### 6.1.1 Primary map



X



Y

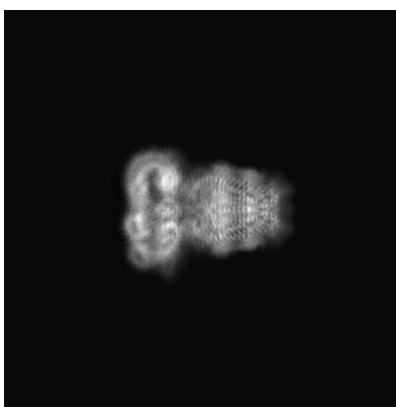


Z

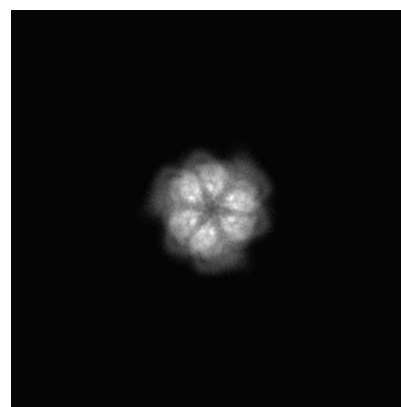
#### 6.1.2 Raw map



X



Y

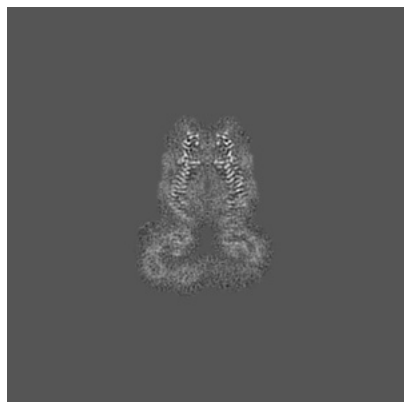


Z

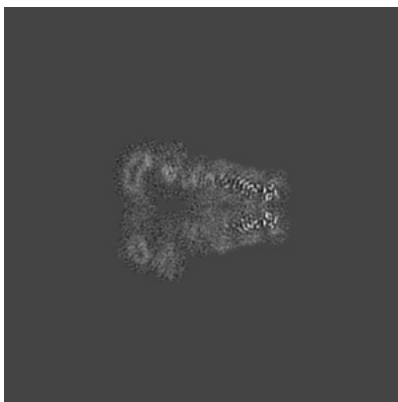
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

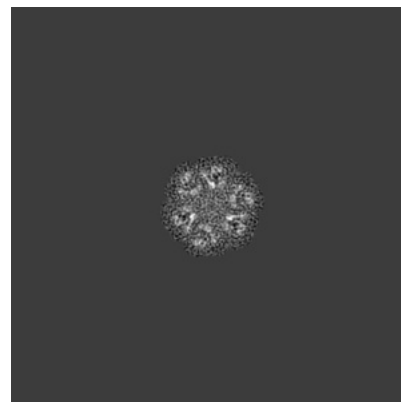
### 6.2.1 Primary map



X Index: 168

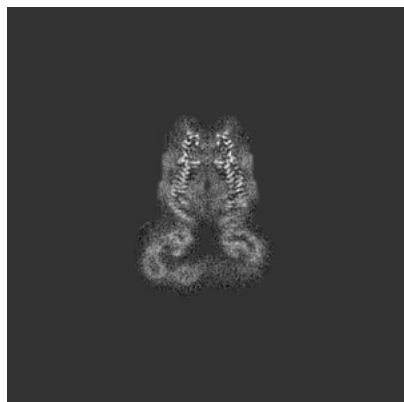


Y Index: 168

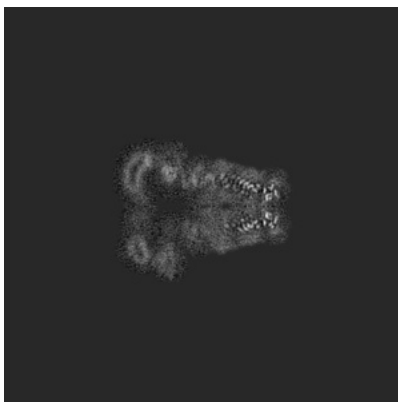


Z Index: 168

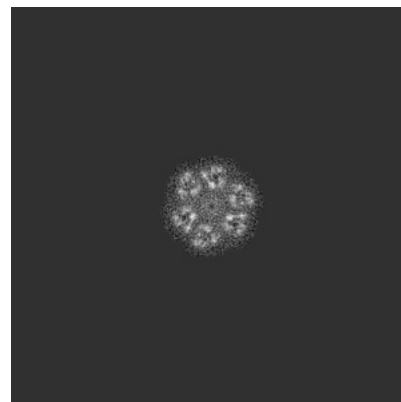
### 6.2.2 Raw map



X Index: 168



Y Index: 168

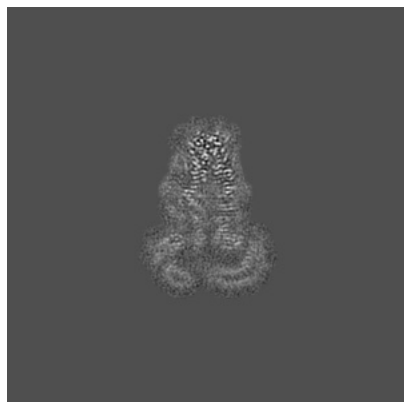


Z Index: 168

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

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

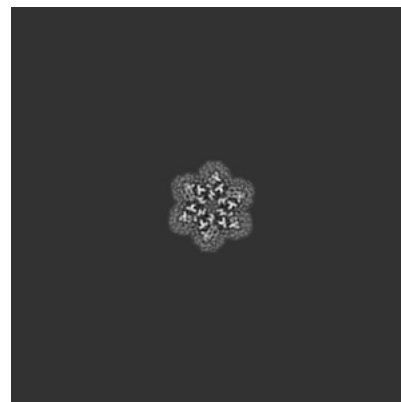
### 6.3.1 Primary map



X Index: 154

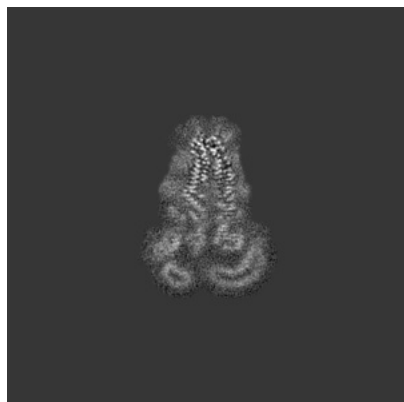


Y Index: 177

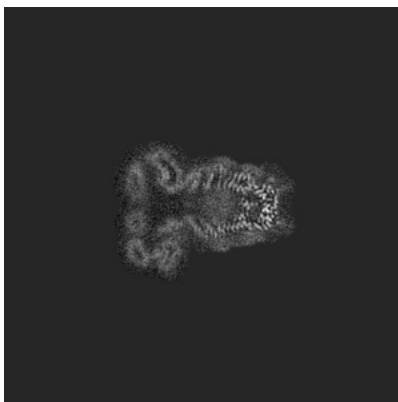


Z Index: 205

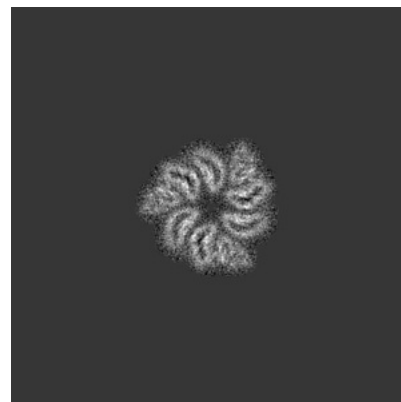
### 6.3.2 Raw map



X Index: 153



Y Index: 177

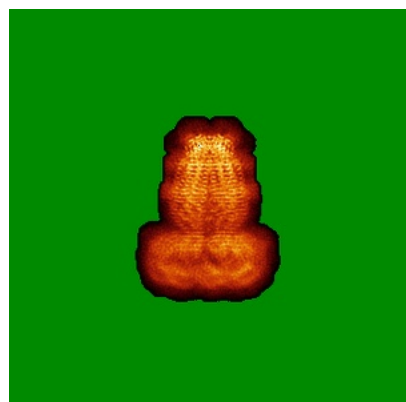


Z Index: 137

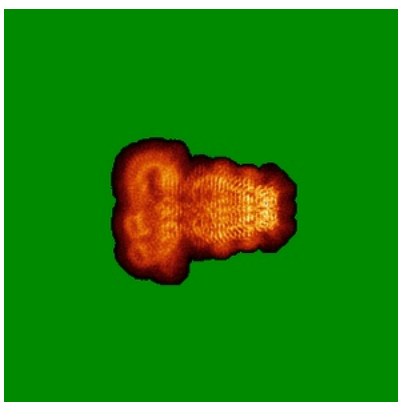
The images above show the largest variance slices of the map in three orthogonal directions.

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

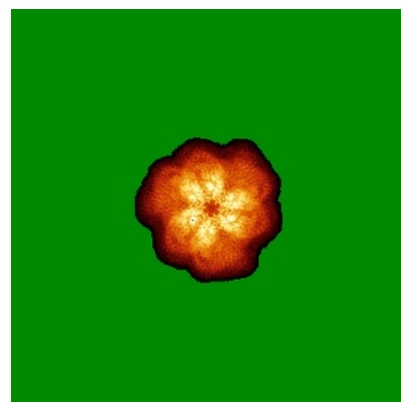
### 6.4.1 Primary map



X

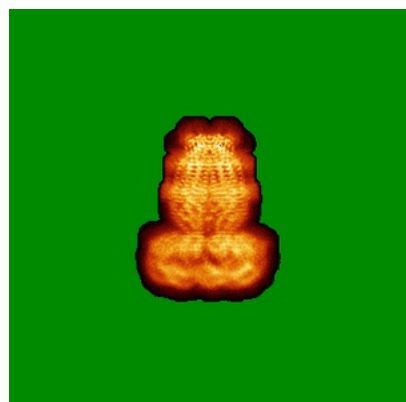


Y

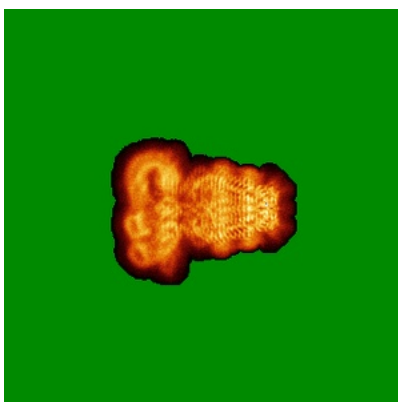


Z

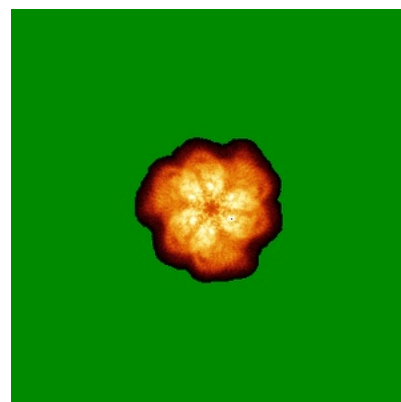
### 6.4.2 Raw map



X



Y

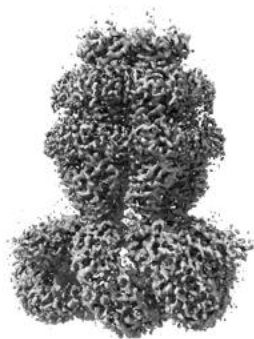


Z

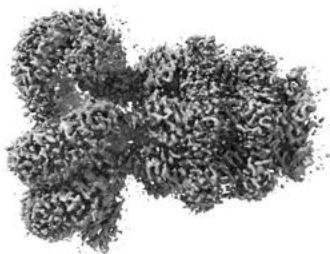
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

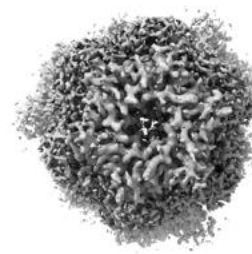
### 6.5.1 Primary map



X



Y



Z

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

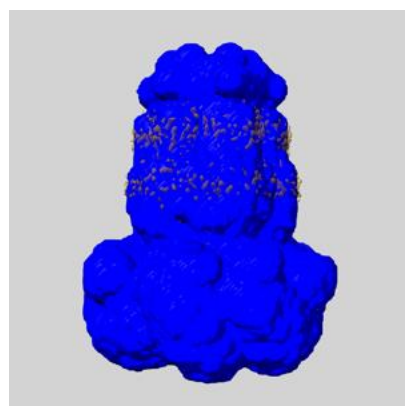
## 6.6 Mask visualisation [i](#)

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

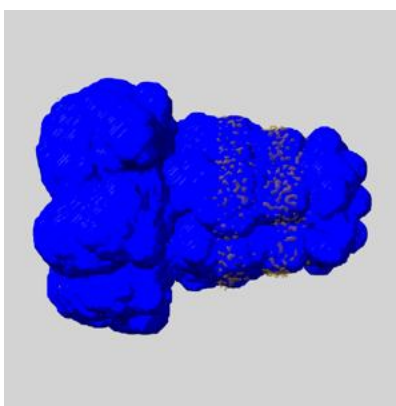
A mask typically either:

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

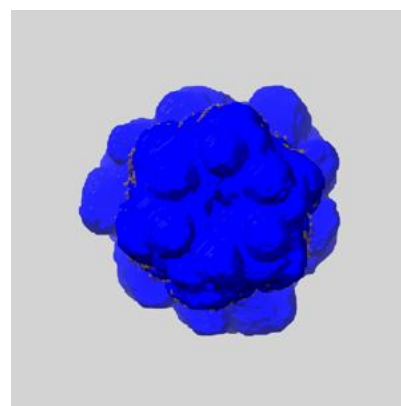
### 6.6.1 emd\_13213\_msk\_1.map [i](#)



X



Y

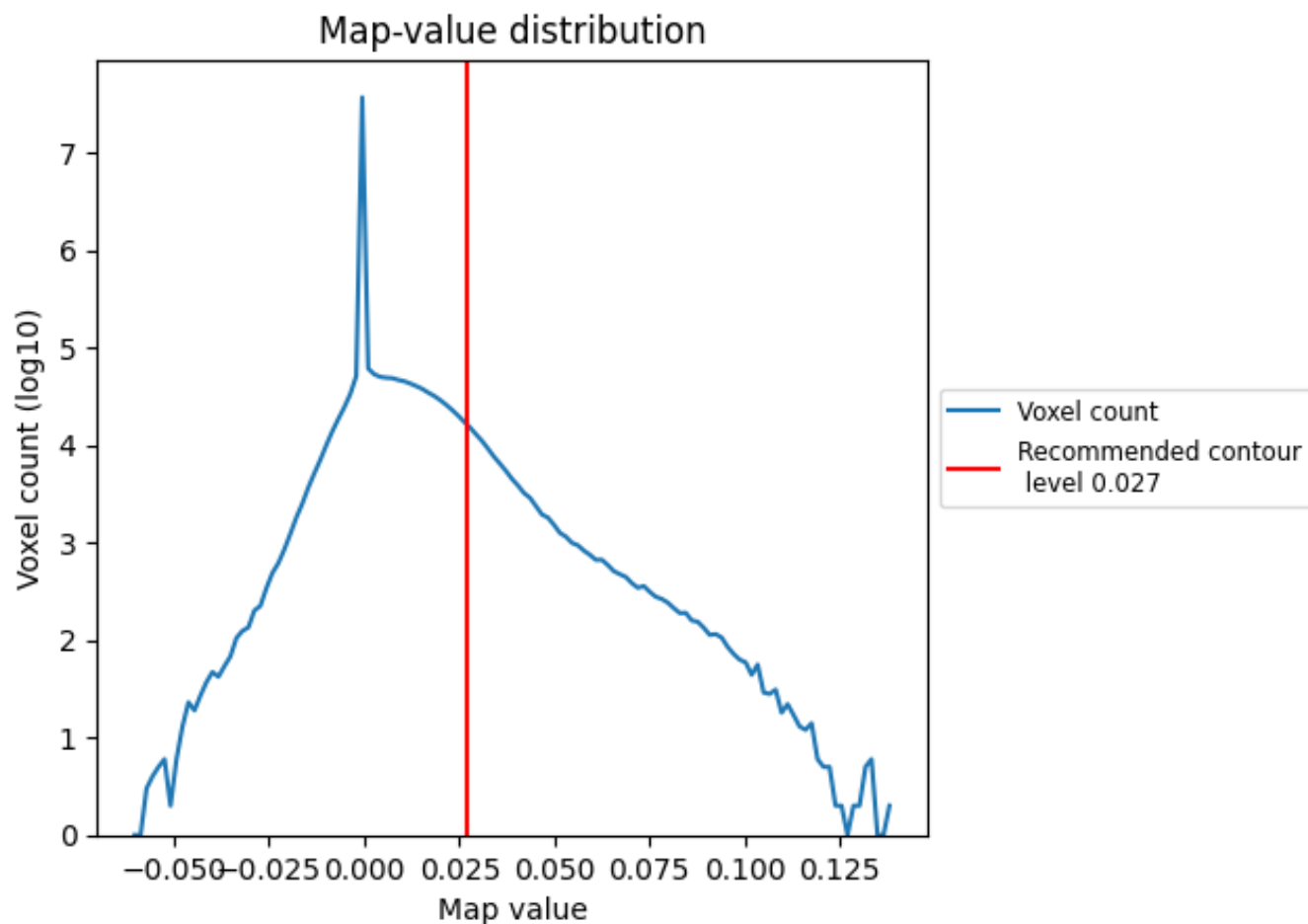


Z

## 7 Map analysis [i](#)

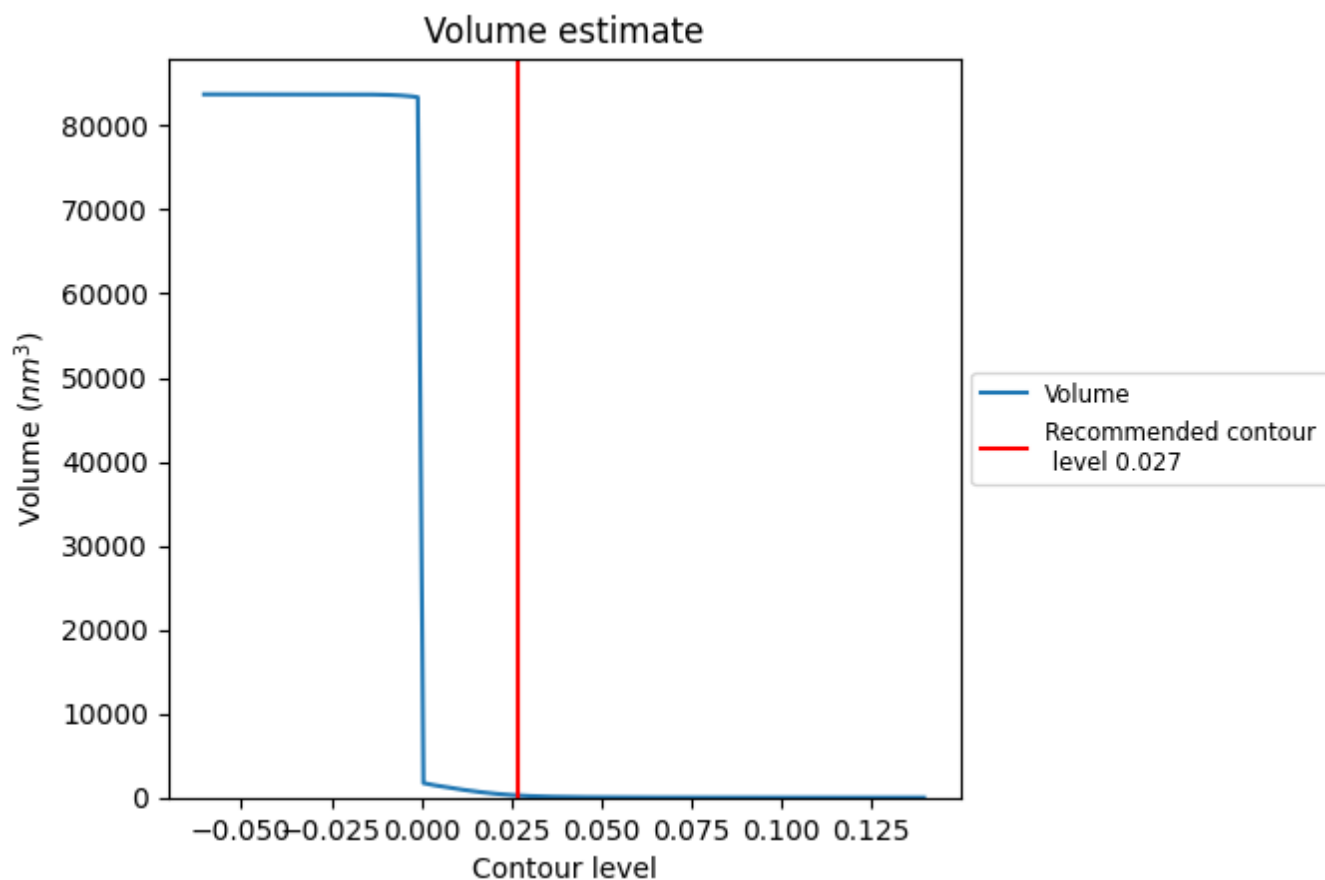
This section contains the results of statistical analysis of the map.

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



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

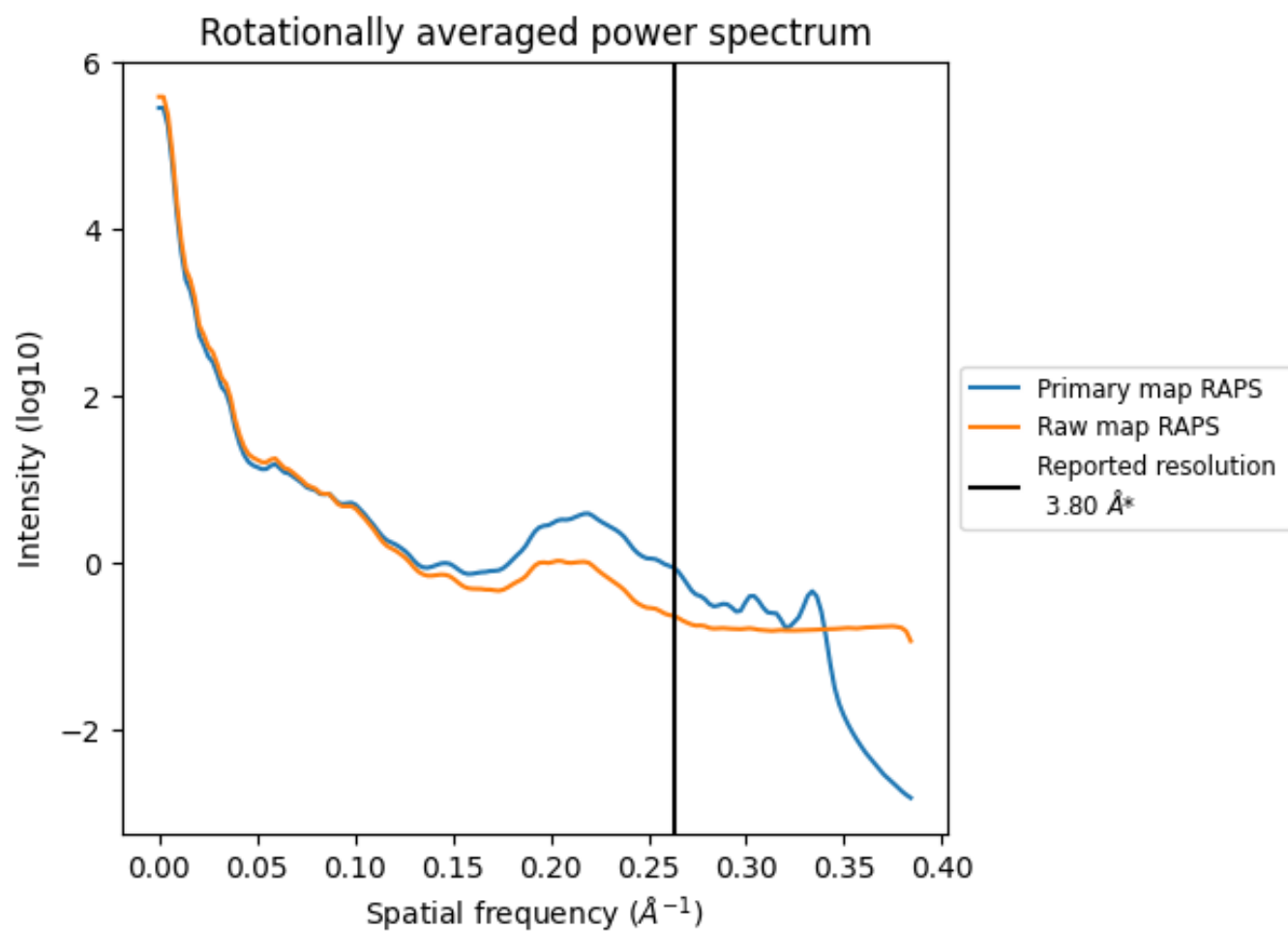
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 248 nm<sup>3</sup>; this corresponds to an approximate mass of 224 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 ⓘ

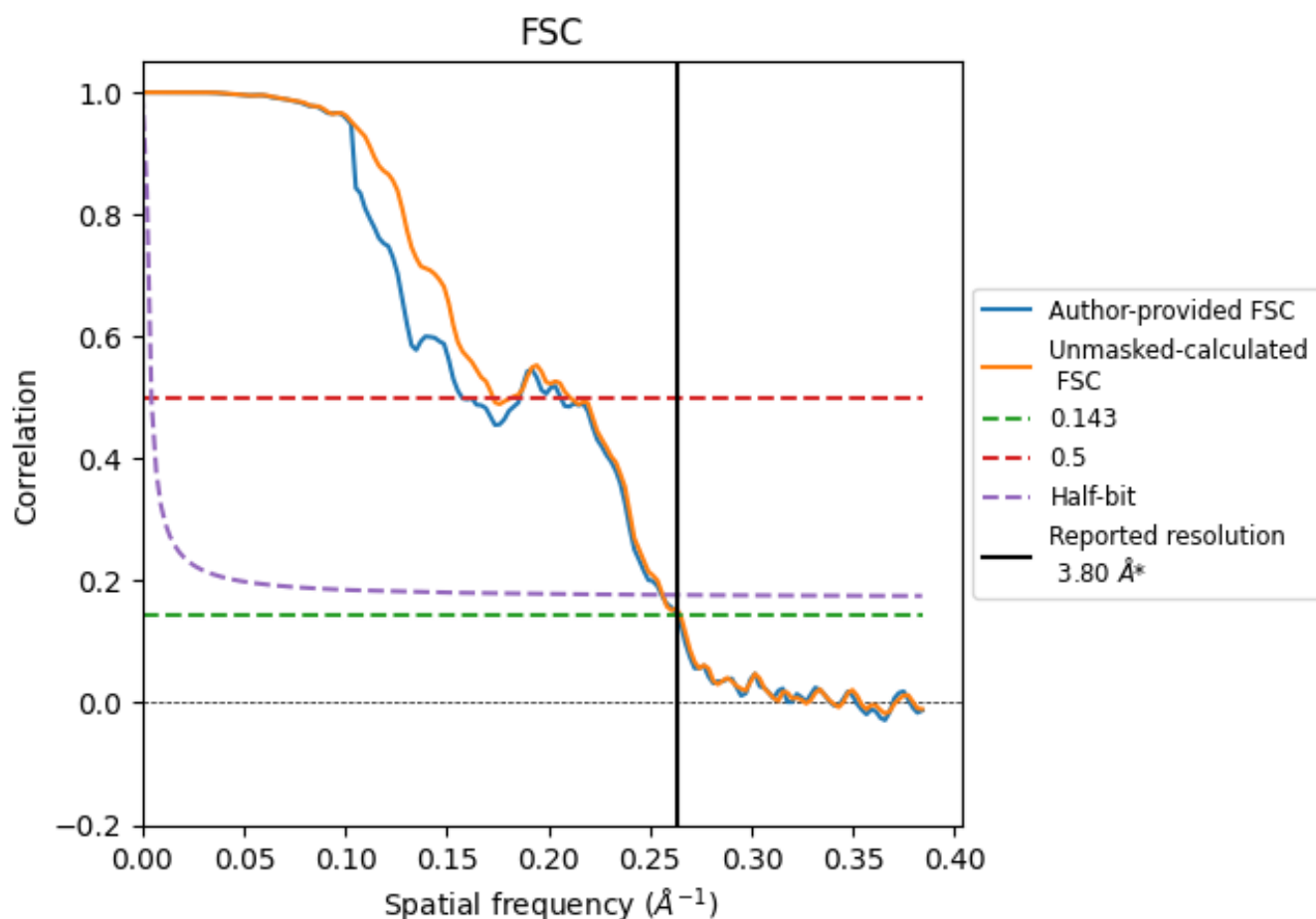


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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  $0.263 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

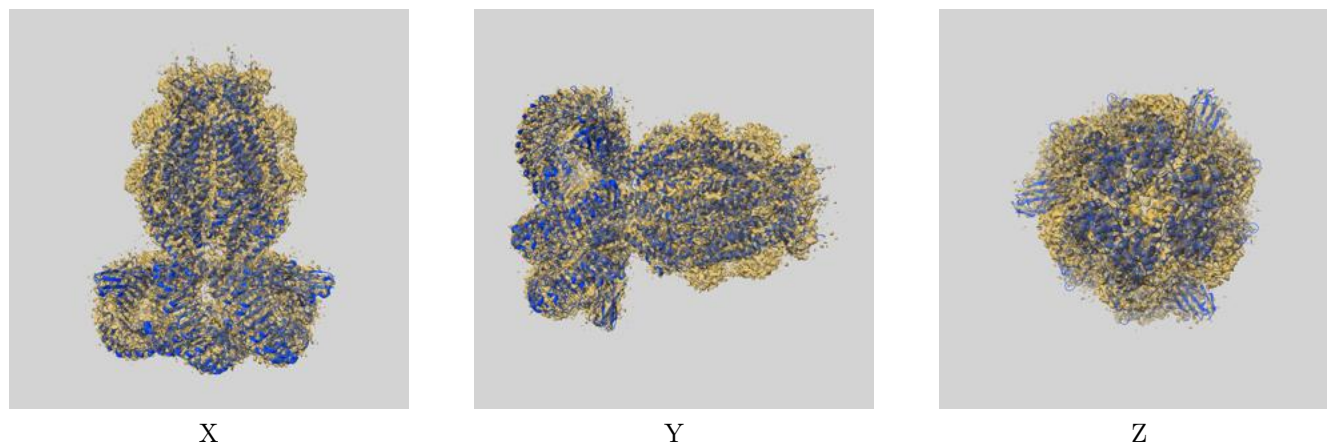
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.80                               | -    | -        |
| Author-provided FSC curve | 3.79                               | 6.35 | 3.91     |
| Unmasked-calculated*      | 3.77                               | 5.79 | 3.90     |

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

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

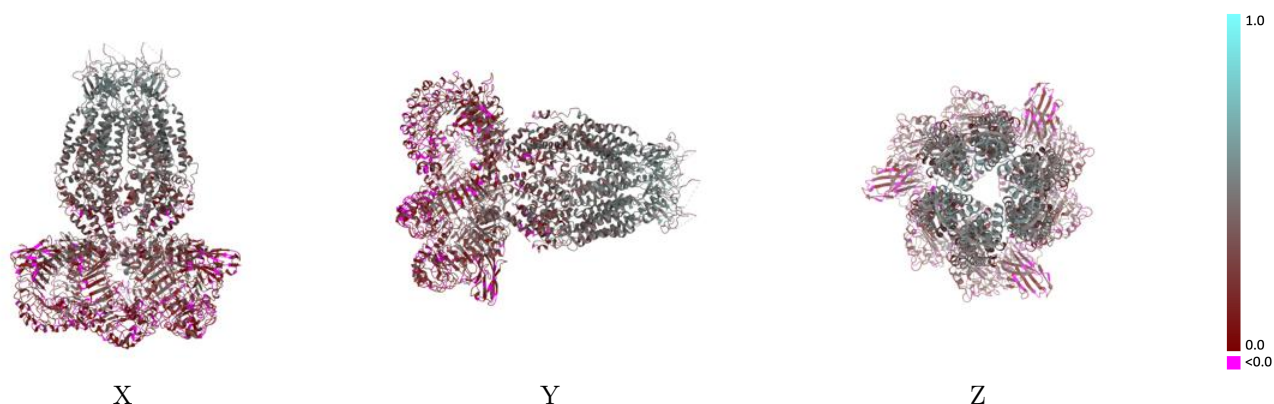
This section contains information regarding the fit between EMDB map EMD-13213 and PDB model 7P60. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



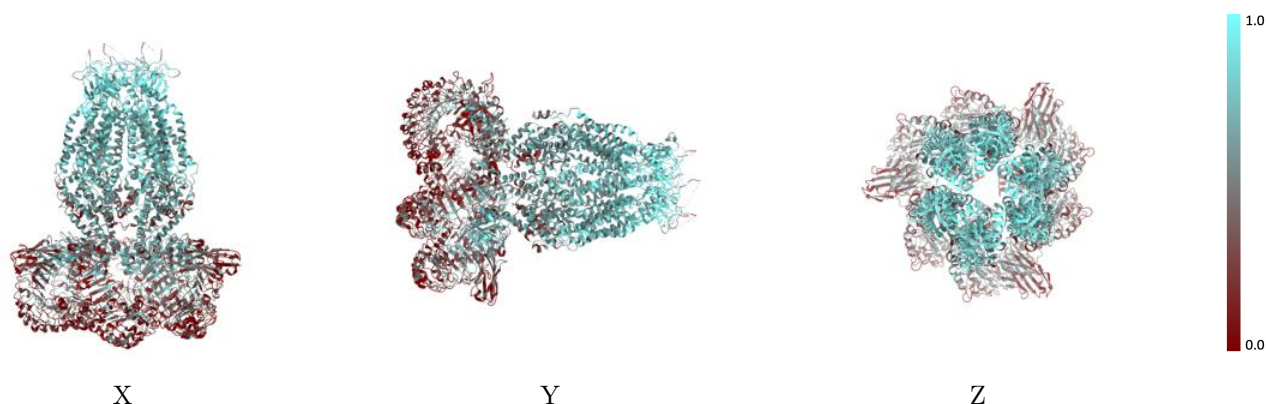
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



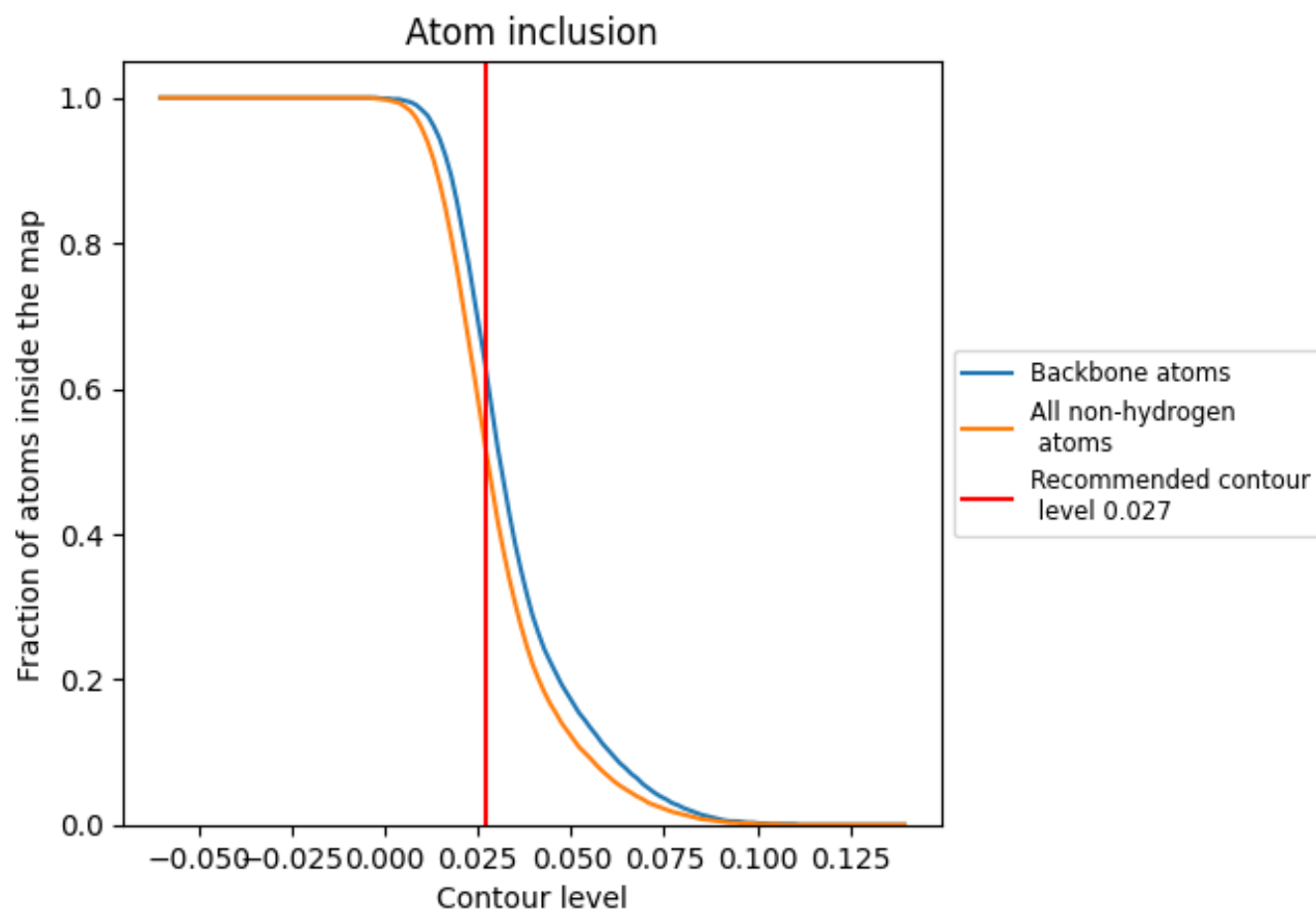
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.027) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.5200 | <div></div> 0.2810 |
| A     | <div></div> 0.5180 | <div></div> 0.2840 |
| B     | <div></div> 0.5500 | <div></div> 0.3040 |
| C     | <div></div> 0.5160 | <div></div> 0.2810 |
| D     | <div></div> 0.5500 | <div></div> 0.3020 |
| E     | <div></div> 0.5210 | <div></div> 0.2830 |
| F     | <div></div> 0.5540 | <div></div> 0.3010 |
| G     | <div></div> 0.3300 | <div></div> 0.1490 |
| H     | <div></div> 0.3290 | <div></div> 0.1520 |
| I     | <div></div> 0.3210 | <div></div> 0.1380 |

1.0

0.0

<0.0