



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:20 PM UTC

PDB ID : 8RD9 / pdb\_00008rd9  
EMDB ID : EMD-19069  
Title : human TRPM4 in SMA NBA  
Authors : Ekundayo, B.; Prakash, A.; Christian, G.; Anne, F.H.; Sabrina, G.; Mey, B.; Daniela, R.; Martin, L.; Jean, S.R.; Henning, S.; Hugues, A.; Dongchun, N.  
Deposited on : 2023-12-07  
Resolution : 4.30 Å(reported)  
Based on initial model : 6BQV

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

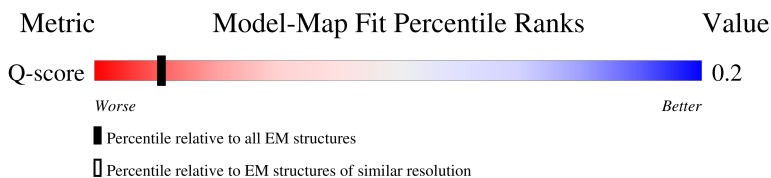
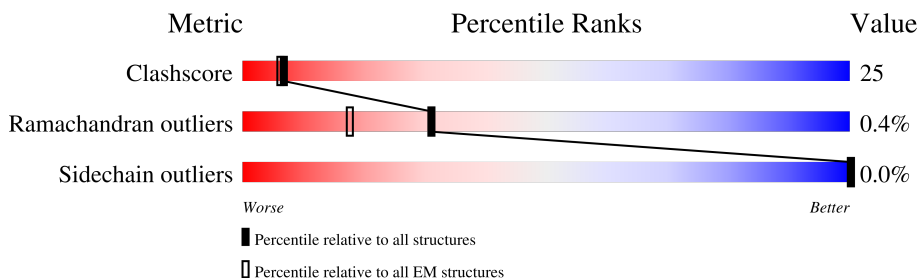
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 4585 ( 3.80 - 4.80 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 749    | <div> <div>9%</div> <div>49%</div> <div>32%</div> <div>19%</div> </div>  |
| 1   | C     | 749    | <div> <div>10%</div> <div>42%</div> <div>38%</div> <div>19%</div> </div> |
| 1   | D     | 749    | <div> <div>9%</div> <div>42%</div> <div>38%</div> <div>19%</div> </div>  |
| 1   | E     | 749    | <div> <div>11%</div> <div>52%</div> <div>28%</div> <div>19%</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | CLR  | A     | 1203 | -         | -        | X       | -                |
| 3   | CLR  | A     | 1205 | -         | -        | X       | -                |
| 3   | CLR  | C     | 1202 | -         | -        | X       | -                |
| 3   | CLR  | D     | 1201 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

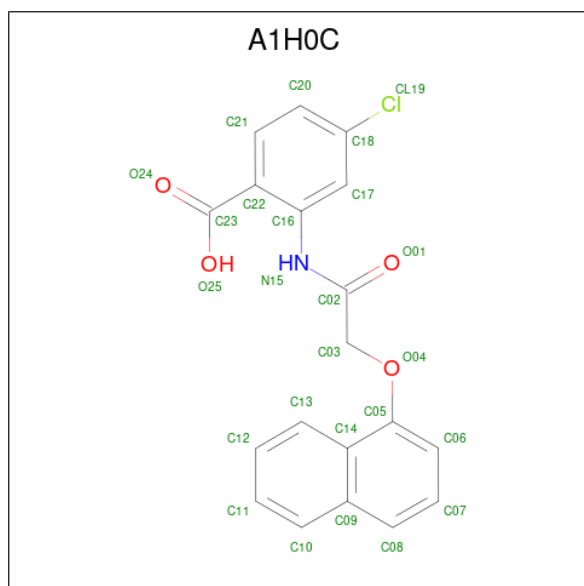
There are 3 unique types of molecules in this entry. The entry contains 20320 atoms, of which 368 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4914  | 3210 | 858 | 815 | 31 |         |       |
| 1   | E     | 605      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4900  | 3199 | 856 | 814 | 31 |         |       |
| 1   | C     | 605      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4900  | 3199 | 856 | 814 | 31 |         |       |
| 1   | D     | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4914  | 3210 | 858 | 815 | 31 |         |       |

- Molecule 2 is 4-chloranyl-2-(2-naphthalen-1-yloxyethanoylamino)benzoic acid (CCD ID: A1H0C) (formula: C<sub>19</sub>H<sub>14</sub>ClNO<sub>4</sub>).



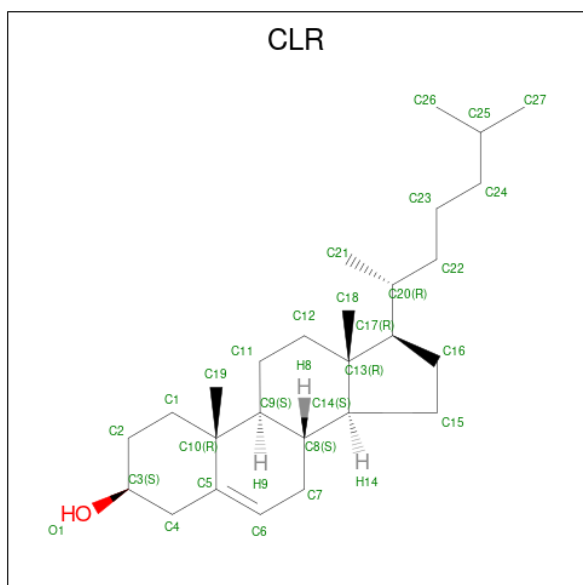
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 2   | A     | 1        | Total | C  | Cl | N | O | 0       |
|     |       |          | 25    | 19 | 1  | 1 | 4 |         |
| 2   | E     | 1        | Total | C  | Cl | N | O | 0       |
|     |       |          | 25    | 19 | 1  | 1 | 4 |         |

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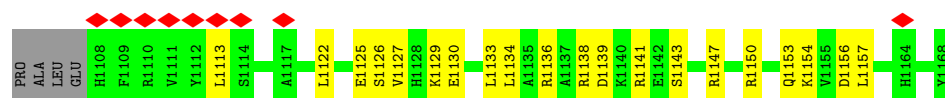
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 2   | C     | 1        | Total | C  | Cl | N | O | 0       |
|     |       |          | 25    | 19 | 1  | 1 | 4 |         |
| 2   | D     | 1        | Total | C  | Cl | N | O | 0       |
|     |       |          | 25    | 19 | 1  | 1 | 4 |         |

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ).

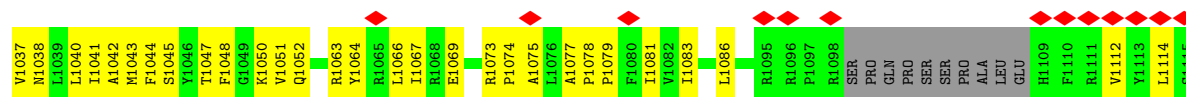
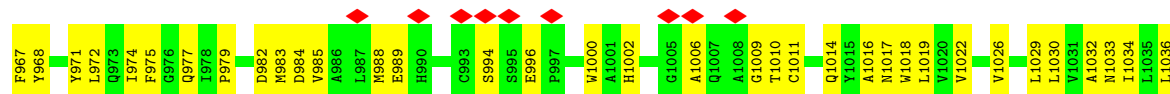
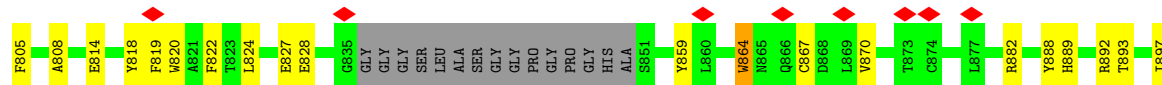
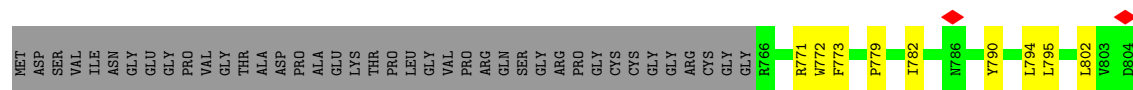
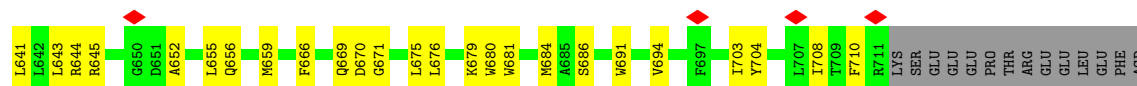
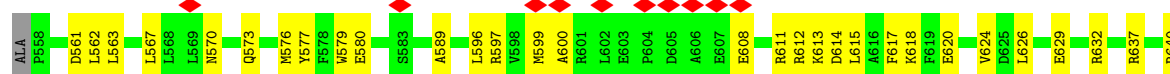
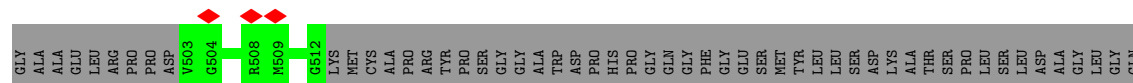
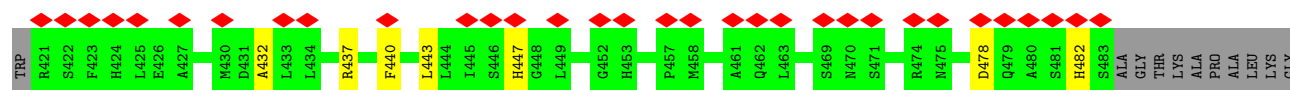


| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 3   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 3   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 3   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 3   | A     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 3   | C     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 3   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 3   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |
| 3   | D     | 1        | Total | C  | H  | O | 0       |
|     |       |          | 74    | 27 | 46 | 1 |         |





- Molecule 1: Transient receptor potential cation channel subfamily M member 4



- Molecule 1: Transient receptor potential cation channel subfamily M member 4







## 4 Experimental information

| Property                             | Value                   | Source    |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE         | Depositor |
| Imposed symmetry                     | POINT, Not provided     |           |
| Number of particles used             | 50000                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF       | Depositor |
| CTF correction method                | NONE                    | Depositor |
| Microscope                           | TFS KRIOS               | Depositor |
| Voltage (kV)                         | 300                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                      | Depositor |
| Minimum defocus (nm)                 | 800                     | Depositor |
| Maximum defocus (nm)                 | 2500                    | Depositor |
| Magnification                        | Not provided            |           |
| Image detector                       | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value                    | 0.562                   | Depositor |
| Minimum map value                    | -0.211                  | Depositor |
| Average map value                    | 0.007                   | Depositor |
| Map value standard deviation         | 0.028                   | Depositor |
| Recommended contour level            | 0.126                   | Depositor |
| Map size ( $\text{\AA}$ )            | 290.4, 290.4, 290.4     | wwPDB     |
| Map dimensions                       | 200, 200, 200           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.452, 1.452, 1.452     | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, A1H0C

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     | 0.16         | 0/5040  | 0.42        | 0/6824         |
| 1   | C     | 0.22         | 0/5024  | 0.62        | 1/6801 (0.0%)  |
| 1   | D     | 0.21         | 0/5040  | 0.61        | 0/6824         |
| 1   | E     | 0.14         | 0/5024  | 0.40        | 0/6801         |
| All | All   | 0.18         | 0/20128 | 0.52        | 1/27250 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | C     | 0                   | 3                   |
| 1   | D     | 0                   | 2                   |
| All | All   | 0                   | 5                   |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 864 | TRP  | N-CA-C | -6.30 | 104.10      | 110.97   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 586 | VAL  | Peptide   |
| 1   | C     | 648 | LEU  | Peptide   |
| 1   | C     | 768 | CYS  | Mainchain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 578 | PHE  | Mainchain |
| 1   | D     | 580 | GLU  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4914  | 0        | 4995     | 223     | 0            |
| 1   | C     | 4900  | 0        | 4985     | 279     | 0            |
| 1   | D     | 4914  | 0        | 4995     | 305     | 0            |
| 1   | E     | 4900  | 0        | 4985     | 215     | 0            |
| 2   | A     | 25    | 0        | 0        | 2       | 0            |
| 2   | C     | 25    | 0        | 0        | 1       | 0            |
| 2   | D     | 25    | 0        | 0        | 5       | 0            |
| 2   | E     | 25    | 0        | 0        | 5       | 0            |
| 3   | A     | 112   | 184      | 181      | 67      | 0            |
| 3   | C     | 28    | 46       | 43       | 36      | 0            |
| 3   | D     | 84    | 138      | 138      | 78      | 0            |
| All | All   | 19952 | 368      | 20322    | 987     | 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 25.

All (987) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:803:VAL:HG22 | 3:D:1201:CLR:C2   | 1.39                     | 1.51              |
| 1:D:803:VAL:CG2  | 3:D:1201:CLR:H22  | 1.37                     | 1.49              |
| 1:A:795:LEU:CD2  | 3:A:1205:CLR:H263 | 1.39                     | 1.47              |
| 1:D:803:VAL:HG21 | 3:D:1201:CLR:C4   | 1.52                     | 1.38              |
| 3:A:1203:CLR:C27 | 1:E:795:LEU:HD22  | 1.55                     | 1.33              |
| 1:A:799:ARG:CG   | 3:A:1205:CLR:C19  | 2.09                     | 1.30              |
| 1:D:794:LEU:CD1  | 3:D:1201:CLR:H25  | 1.59                     | 1.29              |
| 1:D:803:VAL:CG2  | 3:D:1201:CLR:H42  | 1.69                     | 1.22              |
| 1:C:798:SER:OG   | 3:C:1202:CLR:H212 | 1.38                     | 1.18              |
| 1:D:803:VAL:HG22 | 3:D:1201:CLR:C3   | 1.74                     | 1.17              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:795:LEU:CD1   | 3:A:1205:CLR:H162  | 1.76                     | 1.16              |
| 1:D:803:VAL:CG2   | 3:D:1201:CLR:C2    | 2.07                     | 1.15              |
| 1:A:799:ARG:HG2   | 3:A:1205:CLR:C19   | 1.74                     | 1.14              |
| 1:C:803:VAL:HG21  | 3:C:1202:CLR:C2    | 1.76                     | 1.13              |
| 1:A:799:ARG:HG3   | 3:A:1205:CLR:C19   | 1.76                     | 1.12              |
| 1:D:803:VAL:CG2   | 3:D:1201:CLR:C3    | 2.27                     | 1.12              |
| 1:A:799:ARG:HG3   | 3:A:1205:CLR:H191  | 1.31                     | 1.11              |
| 1:C:798:SER:OG    | 3:C:1202:CLR:C21   | 1.99                     | 1.10              |
| 1:D:968:TYR:HB2   | 3:D:1202:CLR:H161  | 1.23                     | 1.10              |
| 1:A:795:LEU:HD22  | 3:A:1205:CLR:C26   | 1.82                     | 1.10              |
| 1:E:1018:TRP:HB2  | 3:D:1202:CLR:C19   | 1.80                     | 1.10              |
| 1:D:794:LEU:HD11  | 3:D:1201:CLR:H25   | 1.11                     | 1.09              |
| 1:D:578:PHE:O     | 1:D:580:GLU:N      | 1.84                     | 1.09              |
| 1:A:799:ARG:HG2   | 3:A:1205:CLR:H192  | 1.33                     | 1.08              |
| 1:E:962:ILE:HD13  | 3:D:1201:CLR:C2    | 1.82                     | 1.08              |
| 1:E:908:HIS:CD2   | 2:E:1201:A1H0C:O24 | 2.08                     | 1.07              |
| 1:A:799:ARG:CG    | 3:A:1205:CLR:H192  | 1.82                     | 1.07              |
| 3:A:1203:CLR:H272 | 1:E:795:LEU:HD22   | 1.11                     | 1.06              |
| 1:D:803:VAL:HG23  | 3:D:1201:CLR:H22   | 1.30                     | 1.05              |
| 1:A:795:LEU:CD2   | 3:A:1205:CLR:C26   | 2.35                     | 1.01              |
| 1:E:962:ILE:HD13  | 3:D:1201:CLR:H21   | 1.43                     | 1.00              |
| 1:D:803:VAL:CG2   | 3:D:1201:CLR:C4    | 2.28                     | 1.00              |
| 1:C:795:LEU:HD22  | 3:C:1202:CLR:C27   | 1.92                     | 1.00              |
| 1:D:794:LEU:HD11  | 3:D:1201:CLR:C25   | 1.92                     | 0.99              |
| 1:A:795:LEU:HD21  | 3:A:1205:CLR:H263  | 1.42                     | 0.98              |
| 1:C:803:VAL:HG21  | 3:C:1202:CLR:H21   | 1.00                     | 0.98              |
| 1:E:1018:TRP:HB2  | 3:D:1202:CLR:H191  | 1.45                     | 0.97              |
| 1:E:962:ILE:HG21  | 3:D:1201:CLR:H12   | 1.47                     | 0.96              |
| 1:C:803:VAL:CG2   | 3:C:1202:CLR:H21   | 1.96                     | 0.96              |
| 1:E:962:ILE:HD13  | 3:D:1201:CLR:C1    | 1.95                     | 0.95              |
| 1:D:951:LEU:HD13  | 1:D:1020:VAL:HG22  | 1.45                     | 0.95              |
| 1:E:1018:TRP:CB   | 3:D:1202:CLR:C19   | 2.45                     | 0.94              |
| 1:A:795:LEU:HD22  | 3:A:1205:CLR:H263  | 0.94                     | 0.93              |
| 3:C:1202:CLR:H213 | 1:D:946:VAL:HG22   | 1.50                     | 0.93              |
| 1:E:908:HIS:NE2   | 2:E:1201:A1H0C:O24 | 2.03                     | 0.92              |
| 1:D:803:VAL:HG23  | 3:D:1201:CLR:H192  | 1.51                     | 0.92              |
| 1:D:794:LEU:HD13  | 3:D:1201:CLR:H25   | 1.50                     | 0.92              |
| 1:D:802:LEU:HD22  | 3:D:1201:CLR:H111  | 1.54                     | 0.90              |
| 1:D:794:LEU:CD1   | 3:D:1201:CLR:C25   | 2.49                     | 0.89              |
| 1:E:962:ILE:HG21  | 3:D:1201:CLR:C1    | 2.03                     | 0.88              |
| 1:D:803:VAL:HG22  | 3:D:1201:CLR:H22   | 0.99                     | 0.88              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C:795:LEU:HD22  | 3:C:1202:CLR:C25   | 2.04                     | 0.88              |
| 3:C:1202:CLR:H41  | 1:D:959:PHE:CD1    | 2.09                     | 0.87              |
| 3:A:1203:CLR:H271 | 1:E:795:LEU:HD22   | 1.56                     | 0.87              |
| 3:A:1203:CLR:C27  | 1:E:795:LEU:CD2    | 2.48                     | 0.86              |
| 3:A:1204:CLR:H162 | 1:C:1025:VAL:HG21  | 1.58                     | 0.85              |
| 1:C:795:LEU:HD22  | 3:C:1202:CLR:H25   | 1.58                     | 0.84              |
| 1:D:1021:VAL:HG11 | 3:D:1204:CLR:H151  | 1.59                     | 0.84              |
| 1:D:798:SER:OG    | 3:D:1201:CLR:H183  | 1.77                     | 0.83              |
| 1:C:586:VAL:O     | 1:C:588:SER:N      | 2.12                     | 0.83              |
| 3:C:1202:CLR:H213 | 1:D:946:VAL:CG2    | 2.08                     | 0.83              |
| 1:D:802:LEU:CD2   | 3:D:1201:CLR:H111  | 2.08                     | 0.82              |
| 1:A:864:TRP:HD1   | 2:A:1201:A1H0C:O24 | 1.63                     | 0.82              |
| 1:E:962:ILE:CD1   | 3:D:1201:CLR:C2    | 2.59                     | 0.81              |
| 3:A:1203:CLR:H151 | 1:E:802:LEU:HD12   | 1.60                     | 0.81              |
| 1:E:962:ILE:CD1   | 3:D:1201:CLR:H21   | 2.10                     | 0.81              |
| 1:A:795:LEU:CD1   | 3:A:1205:CLR:C16   | 2.57                     | 0.81              |
| 1:A:795:LEU:HD13  | 3:A:1205:CLR:H162  | 1.62                     | 0.80              |
| 1:A:1134:LEU:HB3  | 1:A:1138:ARG:HH12  | 1.45                     | 0.80              |
| 1:E:962:ILE:HD13  | 3:D:1201:CLR:H12   | 1.64                     | 0.80              |
| 1:D:791:LEU:HD13  | 1:D:794:LEU:HD21   | 1.64                     | 0.80              |
| 1:E:1018:TRP:CB   | 3:D:1202:CLR:H191  | 2.11                     | 0.79              |
| 1:D:594:LEU:HD22  | 1:D:657:LEU:HD22   | 1.64                     | 0.79              |
| 1:C:599:MET:HB3   | 1:C:612:ARG:HD3    | 1.65                     | 0.79              |
| 3:C:1202:CLR:C21  | 1:D:946:VAL:HG22   | 2.13                     | 0.78              |
| 3:C:1202:CLR:C21  | 1:D:946:VAL:CG2    | 2.61                     | 0.78              |
| 1:C:703:ILE:HA    | 1:C:708:ILE:HD11   | 1.65                     | 0.78              |
| 1:A:795:LEU:HD12  | 3:A:1205:CLR:H152  | 1.67                     | 0.77              |
| 1:C:624:VAL:HG12  | 1:C:666:PHE:HD2    | 1.49                     | 0.77              |
| 1:C:430:MET:SD    | 1:C:459:ARG:NH2    | 2.58                     | 0.77              |
| 1:E:947:ALA:HB2   | 1:D:900:MET:HE3    | 1.66                     | 0.77              |
| 1:A:795:LEU:HD12  | 3:A:1205:CLR:C15   | 2.15                     | 0.76              |
| 1:C:766:ARG:HH21  | 1:C:768:CYS:HB2    | 1.48                     | 0.76              |
| 1:E:1018:TRP:CB   | 3:D:1202:CLR:H192  | 2.13                     | 0.76              |
| 3:A:1203:CLR:H272 | 1:E:795:LEU:CD2    | 2.05                     | 0.76              |
| 3:C:1202:CLR:C4   | 1:D:959:PHE:HD1    | 1.95                     | 0.75              |
| 1:A:1134:LEU:HB3  | 1:A:1138:ARG:NH1   | 2.01                     | 0.75              |
| 1:C:1147:ARG:HH22 | 1:D:1149:LYS:HA    | 1.52                     | 0.75              |
| 1:A:1039:LEU:HG   | 1:A:1043:PHE:CE2   | 2.22                     | 0.74              |
| 1:C:911:THR:HG22  | 1:C:920:ILE:HG21   | 1.69                     | 0.74              |
| 1:D:803:VAL:HG22  | 3:D:1201:CLR:O1    | 1.86                     | 0.74              |
| 1:A:900:MET:HE3   | 1:C:947:ALA:HB2    | 1.67                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:799:ARG:CG    | 3:A:1205:CLR:H191  | 1.94                     | 0.73              |
| 1:A:869:LEU:HD13  | 1:A:872:LEU:HD21   | 1.70                     | 0.73              |
| 1:D:798:SER:OG    | 3:D:1201:CLR:C18   | 2.35                     | 0.73              |
| 1:A:799:ARG:HG2   | 3:A:1205:CLR:H193  | 1.70                     | 0.73              |
| 1:C:583:SER:HB2   | 1:C:1122:LEU:HD11  | 1.71                     | 0.73              |
| 3:A:1203:CLR:H213 | 1:E:795:LEU:HD11   | 1.71                     | 0.73              |
| 1:A:864:TRP:CD1   | 2:A:1201:A1H0C:O24 | 2.42                     | 0.72              |
| 1:C:830:ARG:HH12  | 1:C:1072:ARG:HH21  | 1.36                     | 0.72              |
| 1:D:645:ARG:NH2   | 1:D:646:CYS:SG     | 2.61                     | 0.72              |
| 1:D:803:VAL:HG21  | 3:D:1201:CLR:H42   | 0.76                     | 0.72              |
| 1:D:1136:ARG:NH2  | 1:D:1139:ASP:OD2   | 2.22                     | 0.72              |
| 1:C:595:LEU:O     | 1:C:599:MET:HB2    | 1.89                     | 0.72              |
| 1:C:795:LEU:CD2   | 3:C:1202:CLR:H25   | 2.19                     | 0.72              |
| 1:C:803:VAL:HG21  | 3:C:1202:CLR:C1    | 2.20                     | 0.72              |
| 1:A:1154:LYS:HD2  | 1:C:1159:LEU:HD13  | 1.70                     | 0.72              |
| 1:E:629:GLU:HB2   | 1:E:632:ARG:HH21   | 1.55                     | 0.72              |
| 1:A:629:GLU:HA    | 1:A:632:ARG:HE     | 1.55                     | 0.72              |
| 1:C:644:ARG:NH2   | 1:C:1118:GLU:OE1   | 2.23                     | 0.71              |
| 1:D:703:ILE:HA    | 1:D:708:ILE:HD11   | 1.70                     | 0.71              |
| 1:C:427:ALA:HA    | 1:C:430:MET:HE2    | 1.71                     | 0.71              |
| 1:C:1088:LEU:O    | 1:C:1092:LEU:N     | 2.23                     | 0.71              |
| 1:D:864:TRP:CD1   | 2:D:1203:A1H0C:O24 | 2.44                     | 0.71              |
| 1:D:1089:LEU:O    | 1:D:1093:CYS:N     | 2.22                     | 0.71              |
| 1:E:996:GLU:HB3   | 1:E:1000:TRP:HZ2   | 1.55                     | 0.70              |
| 1:D:968:TYR:HB2   | 3:D:1202:CLR:C16   | 2.13                     | 0.70              |
| 1:A:808:ALA:O     | 1:A:882:ARG:NH2    | 2.24                     | 0.70              |
| 1:D:922:ILE:HG21  | 1:D:1047:PHE:HD1   | 1.56                     | 0.70              |
| 1:E:615:LEU:HD23  | 1:E:618:LYS:HZ2    | 1.57                     | 0.70              |
| 1:C:798:SER:OG    | 3:C:1202:CLR:H211  | 1.91                     | 0.70              |
| 1:C:903:THR:HG21  | 1:D:943:ALA:HB2    | 1.73                     | 0.70              |
| 1:D:908:HIS:CE1   | 2:D:1203:A1H0C:O24 | 2.45                     | 0.69              |
| 1:E:962:ILE:HD12  | 3:D:1201:CLR:H3    | 1.75                     | 0.69              |
| 1:D:618:LYS:O     | 1:D:622:MET:HG3    | 1.92                     | 0.69              |
| 1:E:1158:LEU:HA   | 1:E:1161:LYS:HE2   | 1.73                     | 0.69              |
| 1:D:1119:ARG:HE   | 1:D:1123:THR:HG1   | 1.40                     | 0.69              |
| 1:C:586:VAL:C     | 1:C:588:SER:H      | 2.00                     | 0.69              |
| 1:D:1064:ARG:NH1  | 1:D:1068:GLU:OE2   | 2.26                     | 0.69              |
| 1:C:869:LEU:HD13  | 1:C:872:LEU:HD21   | 1.73                     | 0.69              |
| 1:D:622:MET:HE2   | 1:D:1132:PHE:HE2   | 1.57                     | 0.69              |
| 3:A:1205:CLR:H183 | 3:A:1205:CLR:H212  | 1.75                     | 0.69              |
| 1:C:808:ALA:O     | 1:C:882:ARG:NH2    | 2.25                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:D:579:TRP:O     | 1:D:1129:LYS:NZ    | 2.25                     | 0.68              |
| 1:A:570:ASN:ND2   | 1:A:608:GLU:OE2    | 2.26                     | 0.68              |
| 1:E:808:ALA:O     | 1:E:882:ARG:NH2    | 2.25                     | 0.68              |
| 3:C:1202:CLR:H211 | 1:D:946:VAL:HG21   | 1.74                     | 0.68              |
| 1:A:795:LEU:HD11  | 3:A:1205:CLR:H162  | 1.73                     | 0.68              |
| 1:C:648:LEU:O     | 1:C:650:GLY:N      | 2.24                     | 0.68              |
| 1:A:795:LEU:HD12  | 3:A:1205:CLR:H162  | 1.76                     | 0.68              |
| 1:A:799:ARG:CG    | 3:A:1205:CLR:H193  | 2.22                     | 0.68              |
| 1:D:791:LEU:HD12  | 3:D:1201:CLR:H263  | 1.76                     | 0.68              |
| 1:A:571:ARG:HB3   | 1:A:574:MET:HE2    | 1.77                     | 0.67              |
| 1:D:803:VAL:HG21  | 3:D:1201:CLR:C3    | 2.05                     | 0.67              |
| 1:C:1154:LYS:HB3  | 1:D:1159:LEU:HD11  | 1.76                     | 0.67              |
| 1:A:1157:LEU:HD11 | 1:C:1159:LEU:HD11  | 1.76                     | 0.67              |
| 3:A:1204:CLR:H42  | 1:C:1018:TRP:HB2   | 1.77                     | 0.67              |
| 1:E:570:ASN:ND2   | 1:E:608:GLU:OE2    | 2.28                     | 0.67              |
| 1:E:1034:ILE:HD11 | 1:D:975:PHE:HZ     | 1.60                     | 0.67              |
| 1:C:900:MET:HE3   | 1:D:947:ALA:HB2    | 1.77                     | 0.67              |
| 1:E:1146:SER:O    | 1:D:1147:ARG:NH2   | 2.28                     | 0.67              |
| 1:C:615:LEU:HD23  | 1:C:618:LYS:HE3    | 1.76                     | 0.67              |
| 1:D:475:ASN:OD1   | 1:D:476:LEU:N      | 2.27                     | 0.67              |
| 1:C:645:ARG:NH2   | 1:C:653:THR:OG1    | 2.28                     | 0.67              |
| 1:E:962:ILE:CG2   | 3:D:1201:CLR:H112  | 2.25                     | 0.66              |
| 1:C:899:PHE:HE1   | 1:D:943:ALA:HA     | 1.60                     | 0.66              |
| 1:C:1134:LEU:HB3  | 1:C:1138:ARG:NH1   | 2.09                     | 0.66              |
| 1:A:939:VAL:HG11  | 1:E:907:LEU:HD21   | 1.78                     | 0.66              |
| 1:E:954:PRO:HB3   | 1:E:1009:GLY:HA3   | 1.76                     | 0.66              |
| 1:D:615:LEU:HA    | 1:D:618:LYS:HG2    | 1.76                     | 0.66              |
| 3:A:1203:CLR:H213 | 1:E:795:LEU:CD1    | 2.25                     | 0.66              |
| 1:C:1156:ASP:OD2  | 1:C:1157:LEU:N     | 2.29                     | 0.66              |
| 1:A:704:TYR:HE1   | 1:A:771:ARG:HG2    | 1.60                     | 0.66              |
| 1:C:820:TRP:CH2   | 1:C:1078:PRO:HG3   | 2.31                     | 0.66              |
| 3:C:1202:CLR:H242 | 1:D:942:VAL:HG21   | 1.77                     | 0.66              |
| 1:D:996:GLU:HB3   | 1:D:1000:TRP:HZ2   | 1.60                     | 0.66              |
| 1:E:908:HIS:NE2   | 2:E:1201:A1H0C:C23 | 2.60                     | 0.65              |
| 1:A:432:ALA:HA    | 1:A:437:ARG:HE     | 1.61                     | 0.65              |
| 1:D:702:LEU:HD12  | 1:D:705:THR:HG21   | 1.78                     | 0.65              |
| 1:A:932:PHE:HD1   | 1:E:916:LEU:HD22   | 1.61                     | 0.65              |
| 1:A:996:GLU:HB3   | 1:A:1000:TRP:HZ2   | 1.61                     | 0.65              |
| 1:A:972:LEU:HB3   | 1:A:977:GLN:HB2    | 1.77                     | 0.65              |
| 1:C:827:GLU:HA    | 1:C:830:ARG:HG2    | 1.77                     | 0.65              |
| 1:A:989:GLU:OE2   | 1:A:989:GLU:N      | 2.29                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:D:979:PRO:HB2   | 1:D:982:ASP:HB2    | 1.79                     | 0.65              |
| 1:A:959:PHE:HE1   | 3:A:1203:CLR:H111  | 1.62                     | 0.65              |
| 1:E:979:PRO:HB2   | 1:E:982:ASP:HB2    | 1.79                     | 0.65              |
| 1:C:1094:ARG:O    | 1:C:1094:ARG:NH1   | 2.23                     | 0.64              |
| 1:A:827:GLU:OE2   | 1:A:1072:ARG:NH1   | 2.29                     | 0.64              |
| 1:A:914:LYS:HE2   | 1:A:915:GLN:HE22   | 1.62                     | 0.64              |
| 1:C:426:GLU:HB3   | 1:C:459:ARG:HH22   | 1.62                     | 0.64              |
| 1:C:920:ILE:HG12  | 1:D:936:PHE:HZ     | 1.62                     | 0.64              |
| 1:E:1038:ASN:ND2  | 1:D:1040:ILE:HG12  | 2.13                     | 0.64              |
| 1:D:1088:LEU:O    | 1:D:1092:LEU:N     | 2.31                     | 0.64              |
| 1:A:795:LEU:HD12  | 3:A:1205:CLR:C16   | 2.27                     | 0.64              |
| 3:A:1203:CLR:H212 | 3:A:1203:CLR:H183  | 1.79                     | 0.64              |
| 1:D:596:LEU:O     | 1:D:600:ALA:HB2    | 1.98                     | 0.64              |
| 1:A:615:LEU:O     | 1:A:618:LYS:HG3    | 1.98                     | 0.64              |
| 1:D:791:LEU:CD1   | 3:D:1201:CLR:H263  | 2.28                     | 0.64              |
| 1:C:443:LEU:O     | 1:C:447:HIS:ND1    | 2.31                     | 0.63              |
| 1:E:1073:ARG:HD3  | 1:E:1074:PRO:HD2   | 1.80                     | 0.63              |
| 3:C:1202:CLR:H212 | 3:C:1202:CLR:H121  | 1.79                     | 0.63              |
| 1:D:577:TYR:O     | 1:D:581:MET:HG3    | 1.99                     | 0.63              |
| 1:E:962:ILE:CD1   | 3:D:1201:CLR:C3    | 2.77                     | 0.63              |
| 1:C:640:ARG:HB2   | 1:C:1113:LEU:HD11  | 1.80                     | 0.63              |
| 1:D:802:LEU:HD23  | 3:D:1201:CLR:H11   | 1.79                     | 0.63              |
| 1:C:438:PRO:O     | 1:C:442:ARG:HG2    | 1.99                     | 0.62              |
| 1:C:1031:ALA:HA   | 1:C:1035:LEU:HD23  | 1.81                     | 0.62              |
| 1:D:808:ALA:O     | 1:D:882:ARG:NH2    | 2.32                     | 0.62              |
| 1:A:579:TRP:HE1   | 1:A:585:ALA:HB1    | 1.65                     | 0.62              |
| 1:E:644:ARG:HH22  | 1:E:1119:GLU:HB2   | 1.65                     | 0.62              |
| 1:D:908:HIS:HE1   | 2:D:1203:A1H0C:O24 | 1.81                     | 0.62              |
| 1:C:964:ARG:NH2   | 1:D:984:ASP:OD2    | 2.24                     | 0.62              |
| 1:E:898:ASP:HA    | 1:E:901:VAL:HG22   | 1.82                     | 0.62              |
| 1:E:644:ARG:HD3   | 1:E:645:ARG:N      | 2.15                     | 0.62              |
| 1:C:584:ASN:O     | 1:C:588:SER:HB3    | 2.00                     | 0.62              |
| 1:D:917:GLY:HA3   | 1:D:1058:TRP:CD1   | 2.35                     | 0.62              |
| 1:A:1031:ALA:HA   | 1:A:1035:LEU:HD12  | 1.82                     | 0.61              |
| 1:C:503:VAL:HG21  | 1:C:598:VAL:HG21   | 1.81                     | 0.61              |
| 1:D:794:LEU:HD13  | 3:D:1201:CLR:C25   | 2.26                     | 0.61              |
| 1:D:803:VAL:CG2   | 3:D:1201:CLR:O1    | 2.44                     | 0.61              |
| 1:E:904:VAL:HA    | 1:E:907:LEU:HD23   | 1.80                     | 0.61              |
| 1:C:913:ASN:HB3   | 1:C:916:LEU:HB2    | 1.83                     | 0.61              |
| 1:E:643:LEU:HD13  | 1:E:1112:VAL:HB    | 1.81                     | 0.61              |
| 1:E:1014:GLN:O    | 1:E:1017:ASN:ND2   | 2.33                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:681:TRP:HE3   | 1:E:686:SER:HB3   | 1.66                     | 0.61              |
| 1:D:473:ILE:HG23  | 1:D:568:LEU:HD13  | 1.81                     | 0.61              |
| 3:D:1202:CLR:H183 | 3:D:1202:CLR:H212 | 1.83                     | 0.61              |
| 1:E:1033:ASN:ND2  | 1:E:1033:ASN:O    | 2.33                     | 0.61              |
| 3:C:1202:CLR:C21  | 1:D:946:VAL:HG21  | 2.29                     | 0.61              |
| 1:A:947:ALA:HB2   | 1:E:900:MET:SD    | 2.40                     | 0.61              |
| 1:E:951:LEU:HD11  | 1:E:1019:LEU:HD23 | 1.82                     | 0.61              |
| 1:D:700:PRO:O     | 1:D:703:ILE:HG12  | 2.00                     | 0.61              |
| 3:D:1204:CLR:H183 | 3:D:1204:CLR:H212 | 1.83                     | 0.61              |
| 1:C:1089:LEU:O    | 1:C:1093:CYS:N    | 2.32                     | 0.60              |
| 1:D:610:ALA:HA    | 1:D:613:LYS:HG2   | 1.82                     | 0.60              |
| 3:A:1203:CLR:H273 | 1:E:794:LEU:HB3   | 1.81                     | 0.60              |
| 1:C:599:MET:O     | 1:C:603:GLU:HG2   | 2.00                     | 0.60              |
| 1:C:1134:LEU:HB3  | 1:C:1138:ARG:HH12 | 1.64                     | 0.60              |
| 1:A:1136:ARG:NH2  | 1:A:1139:ASP:OD2  | 2.32                     | 0.60              |
| 1:C:1053:ASN:HA   | 1:C:1056:LEU:HG   | 1.81                     | 0.60              |
| 1:C:629:GLU:HA    | 1:C:632:ARG:HE    | 1.66                     | 0.60              |
| 1:D:799:ARG:HA    | 3:D:1201:CLR:C19  | 2.30                     | 0.60              |
| 1:C:996:GLU:HB3   | 1:C:1000:TRP:HZ2  | 1.66                     | 0.60              |
| 1:D:1055:ASP:OD2  | 1:D:1059:LYS:NZ   | 2.34                     | 0.60              |
| 1:C:1119:ARG:NH1  | 1:C:1119:ARG:HA   | 2.17                     | 0.60              |
| 1:D:799:ARG:HA    | 3:D:1201:CLR:H191 | 1.84                     | 0.60              |
| 1:A:922:ILE:HD11  | 1:A:1051:GLN:HA   | 1.83                     | 0.60              |
| 1:C:475:ASN:OD1   | 1:C:476:LEU:N     | 2.33                     | 0.60              |
| 1:D:480:ALA:HA    | 1:D:508:ARG:HH12  | 1.67                     | 0.60              |
| 1:D:677:THR:OG1   | 1:D:1062:ARG:NH2  | 2.35                     | 0.60              |
| 1:D:1037:ASN:HA   | 1:D:1040:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:941:LEU:HD21  | 1:A:967:PHE:HA    | 1.83                     | 0.59              |
| 1:C:802:LEU:HD12  | 3:C:1202:CLR:H112 | 1.84                     | 0.59              |
| 1:A:963:LEU:HD13  | 1:A:967:PHE:HE2   | 1.65                     | 0.59              |
| 1:E:561:ASP:OD1   | 1:E:562:LEU:N     | 2.35                     | 0.59              |
| 1:E:962:ILE:CD1   | 3:D:1201:CLR:H3   | 2.32                     | 0.59              |
| 1:C:618:LYS:O     | 1:C:622:MET:HG3   | 2.02                     | 0.59              |
| 1:E:437:ARG:HG3   | 1:E:440:PHE:HB2   | 1.84                     | 0.59              |
| 1:C:584:ASN:O     | 1:C:588:SER:CB    | 2.51                     | 0.59              |
| 1:C:641:LEU:HD11  | 1:C:1124:TRP:HZ3  | 1.67                     | 0.59              |
| 1:A:790:TYR:HB3   | 1:A:906:LEU:HD11  | 1.84                     | 0.59              |
| 1:E:914:LYS:HE2   | 1:E:915:GLN:HE22  | 1.67                     | 0.59              |
| 1:A:794:LEU:HD11  | 1:A:906:LEU:HG    | 1.84                     | 0.59              |
| 1:E:596:LEU:HD22  | 1:E:612:ARG:HG3   | 1.83                     | 0.59              |
| 1:A:1057:TYR:O    | 1:A:1061:GLN:HG2  | 2.03                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C:573:GLN:N     | 1:C:573:GLN:OE1    | 2.33                     | 0.58              |
| 1:A:561:ASP:OD1   | 1:A:562:LEU:N      | 2.35                     | 0.58              |
| 1:E:984:ASP:OD2   | 1:D:964:ARG:NH2    | 2.32                     | 0.58              |
| 1:A:828:GLU:OE2   | 1:A:859:TYR:OH     | 2.21                     | 0.58              |
| 1:E:962:ILE:HG21  | 3:D:1201:CLR:H11   | 1.83                     | 0.58              |
| 3:A:1202:CLR:H183 | 3:A:1202:CLR:H212  | 1.84                     | 0.58              |
| 1:D:790:TYR:HB3   | 1:D:906:LEU:HD11   | 1.85                     | 0.58              |
| 1:C:1127:VAL:O    | 1:C:1130:GLU:HG3   | 2.04                     | 0.58              |
| 1:D:793:PHE:CD1   | 1:D:820:TRP:CD1    | 2.91                     | 0.58              |
| 1:E:951:LEU:HD12  | 1:E:1016:ALA:HB3   | 1.86                     | 0.58              |
| 1:E:1018:TRP:HB3  | 3:D:1202:CLR:C19   | 2.34                     | 0.58              |
| 1:D:1033:ILE:O    | 1:D:1037:ASN:ND2   | 2.36                     | 0.58              |
| 1:A:933:PHE:CD1   | 1:A:1039:LEU:HD22  | 2.38                     | 0.58              |
| 1:E:645:ARG:HH22  | 1:E:652:ALA:C      | 2.12                     | 0.58              |
| 1:E:1047:THR:O    | 1:E:1051:VAL:HG12  | 2.03                     | 0.58              |
| 1:D:656:GLN:HA    | 1:D:659:MET:HE3    | 1.86                     | 0.58              |
| 1:A:669:GLN:NE2   | 1:A:670:ASP:OD1    | 2.36                     | 0.58              |
| 1:E:680:TRP:HD1   | 1:E:779:PRO:HB2    | 1.69                     | 0.58              |
| 1:D:821:ALA:HA    | 1:D:824:LEU:HG     | 1.85                     | 0.58              |
| 1:C:820:TRP:O     | 1:C:823:THR:OG1    | 2.19                     | 0.57              |
| 1:D:670:ASP:OD1   | 1:D:671:GLY:N      | 2.37                     | 0.57              |
| 1:E:615:LEU:HD23  | 1:E:618:LYS:NZ     | 2.19                     | 0.57              |
| 1:C:1119:ARG:HA   | 1:C:1119:ARG:HH11  | 1.67                     | 0.57              |
| 1:D:615:LEU:HD22  | 1:D:619:PHE:HE1    | 1.69                     | 0.57              |
| 1:E:908:HIS:HE2   | 2:E:1201:A1H0C:C23 | 2.17                     | 0.57              |
| 1:E:1040:LEU:HA   | 1:E:1043:MET:HE2   | 1.87                     | 0.57              |
| 1:A:1127:VAL:O    | 1:A:1130:GLU:HG3   | 2.05                     | 0.57              |
| 1:C:429:LEU:HD22  | 1:C:449:LEU:HG     | 1.85                     | 0.57              |
| 1:A:799:ARG:HG3   | 3:A:1205:CLR:H192  | 1.61                     | 0.57              |
| 1:A:987:LEU:HD23  | 1:E:1006:ALA:HB3   | 1.86                     | 0.57              |
| 3:A:1203:CLR:H271 | 1:E:795:LEU:CD2    | 2.27                     | 0.57              |
| 3:A:1204:CLR:H222 | 1:C:1025:VAL:HG11  | 1.84                     | 0.57              |
| 1:C:620:GLU:O     | 1:C:624:VAL:HG13   | 2.05                     | 0.57              |
| 1:C:831:GLN:NE2   | 1:C:859:TYR:OH     | 2.37                     | 0.57              |
| 1:D:1021:VAL:HG11 | 3:D:1204:CLR:C15   | 2.32                     | 0.57              |
| 1:C:953:ARG:HB3   | 1:C:955:ARG:HH21   | 1.70                     | 0.57              |
| 1:C:768:CYS:O     | 1:C:770:ARG:N      | 2.38                     | 0.56              |
| 1:C:1089:LEU:HA   | 1:C:1092:LEU:HB2   | 1.87                     | 0.56              |
| 1:D:985:VAL:HB    | 1:D:1017:ASN:ND2   | 2.20                     | 0.56              |
| 1:E:443:LEU:O     | 1:E:447:HIS:ND1    | 2.36                     | 0.56              |
| 1:C:954:PRO:HB3   | 1:C:1009:GLY:HA3   | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:974:ILE:HG23  | 1:E:975:PHE:CD1   | 2.40                     | 0.56              |
| 1:C:472:LEU:HD21  | 1:C:604:PRO:HD2   | 1.87                     | 0.56              |
| 1:D:597:ARG:HB3   | 1:D:661:ALA:HB1   | 1.85                     | 0.56              |
| 1:D:1127:VAL:O    | 1:D:1130:GLU:HG3  | 2.05                     | 0.56              |
| 1:A:569:LEU:HG    | 1:A:571:ARG:HH11  | 1.71                     | 0.56              |
| 1:A:981:GLU:N     | 1:A:981:GLU:OE2   | 2.37                     | 0.56              |
| 1:C:478:ASP:O     | 1:C:482:HIS:ND1   | 2.39                     | 0.56              |
| 1:D:575:ALA:O     | 1:D:578:PHE:HB2   | 2.06                     | 0.56              |
| 1:D:596:LEU:O     | 1:D:600:ALA:CB    | 2.54                     | 0.56              |
| 1:D:791:LEU:CD1   | 3:D:1201:CLR:C26  | 2.84                     | 0.56              |
| 1:C:622:MET:HA    | 1:C:625:ASP:OD1   | 2.06                     | 0.56              |
| 1:C:630:CYS:HB2   | 1:C:1124:TRP:CH2  | 2.41                     | 0.56              |
| 1:C:1161:GLN:HE22 | 1:D:1162:LEU:HB3  | 1.71                     | 0.56              |
| 1:E:629:GLU:HA    | 1:E:632:ARG:HE    | 1.70                     | 0.56              |
| 1:C:790:TYR:HB3   | 1:C:906:LEU:HD11  | 1.87                     | 0.56              |
| 1:C:802:LEU:HD12  | 3:C:1202:CLR:C12  | 2.35                     | 0.56              |
| 1:E:953:ARG:HD3   | 1:D:892:ARG:HH12  | 1.70                     | 0.56              |
| 1:C:768:CYS:O     | 1:C:771:ARG:N     | 2.39                     | 0.56              |
| 1:C:1002:HIS:ND1  | 1:C:1010:THR:O    | 2.28                     | 0.56              |
| 1:D:469:SER:HA    | 1:D:474:ARG:HG2   | 1.87                     | 0.56              |
| 1:D:579:TRP:CZ3   | 1:D:622:MET:HE1   | 2.41                     | 0.56              |
| 1:D:640:ARG:HB2   | 1:D:1113:LEU:HD11 | 1.87                     | 0.56              |
| 1:D:1138:ARG:HA   | 1:D:1141:ARG:HB2  | 1.87                     | 0.56              |
| 1:A:443:LEU:O     | 1:A:447:HIS:ND1   | 2.38                     | 0.55              |
| 1:A:1036:VAL:O    | 1:A:1040:ILE:HG13 | 2.07                     | 0.55              |
| 1:D:429:LEU:HD22  | 1:D:449:LEU:HG    | 1.89                     | 0.55              |
| 1:D:820:TRP:O     | 1:D:823:THR:OG1   | 2.23                     | 0.55              |
| 1:D:1134:LEU:HB3  | 1:D:1138:ARG:HH21 | 1.70                     | 0.55              |
| 1:A:1147:ARG:HH22 | 1:C:1149:LYS:HA   | 1.71                     | 0.55              |
| 1:E:1018:TRP:HB3  | 3:D:1202:CLR:H192 | 1.88                     | 0.55              |
| 1:D:594:LEU:HD12  | 1:D:661:ALA:HB2   | 1.87                     | 0.55              |
| 1:D:1115:LYS:O    | 1:D:1116:GLU:HG2  | 2.06                     | 0.55              |
| 1:E:629:GLU:HA    | 1:E:632:ARG:NE    | 2.22                     | 0.55              |
| 1:C:1087:LEU:HD12 | 1:C:1090:ARG:HB2  | 1.89                     | 0.55              |
| 1:E:637:ARG:O     | 1:E:641:LEU:HG    | 2.07                     | 0.55              |
| 1:C:442:ARG:HH12  | 1:C:574:MET:HE1   | 1.72                     | 0.55              |
| 1:C:798:SER:CB    | 3:C:1202:CLR:H211 | 2.36                     | 0.55              |
| 1:C:803:VAL:CG2   | 3:C:1202:CLR:C1   | 2.85                     | 0.55              |
| 3:A:1204:CLR:C16  | 1:C:1025:VAL:HG21 | 2.32                     | 0.55              |
| 1:C:830:ARG:HH12  | 1:C:1072:ARG:NH2  | 2.05                     | 0.55              |
| 1:C:933:PHE:HB2   | 1:C:1039:LEU:HD13 | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1045:TYR:O    | 1:C:1049:LYS:HG2  | 2.07                     | 0.55              |
| 1:E:478:ASP:O     | 1:E:482:HIS:ND1   | 2.38                     | 0.54              |
| 1:D:968:TYR:CB    | 3:D:1202:CLR:H161 | 2.16                     | 0.54              |
| 1:E:955:ARG:HG2   | 1:E:1011:CYS:HB3  | 1.89                     | 0.54              |
| 1:C:579:TRP:CZ3   | 1:C:622:MET:HE1   | 2.41                     | 0.54              |
| 1:D:629:GLU:OE2   | 1:D:1128:HIS:HB3  | 2.08                     | 0.54              |
| 3:A:1202:CLR:H212 | 3:A:1202:CLR:H121 | 1.89                     | 0.54              |
| 1:C:426:GLU:HB3   | 1:C:459:ARG:NH2   | 2.22                     | 0.54              |
| 1:A:605:ASP:OD1   | 1:A:608:GLU:HB3   | 2.06                     | 0.54              |
| 1:E:971:TYR:O     | 1:E:974:ILE:HG22  | 2.06                     | 0.54              |
| 1:E:1077:ALA:O    | 1:E:1081:ILE:HG13 | 2.08                     | 0.54              |
| 1:D:933:PHE:CG    | 1:D:1039:LEU:HD22 | 2.42                     | 0.54              |
| 1:E:599:MET:HB3   | 1:E:612:ARG:HD3   | 1.89                     | 0.54              |
| 1:E:1030:LEU:HA   | 1:E:1034:ILE:HD13 | 1.89                     | 0.54              |
| 1:E:929:ASP:HB3   | 1:E:1043:MET:HE3  | 1.88                     | 0.54              |
| 1:C:798:SER:CB    | 3:C:1202:CLR:C21  | 2.84                     | 0.54              |
| 1:C:1119:ARG:HH12 | 1:C:1122:LEU:HD22 | 1.73                     | 0.54              |
| 1:A:610:ALA:HA    | 1:A:613:LYS:HG2   | 1.88                     | 0.54              |
| 1:A:875:PHE:HD2   | 1:A:876:LEU:HD22  | 1.73                     | 0.54              |
| 1:A:955:ARG:HG2   | 1:A:1011:CYS:HB3  | 1.90                     | 0.54              |
| 1:A:1033:ILE:O    | 1:A:1037:ASN:ND2  | 2.40                     | 0.54              |
| 1:E:864:TRP:CE3   | 1:E:864:TRP:C     | 2.86                     | 0.54              |
| 1:E:1128:VAL:O    | 1:E:1131:GLU:HG3  | 2.07                     | 0.54              |
| 1:D:901:VAL:HA    | 1:D:904:VAL:HG22  | 1.89                     | 0.54              |
| 1:A:637:ARG:O     | 1:A:641:LEU:HG    | 2.08                     | 0.54              |
| 1:C:892:ARG:NE    | 1:D:950:GLY:O     | 2.39                     | 0.54              |
| 1:D:599:MET:HA    | 1:D:602:LEU:HB2   | 1.89                     | 0.54              |
| 1:D:600:ALA:HA    | 1:D:603:GLU:HG2   | 1.90                     | 0.54              |
| 1:A:459:ARG:HA    | 1:A:462:GLN:OE1   | 2.08                     | 0.54              |
| 1:E:962:ILE:CD1   | 3:D:1201:CLR:H12  | 2.34                     | 0.54              |
| 1:C:793:PHE:HB2   | 1:C:820:TRP:CZ2   | 2.43                     | 0.54              |
| 1:A:629:GLU:HA    | 1:A:632:ARG:NE    | 2.21                     | 0.53              |
| 1:C:594:LEU:HA    | 1:C:661:ALA:HB2   | 1.89                     | 0.53              |
| 1:A:483:SER:OG    | 1:A:508:ARG:NH1   | 2.41                     | 0.53              |
| 1:E:972:LEU:HB3   | 1:E:977:GLN:HB2   | 1.89                     | 0.53              |
| 1:E:1066:LEU:O    | 1:E:1069:GLU:HG3  | 2.09                     | 0.53              |
| 1:C:830:ARG:HE    | 1:C:1087:LEU:HD23 | 1.74                     | 0.53              |
| 1:C:1160:LYS:O    | 1:C:1164:HIS:ND1  | 2.41                     | 0.53              |
| 1:D:953:ARG:HB3   | 1:D:955:ARG:HH21  | 1.72                     | 0.53              |
| 1:D:1126:SER:O    | 1:D:1129:LYS:HG2  | 2.08                     | 0.53              |
| 1:D:598:VAL:O     | 1:D:601:ARG:HG2   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:D:630:CYS:HB2   | 1:D:1124:TRP:CH2   | 2.43                     | 0.53              |
| 1:E:908:HIS:CD2   | 2:E:1201:A1H0C:C23 | 2.91                     | 0.53              |
| 1:C:566:ALA:O     | 1:C:570:ASN:N      | 2.42                     | 0.53              |
| 1:C:999:PHE:HB2   | 1:C:1014:GLN:HE21  | 1.74                     | 0.53              |
| 1:D:599:MET:O     | 1:D:603:GLU:HG2    | 2.08                     | 0.53              |
| 1:C:922:ILE:HD11  | 1:C:1051:GLN:HA    | 1.89                     | 0.53              |
| 1:C:933:PHE:CD2   | 1:C:1039:LEU:HD22  | 2.44                     | 0.53              |
| 1:A:597:ARG:HH22  | 1:A:616:ALA:HB3    | 1.72                     | 0.53              |
| 1:A:900:MET:HE1   | 1:C:943:ALA:O      | 2.08                     | 0.53              |
| 1:A:936:PHE:CE1   | 1:A:1035:LEU:HD21  | 2.43                     | 0.53              |
| 3:A:1204:CLR:H72  | 1:C:1021:VAL:HG11  | 1.90                     | 0.53              |
| 1:D:1065:LEU:HA   | 1:D:1068:GLU:OE1   | 2.09                     | 0.53              |
| 1:A:611:ARG:O     | 1:A:615:LEU:HG     | 2.09                     | 0.53              |
| 1:A:803:VAL:HG21  | 3:A:1205:CLR:C2    | 2.39                     | 0.53              |
| 1:D:696:ALA:HB1   | 1:D:708:ILE:HD13   | 1.90                     | 0.53              |
| 1:D:820:TRP:HZ3   | 1:D:1078:PRO:HB3   | 1.74                     | 0.53              |
| 1:D:972:LEU:HB3   | 1:D:977:GLN:HB2    | 1.90                     | 0.53              |
| 1:E:624:VAL:HG12  | 1:E:666:PHE:HD1    | 1.73                     | 0.53              |
| 1:E:962:ILE:HG21  | 3:D:1201:CLR:H112  | 1.90                     | 0.53              |
| 1:C:570:ASN:HD22  | 1:C:608:GLU:HG3    | 1.74                     | 0.53              |
| 1:C:979:PRO:HB2   | 1:C:982:ASP:HB2    | 1.91                     | 0.53              |
| 1:C:1072:ARG:CZ   | 1:C:1072:ARG:HA    | 2.39                     | 0.53              |
| 1:D:696:ALA:HB2   | 1:D:708:ILE:HG21   | 1.90                     | 0.53              |
| 1:D:954:PRO:HB3   | 1:D:1009:GLY:HA3   | 1.91                     | 0.52              |
| 1:C:908:HIS:NE2   | 2:C:1201:A1H0C:O24 | 2.42                     | 0.52              |
| 1:A:984:ASP:OD2   | 1:E:964:ARG:NH2    | 2.35                     | 0.52              |
| 1:A:480:ALA:HA    | 1:A:508:ARG:HH12   | 1.74                     | 0.52              |
| 1:A:867:CYS:HA    | 1:A:870:VAL:HG12   | 1.91                     | 0.52              |
| 1:C:1150:ARG:O    | 1:C:1154:LYS:HG2   | 2.10                     | 0.52              |
| 1:E:794:LEU:HD11  | 1:E:906:LEU:HG     | 1.91                     | 0.52              |
| 1:E:1038:ASN:HD22 | 1:E:1041:ILE:HD12  | 1.75                     | 0.52              |
| 1:C:805:PHE:HD2   | 1:C:892:ARG:HH11   | 1.57                     | 0.52              |
| 1:A:614:ASP:HA    | 1:A:617:PHE:CD2    | 2.45                     | 0.52              |
| 1:C:594:LEU:O     | 1:C:598:VAL:HG12   | 2.08                     | 0.52              |
| 1:A:677:THR:OG1   | 1:A:1062:ARG:NH2   | 2.42                     | 0.52              |
| 1:C:901:VAL:HA    | 1:C:904:VAL:HG22   | 1.91                     | 0.52              |
| 1:D:1029:LEU:HA   | 1:D:1033:ILE:HD13  | 1.92                     | 0.52              |
| 1:A:704:TYR:CE1   | 1:A:771:ARG:HG2    | 2.44                     | 0.52              |
| 1:A:979:PRO:HB2   | 1:A:982:ASP:HB2    | 1.92                     | 0.52              |
| 1:D:820:TRP:CD1   | 1:D:824:LEU:HD23   | 2.44                     | 0.52              |
| 1:C:608:GLU:HA    | 1:C:611:ARG:HG2    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:981:GLU:HG3   | 1:C:987:LEU:HD13  | 1.91                     | 0.51              |
| 1:C:996:GLU:HB3   | 1:C:1000:TRP:CZ2  | 2.46                     | 0.51              |
| 1:D:805:PHE:HE1   | 1:D:892:ARG:HG2   | 1.74                     | 0.51              |
| 1:D:1152:SER:HA   | 1:D:1155:VAL:HG12 | 1.91                     | 0.51              |
| 1:A:617:PHE:HA    | 1:A:620:GLU:OE1   | 2.10                     | 0.51              |
| 1:A:795:LEU:HD21  | 3:A:1205:CLR:C26  | 2.21                     | 0.51              |
| 1:A:898:ASP:HA    | 1:A:901:VAL:HG22  | 1.93                     | 0.51              |
| 1:A:1076:ALA:O    | 1:A:1080:ILE:N    | 2.44                     | 0.51              |
| 1:E:670:ASP:OD1   | 1:E:671:GLY:N     | 2.43                     | 0.51              |
| 1:C:802:LEU:HD12  | 3:C:1202:CLR:C11  | 2.41                     | 0.51              |
| 1:D:478:ASP:O     | 1:D:482:HIS:ND1   | 2.43                     | 0.51              |
| 1:D:624:VAL:HG22  | 1:D:669:GLN:HG3   | 1.91                     | 0.51              |
| 1:C:1122:LEU:O    | 1:C:1125:GLU:HG3  | 2.11                     | 0.51              |
| 1:D:974:ILE:HG23  | 1:D:975:PHE:CD1   | 2.46                     | 0.51              |
| 1:A:942:VAL:HG21  | 3:A:1203:CLR:H242 | 1.92                     | 0.51              |
| 1:A:1039:LEU:HA   | 1:A:1042:MET:HG3  | 1.93                     | 0.51              |
| 1:C:571:ARG:HB3   | 1:C:574:MET:HB2   | 1.91                     | 0.51              |
| 1:C:1162:LEU:HA   | 1:C:1165:ILE:HG12 | 1.93                     | 0.51              |
| 1:D:579:TRP:CH2   | 1:D:622:MET:HE1   | 2.44                     | 0.51              |
| 1:A:624:VAL:HG12  | 1:A:666:PHE:HD1   | 1.75                     | 0.51              |
| 3:A:1203:CLR:C25  | 1:E:795:LEU:HD22  | 2.33                     | 0.51              |
| 1:E:989:GLU:N     | 1:E:989:GLU:OE2   | 2.43                     | 0.51              |
| 1:D:1036:VAL:O    | 1:D:1040:ILE:HG13 | 2.11                     | 0.51              |
| 1:A:901:VAL:HA    | 1:A:904:VAL:HG22  | 1.93                     | 0.51              |
| 1:A:968:TYR:HB2   | 3:A:1204:CLR:H151 | 1.91                     | 0.51              |
| 1:E:900:MET:HA    | 1:E:903:THR:HG22  | 1.91                     | 0.51              |
| 1:A:1147:ARG:HH22 | 1:C:1149:LYS:HD3  | 1.75                     | 0.51              |
| 1:C:670:ASP:OD1   | 1:C:671:GLY:N     | 2.44                     | 0.51              |
| 1:A:1143:SER:O    | 1:A:1147:ARG:HG3  | 2.11                     | 0.51              |
| 1:E:867:CYS:HA    | 1:E:870:VAL:HG12  | 1.92                     | 0.51              |
| 1:E:943:ALA:C     | 1:D:900:MET:HE1   | 2.36                     | 0.50              |
| 1:D:794:LEU:HD11  | 3:D:1201:CLR:C24  | 2.40                     | 0.50              |
| 1:D:999:PHE:HB2   | 1:D:1014:GLN:NE2  | 2.26                     | 0.50              |
| 1:D:1132:PHE:HE1  | 1:D:1136:ARG:HH11 | 1.57                     | 0.50              |
| 1:A:951:LEU:HD12  | 1:A:1016:ALA:HB3  | 1.94                     | 0.50              |
| 1:E:1002:HIS:ND1  | 1:E:1010:THR:O    | 2.31                     | 0.50              |
| 1:D:1115:LYS:C    | 1:D:1117:ALA:H    | 2.20                     | 0.50              |
| 1:A:900:MET:HE1   | 1:C:943:ALA:C     | 2.36                     | 0.50              |
| 1:A:933:PHE:HB2   | 1:A:1039:LEU:HD13 | 1.93                     | 0.50              |
| 1:A:1068:GLU:O    | 1:A:1072:ARG:HG2  | 2.11                     | 0.50              |
| 1:E:617:PHE:O     | 1:E:620:GLU:HG2   | 2.10                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1014:GLN:HB2  | 1:E:1017:ASN:HD22 | 1.77                     | 0.50              |
| 1:C:631:TYR:OH    | 1:C:674:SER:OG    | 2.23                     | 0.50              |
| 1:C:700:PRO:HG2   | 1:C:701:PRO:HD3   | 1.93                     | 0.50              |
| 1:C:1076:ALA:O    | 1:C:1080:ILE:N    | 2.44                     | 0.50              |
| 1:D:594:LEU:HA    | 1:D:661:ALA:HB2   | 1.93                     | 0.50              |
| 1:A:985:VAL:HB    | 1:A:1017:ASN:HD22 | 1.77                     | 0.50              |
| 1:A:1069:PHE:HA   | 1:A:1072:ARG:HG2  | 1.92                     | 0.50              |
| 1:E:942:VAL:CG2   | 3:D:1201:CLR:H211 | 2.41                     | 0.50              |
| 1:E:1047:THR:HA   | 1:E:1050:LYS:NZ   | 2.27                     | 0.50              |
| 1:E:864:TRP:CD1   | 1:E:908:HIS:CE1   | 3.00                     | 0.50              |
| 1:D:787:VAL:O     | 1:D:791:LEU:HD23  | 2.12                     | 0.50              |
| 1:A:579:TRP:CH2   | 1:A:1133:LEU:HD21 | 2.47                     | 0.50              |
| 1:A:656:GLN:HA    | 1:A:659:MET:HE3   | 1.94                     | 0.50              |
| 1:A:978:ILE:HD12  | 1:E:977:GLN:HG2   | 1.94                     | 0.50              |
| 1:E:962:ILE:HG22  | 3:D:1201:CLR:H112 | 1.91                     | 0.50              |
| 1:C:469:SER:HA    | 1:C:474:ARG:HG2   | 1.93                     | 0.50              |
| 1:D:610:ALA:HA    | 1:D:613:LYS:HZ2   | 1.75                     | 0.50              |
| 1:D:621:GLY:HA2   | 1:D:624:VAL:HG12  | 1.94                     | 0.50              |
| 1:A:437:ARG:HB2   | 1:A:440:PHE:HD2   | 1.77                     | 0.50              |
| 1:A:790:TYR:CE2   | 1:A:909:ILE:HD13  | 2.47                     | 0.50              |
| 1:E:669:GLN:NE2   | 1:E:670:ASP:OD1   | 2.45                     | 0.50              |
| 1:D:971:TYR:O     | 1:D:974:ILE:HG22  | 2.11                     | 0.50              |
| 1:D:1045:TYR:CE1  | 1:D:1049:LYS:HE2  | 2.47                     | 0.50              |
| 1:A:700:PRO:HG2   | 1:A:701:PRO:HD3   | 1.93                     | 0.50              |
| 1:A:799:ARG:CB    | 3:A:1205:CLR:C19  | 2.86                     | 0.50              |
| 1:A:820:TRP:CH2   | 1:A:1078:PRO:HG3  | 2.46                     | 0.50              |
| 1:E:922:ILE:HD11  | 1:E:1052:GLN:HA   | 1.93                     | 0.50              |
| 1:E:1116:LYS:O    | 1:E:1119:GLU:HB3  | 2.12                     | 0.50              |
| 1:D:1021:VAL:CG1  | 3:D:1204:CLR:C15  | 2.90                     | 0.50              |
| 1:D:637:ARG:O     | 1:D:641:LEU:HG    | 2.12                     | 0.49              |
| 1:D:790:TYR:CB    | 1:D:906:LEU:HD11  | 2.42                     | 0.49              |
| 1:E:946:VAL:CG2   | 3:D:1201:CLR:H212 | 2.42                     | 0.49              |
| 1:C:824:LEU:O     | 1:C:827:GLU:HG3   | 2.12                     | 0.49              |
| 1:D:637:ARG:HD2   | 1:D:1124:TRP:CD2  | 2.47                     | 0.49              |
| 1:D:797:PHE:HD1   | 1:D:817:LEU:HD11  | 1.77                     | 0.49              |
| 1:D:1045:TYR:O    | 1:D:1049:LYS:HG2  | 2.12                     | 0.49              |
| 3:D:1202:CLR:H212 | 3:D:1202:CLR:H121 | 1.94                     | 0.49              |
| 1:A:478:ASP:O     | 1:A:482:HIS:ND1   | 2.31                     | 0.49              |
| 1:A:626:LEU:O     | 1:A:629:GLU:HG3   | 2.12                     | 0.49              |
| 1:A:627:PHE:CE1   | 1:A:642:LEU:HD21  | 2.47                     | 0.49              |
| 1:E:615:LEU:HA    | 1:E:618:LYS:HZ2   | 1.76                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:644:ARG:HH12 | 1:E:1119:GLU:HB2  | 1.77                     | 0.49              |
| 1:C:626:LEU:O    | 1:C:629:GLU:HG3   | 2.13                     | 0.49              |
| 1:C:1087:LEU:HA  | 1:C:1090:ARG:HB2  | 1.94                     | 0.49              |
| 1:D:948:THR:O    | 1:D:952:LEU:HG    | 2.12                     | 0.49              |
| 1:C:933:PHE:CE1  | 1:C:937:LEU:HD23  | 2.47                     | 0.49              |
| 1:C:969:ARG:HB3  | 1:C:970:PRO:HD3   | 1.95                     | 0.49              |
| 1:C:1147:ARG:NH2 | 1:D:1149:LYS:HA   | 2.22                     | 0.49              |
| 1:A:926:MET:SD   | 1:A:1043:PHE:HD1  | 2.36                     | 0.49              |
| 1:E:656:GLN:O    | 1:E:659:MET:HG2   | 2.12                     | 0.49              |
| 1:E:704:TYR:HE1  | 1:E:771:ARG:HG2   | 1.77                     | 0.49              |
| 1:E:1047:THR:HA  | 1:E:1050:LYS:HZ3  | 1.77                     | 0.49              |
| 1:C:795:LEU:CD2  | 3:C:1202:CLR:C25  | 2.79                     | 0.49              |
| 1:E:921:VAL:O    | 1:E:924:SER:OG    | 2.26                     | 0.49              |
| 1:C:867:CYS:HA   | 1:C:870:VAL:HG12  | 1.95                     | 0.49              |
| 1:A:996:GLU:HB3  | 1:A:1000:TRP:CZ2  | 2.45                     | 0.49              |
| 1:E:828:GLU:OE2  | 1:E:859:TYR:OH    | 2.30                     | 0.49              |
| 1:C:1086:ARG:O   | 1:C:1090:ARG:N    | 2.43                     | 0.49              |
| 1:D:937:LEU:HG   | 1:D:941:LEU:HD23  | 1.95                     | 0.49              |
| 1:A:968:TYR:CD1  | 3:A:1204:CLR:H151 | 2.47                     | 0.49              |
| 1:E:906:LEU:HA   | 1:E:909:ILE:HD12  | 1.95                     | 0.49              |
| 1:E:908:HIS:HA   | 1:E:911:THR:HG23  | 1.94                     | 0.49              |
| 1:C:559:TRP:HZ3  | 1:C:578:PHE:CD1   | 2.31                     | 0.49              |
| 1:C:597:ARG:HG2  | 1:C:661:ALA:O     | 2.13                     | 0.49              |
| 1:C:675:LEU:O    | 1:C:679:LYS:HG2   | 2.12                     | 0.49              |
| 1:D:973:GLN:NE2  | 1:D:979:PRO:HD2   | 2.28                     | 0.49              |
| 1:D:1076:ALA:C   | 1:D:1078:PRO:HD2  | 2.37                     | 0.49              |
| 3:A:1203:CLR:C15 | 1:E:802:LEU:HD12  | 2.37                     | 0.49              |
| 1:E:703:ILE:HG23 | 1:E:704:TYR:CD1   | 2.48                     | 0.49              |
| 1:E:1040:LEU:HA  | 1:E:1043:MET:HG2  | 1.95                     | 0.49              |
| 1:C:966:VAL:HG13 | 1:C:967:PHE:CD2   | 2.47                     | 0.49              |
| 1:D:820:TRP:CZ3  | 1:D:1078:PRO:HB3  | 2.48                     | 0.49              |
| 1:A:862:ASP:OD1  | 1:A:864:TRP:NE1   | 2.46                     | 0.49              |
| 1:E:626:LEU:O    | 1:E:629:GLU:HG3   | 2.12                     | 0.49              |
| 1:D:814:GLU:HG2  | 1:D:818:TYR:CZ    | 2.48                     | 0.49              |
| 1:D:432:ALA:HB1  | 1:D:441:VAL:HG22  | 1.95                     | 0.48              |
| 1:D:683:ASP:O    | 1:D:684:MET:HE2   | 2.13                     | 0.48              |
| 1:E:1077:ALA:C   | 1:E:1081:ILE:HG13 | 2.38                     | 0.48              |
| 1:C:637:ARG:O    | 1:C:641:LEU:HG    | 2.13                     | 0.48              |
| 1:C:1037:ASN:HA  | 1:C:1040:ILE:HG12 | 1.95                     | 0.48              |
| 1:A:608:GLU:HA   | 1:A:611:ARG:HG2   | 1.94                     | 0.48              |
| 1:A:645:ARG:HG2  | 1:A:645:ARG:HH11  | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:805:PHE:CE2   | 1:A:892:ARG:HB3   | 2.49                     | 0.48              |
| 1:D:862:ASP:OD1   | 1:D:864:TRP:NE1   | 2.46                     | 0.48              |
| 1:D:666:PHE:O     | 1:D:672:VAL:HG11  | 2.13                     | 0.48              |
| 1:D:952:LEU:HD12  | 1:D:954:PRO:HD3   | 1.95                     | 0.48              |
| 1:D:959:PHE:HB3   | 1:D:960:PRO:HD3   | 1.96                     | 0.48              |
| 1:E:805:PHE:CE2   | 1:E:892:ARG:HB2   | 2.49                     | 0.48              |
| 1:E:968:TYR:CE2   | 1:E:972:LEU:HD11  | 2.48                     | 0.48              |
| 1:C:456:THR:H     | 1:C:459:ARG:HD3   | 1.79                     | 0.48              |
| 1:C:559:TRP:O     | 1:C:563:LEU:HB2   | 2.13                     | 0.48              |
| 1:C:656:GLN:HA    | 1:C:659:MET:HG2   | 1.94                     | 0.48              |
| 1:C:683:ASP:O     | 1:C:684:MET:HE2   | 2.13                     | 0.48              |
| 1:D:592:ALA:O     | 1:D:596:LEU:HG    | 2.12                     | 0.48              |
| 1:D:598:VAL:HG12  | 1:D:599:MET:HE2   | 1.95                     | 0.48              |
| 1:D:927:MET:HA    | 1:D:930:VAL:HG12  | 1.94                     | 0.48              |
| 1:E:579:TRP:NE1   | 1:E:589:ALA:HB2   | 2.28                     | 0.48              |
| 1:C:426:GLU:OE1   | 1:C:459:ARG:NH2   | 2.47                     | 0.48              |
| 1:A:459:ARG:O     | 1:A:463:LEU:HD23  | 2.13                     | 0.48              |
| 3:A:1203:CLR:H212 | 3:A:1203:CLR:H121 | 1.95                     | 0.48              |
| 3:A:1204:CLR:H212 | 3:A:1204:CLR:H183 | 1.94                     | 0.48              |
| 1:C:566:ALA:HB1   | 1:C:571:ARG:HB2   | 1.95                     | 0.48              |
| 1:C:570:ASN:ND2   | 1:C:608:GLU:HG3   | 2.28                     | 0.48              |
| 1:C:677:THR:OG1   | 1:C:1062:ARG:NH2  | 2.45                     | 0.48              |
| 1:C:702:LEU:HD12  | 1:C:705:THR:HG21  | 1.96                     | 0.48              |
| 1:A:429:LEU:HD22  | 1:A:449:LEU:HG    | 1.95                     | 0.48              |
| 1:A:913:ASN:HB2   | 1:A:916:LEU:HB2   | 1.96                     | 0.48              |
| 1:C:680:TRP:HD1   | 1:C:779:PRO:HB2   | 1.78                     | 0.48              |
| 1:D:949:GLU:OE2   | 1:D:962:ILE:HG23  | 2.13                     | 0.48              |
| 1:C:584:ASN:O     | 1:C:588:SER:OG    | 2.32                     | 0.48              |
| 1:D:824:LEU:HA    | 1:D:827:GLU:HG3   | 1.95                     | 0.48              |
| 1:D:881:CYS:SG    | 1:D:887:LEU:HB3   | 2.53                     | 0.48              |
| 1:A:645:ARG:NH1   | 1:A:651:ASP:OD1   | 2.47                     | 0.48              |
| 1:A:970:PRO:O     | 1:A:973:GLN:HB2   | 2.14                     | 0.48              |
| 1:E:611:ARG:HA    | 1:E:614:ASP:OD2   | 2.13                     | 0.48              |
| 1:C:585:ALA:HB3   | 1:C:1125:GLU:OE1  | 2.14                     | 0.48              |
| 1:A:954:PRO:HB3   | 1:A:1009:GLY:HA3  | 1.95                     | 0.47              |
| 1:D:605:ASP:OD2   | 1:D:608:GLU:HB3   | 2.13                     | 0.47              |
| 1:D:802:LEU:CD2   | 3:D:1201:CLR:C11  | 2.86                     | 0.47              |
| 1:D:1087:LEU:HA   | 1:D:1090:ARG:HB2  | 1.96                     | 0.47              |
| 1:A:459:ARG:HA    | 1:A:462:GLN:CD    | 2.39                     | 0.47              |
| 1:A:959:PHE:CD1   | 3:A:1203:CLR:H22  | 2.49                     | 0.47              |
| 1:A:975:PHE:CE2   | 1:C:1028:LEU:HB3  | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:959:PHE:HB3   | 1:C:960:PRO:HD3   | 1.96                     | 0.47              |
| 3:C:1202:CLR:H211 | 1:D:946:VAL:CG2   | 2.36                     | 0.47              |
| 1:D:505:HIS:HE2   | 1:D:650:GLY:HA3   | 1.79                     | 0.47              |
| 1:D:562:LEU:HB3   | 1:D:578:PHE:CE2   | 2.49                     | 0.47              |
| 1:D:627:PHE:CE1   | 1:D:642:LEU:HD21  | 2.49                     | 0.47              |
| 1:A:703:ILE:HG23  | 1:A:704:TYR:CD1   | 2.49                     | 0.47              |
| 1:E:824:LEU:O     | 1:E:827:GLU:HG3   | 2.14                     | 0.47              |
| 1:C:585:ALA:HB2   | 1:C:1129:LYS:HD2  | 1.97                     | 0.47              |
| 1:C:627:PHE:HA    | 1:C:630:CYS:SG    | 2.54                     | 0.47              |
| 1:C:865:ASN:O     | 1:C:869:LEU:HD23  | 2.15                     | 0.47              |
| 1:D:994:SER:HB3   | 1:D:1000:TRP:CE2  | 2.49                     | 0.47              |
| 1:C:941:LEU:HD11  | 1:C:970:PRO:HB2   | 1.96                     | 0.47              |
| 1:C:975:PHE:HZ    | 1:D:1033:ILE:HD11 | 1.79                     | 0.47              |
| 1:D:1077:PRO:N    | 1:D:1078:PRO:HD2  | 2.29                     | 0.47              |
| 1:A:932:PHE:CD1   | 1:E:916:LEU:HD22  | 2.47                     | 0.47              |
| 1:E:979:PRO:HG2   | 1:E:983:MET:HE2   | 1.95                     | 0.47              |
| 1:C:920:ILE:O     | 1:C:923:VAL:HG12  | 2.13                     | 0.47              |
| 1:C:921:VAL:O     | 1:C:924:SER:OG    | 2.29                     | 0.47              |
| 1:C:952:LEU:HD12  | 1:C:954:PRO:HD3   | 1.96                     | 0.47              |
| 1:C:1040:ILE:HG22 | 1:D:1037:ASN:HB3  | 1.96                     | 0.47              |
| 1:D:432:ALA:HA    | 1:D:437:ARG:HE    | 1.79                     | 0.47              |
| 1:D:579:TRP:HZ2   | 1:D:589:ALA:HB2   | 1.79                     | 0.47              |
| 1:A:1156:ASP:OD1  | 1:A:1157:LEU:N    | 2.47                     | 0.47              |
| 1:C:572:ALA:HB1   | 1:C:615:LEU:HD21  | 1.95                     | 0.47              |
| 1:D:437:ARG:HB2   | 1:D:440:PHE:HD2   | 1.78                     | 0.47              |
| 1:D:579:TRP:CZ2   | 1:D:589:ALA:HB2   | 2.50                     | 0.47              |
| 1:D:918:PRO:O     | 1:D:922:ILE:HG12  | 2.13                     | 0.47              |
| 1:A:1041:ALA:O    | 1:A:1044:SER:OG   | 2.26                     | 0.47              |
| 1:E:782:ILE:HD12  | 1:E:1075:ALA:HA   | 1.97                     | 0.47              |
| 1:E:920:ILE:O     | 1:E:923:VAL:HG12  | 2.15                     | 0.47              |
| 1:E:1029:LEU:HB3  | 1:D:975:PHE:CE2   | 2.49                     | 0.47              |
| 1:E:1130:LYS:O    | 1:E:1134:LEU:HD23 | 2.14                     | 0.47              |
| 1:E:1157:ASP:OD1  | 1:E:1158:LEU:N    | 2.47                     | 0.47              |
| 1:D:956:ASP:OD2   | 1:D:1010:THR:N    | 2.47                     | 0.47              |
| 1:A:936:PHE:HE1   | 1:A:1035:LEU:HD21 | 1.78                     | 0.47              |
| 1:E:563:LEU:O     | 1:E:567:LEU:HD23  | 2.15                     | 0.47              |
| 1:D:1138:ARG:O    | 1:D:1141:ARG:N    | 2.39                     | 0.47              |
| 1:A:659:MET:HE2   | 1:A:1063:TYR:HE2  | 1.79                     | 0.47              |
| 1:E:600:ALA:HB3   | 1:E:613:LYS:HE2   | 1.96                     | 0.47              |
| 1:E:966:VAL:HG13  | 1:E:967:PHE:CD1   | 2.50                     | 0.47              |
| 1:E:1123:LEU:O    | 1:E:1126:GLU:HG3  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:1202:CLR:C24 | 1:D:942:VAL:HG21  | 2.45                     | 0.47              |
| 1:A:865:ASN:O    | 1:A:869:LEU:HD23  | 2.15                     | 0.47              |
| 1:A:972:LEU:HD12 | 1:A:977:GLN:HG3   | 1.96                     | 0.47              |
| 1:C:454:PHE:HD2  | 1:C:455:LEU:HG    | 1.79                     | 0.47              |
| 1:D:563:LEU:O    | 1:D:567:LEU:HD23  | 2.15                     | 0.47              |
| 1:E:644:ARG:HH21 | 1:E:1114:LEU:HB3  | 1.79                     | 0.46              |
| 1:E:927:MET:HE2  | 1:E:927:MET:HA    | 1.97                     | 0.46              |
| 1:C:445:ILE:HG13 | 1:C:449:LEU:HD23  | 1.97                     | 0.46              |
| 1:C:828:GLU:OE2  | 1:C:831:GLN:NE2   | 2.48                     | 0.46              |
| 1:D:803:VAL:CG2  | 3:D:1201:CLR:H192 | 2.34                     | 0.46              |
| 1:D:1082:ILE:O   | 1:D:1085:LEU:HG   | 2.15                     | 0.46              |
| 1:C:828:GLU:CD   | 1:C:831:GLN:HE21  | 2.22                     | 0.46              |
| 1:A:1003:PRO:HD3 | 1:A:1012:VAL:HG22 | 1.98                     | 0.46              |
| 1:C:1141:ARG:NH2 | 1:C:1150:ARG:HH12 | 2.12                     | 0.46              |
| 1:D:1064:ARG:NH1 | 1:D:1067:ARG:HH21 | 2.13                     | 0.46              |
| 1:E:814:GLU:HG2  | 1:E:818:TYR:CZ    | 2.51                     | 0.46              |
| 1:E:1032:ALA:HA  | 1:E:1036:LEU:HD12 | 1.96                     | 0.46              |
| 1:C:793:PHE:HB2  | 1:C:820:TRP:CE2   | 2.50                     | 0.46              |
| 1:C:1161:GLN:NE2 | 1:D:1162:LEU:HB3  | 2.30                     | 0.46              |
| 1:A:430:MET:HE1  | 1:A:463:LEU:HD22  | 1.96                     | 0.46              |
| 1:A:1126:SER:HA  | 1:A:1129:LYS:HD3  | 1.97                     | 0.46              |
| 1:E:675:LEU:O    | 1:E:679:LYS:HG2   | 2.16                     | 0.46              |
| 1:E:691:TRP:HA   | 1:E:694:VAL:HG12  | 1.98                     | 0.46              |
| 1:C:805:PHE:CE1  | 1:C:882:ARG:HD3   | 2.51                     | 0.46              |
| 1:D:474:ARG:HA   | 1:D:477:LEU:HB2   | 1.97                     | 0.46              |
| 1:D:622:MET:HE2  | 1:D:1132:PHE:CE2  | 2.43                     | 0.46              |
| 1:D:824:LEU:O    | 1:D:827:GLU:HG3   | 2.15                     | 0.46              |
| 1:D:1086:ARG:O   | 1:D:1090:ARG:N    | 2.39                     | 0.46              |
| 1:A:563:LEU:O    | 1:A:567:LEU:HD23  | 2.15                     | 0.46              |
| 1:A:611:ARG:HA   | 1:A:614:ASP:OD2   | 2.15                     | 0.46              |
| 1:A:949:GLU:OE2  | 1:A:965:ARG:HB3   | 2.16                     | 0.46              |
| 1:C:802:LEU:HD12 | 3:C:1202:CLR:H121 | 1.97                     | 0.46              |
| 1:C:814:GLU:HG2  | 1:C:818:TYR:CZ    | 2.50                     | 0.46              |
| 1:C:989:GLU:OE1  | 1:C:989:GLU:N     | 2.47                     | 0.46              |
| 1:A:889:HIS:O    | 1:A:893:THR:HG23  | 2.15                     | 0.46              |
| 1:E:637:ARG:HG3  | 1:E:640:ARG:HE    | 1.80                     | 0.46              |
| 1:E:1077:ALA:O   | 1:E:1081:ILE:N    | 2.49                     | 0.46              |
| 1:E:1144:SER:O   | 1:E:1148:ARG:HG3  | 2.16                     | 0.46              |
| 1:C:656:GLN:HA   | 1:C:659:MET:HE3   | 1.97                     | 0.46              |
| 1:C:830:ARG:NH1  | 1:C:1072:ARG:HH21 | 2.07                     | 0.46              |
| 1:D:794:LEU:CD1  | 3:D:1201:CLR:C24  | 2.94                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:629:GLU:OE2   | 1:C:1128:HIS:HB3  | 2.15                     | 0.46              |
| 1:D:1017:ASN:HA   | 1:D:1020:VAL:CG2  | 2.45                     | 0.46              |
| 1:A:681:TRP:HE3   | 1:A:686:SER:HB3   | 1.81                     | 0.46              |
| 1:C:610:ALA:HA    | 1:C:613:LYS:HG2   | 1.98                     | 0.46              |
| 1:C:627:PHE:O     | 1:C:631:TYR:HB2   | 2.16                     | 0.46              |
| 1:C:819:PHE:O     | 1:C:823:THR:HG23  | 2.15                     | 0.46              |
| 1:D:579:TRP:HE1   | 1:D:589:ALA:HA    | 1.79                     | 0.46              |
| 1:D:965:ARG:HD3   | 1:D:1008:ALA:HA   | 1.98                     | 0.46              |
| 1:D:1064:ARG:CZ   | 1:D:1067:ARG:HH21 | 2.28                     | 0.46              |
| 3:D:1204:CLR:H212 | 3:D:1204:CLR:H121 | 1.97                     | 0.46              |
| 1:A:899:PHE:O     | 1:A:903:THR:HG23  | 2.15                     | 0.46              |
| 1:E:1078:PRO:HA   | 1:E:1081:ILE:HD12 | 1.98                     | 0.46              |
| 1:E:1083:ILE:O    | 1:E:1086:LEU:HG   | 2.16                     | 0.46              |
| 1:E:1157:ASP:O    | 1:E:1161:LYS:HG3  | 2.16                     | 0.46              |
| 1:A:599:MET:O     | 1:A:603:GLU:HG2   | 2.16                     | 0.45              |
| 1:C:563:LEU:O     | 1:C:567:LEU:HD23  | 2.16                     | 0.45              |
| 1:C:899:PHE:CE1   | 1:D:943:ALA:HA    | 2.47                     | 0.45              |
| 1:C:907:LEU:HD11  | 1:D:936:PHE:CE1   | 2.51                     | 0.45              |
| 1:D:1076:ALA:O    | 1:D:1080:ILE:N    | 2.49                     | 0.45              |
| 1:A:959:PHE:HB3   | 1:A:960:PRO:HD3   | 1.98                     | 0.45              |
| 1:E:985:VAL:HA    | 1:E:988:MET:HG2   | 1.98                     | 0.45              |
| 1:C:1147:ARG:HH22 | 1:D:1149:LYS:HD2  | 1.81                     | 0.45              |
| 1:D:616:ALA:O     | 1:D:620:GLU:HB3   | 2.15                     | 0.45              |
| 1:D:828:GLU:OE2   | 1:D:859:TYR:OH    | 2.34                     | 0.45              |
| 1:D:963:LEU:HD22  | 1:D:967:PHE:HE1   | 1.82                     | 0.45              |
| 1:D:1046:THR:O    | 1:D:1050:VAL:HG12 | 2.16                     | 0.45              |
| 1:A:584:ASN:O     | 1:A:584:ASN:ND2   | 2.49                     | 0.45              |
| 1:E:959:PHE:HE1   | 3:D:1201:CLR:H71  | 1.81                     | 0.45              |
| 1:A:421:ARG:HB2   | 1:A:424:HIS:ND1   | 2.32                     | 0.45              |
| 1:A:893:THR:O     | 1:A:897:ILE:HD12  | 2.17                     | 0.45              |
| 1:A:1037:ASN:HA   | 1:A:1040:ILE:HD12 | 1.98                     | 0.45              |
| 1:E:929:ASP:HB2   | 1:E:1044:PHE:HE1  | 1.82                     | 0.45              |
| 1:E:936:PHE:CD1   | 1:E:1036:LEU:HD21 | 2.52                     | 0.45              |
| 1:C:803:VAL:CG2   | 3:C:1202:CLR:H11  | 2.46                     | 0.45              |
| 1:A:691:TRP:HA    | 1:A:694:VAL:HG22  | 1.99                     | 0.45              |
| 3:A:1205:CLR:H212 | 3:A:1205:CLR:H121 | 1.99                     | 0.45              |
| 1:C:586:VAL:C     | 1:C:588:SER:N     | 2.65                     | 0.45              |
| 1:C:956:ASP:OD2   | 1:C:1010:THR:N    | 2.41                     | 0.45              |
| 1:C:985:VAL:HB    | 1:C:1017:ASN:HD22 | 1.82                     | 0.45              |
| 1:A:1017:ASN:O    | 1:A:1021:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:1122:LEU:O    | 1:A:1125:GLU:HG3  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:969:ARG:HB3  | 1:A:970:PRO:HD3   | 1.98                     | 0.45              |
| 3:A:1203:CLR:C27 | 1:E:794:LEU:HB3   | 2.47                     | 0.45              |
| 1:E:656:GLN:HA   | 1:E:659:MET:SD    | 2.57                     | 0.45              |
| 1:E:864:TRP:CE3  | 1:E:864:TRP:O     | 2.70                     | 0.45              |
| 1:D:624:VAL:HA   | 1:D:627:PHE:HB3   | 1.99                     | 0.45              |
| 1:A:920:ILE:O    | 1:A:923:VAL:HG12  | 2.16                     | 0.45              |
| 1:A:1028:LEU:HB3 | 1:E:975:PHE:CE2   | 2.52                     | 0.45              |
| 1:E:573:GLN:HA   | 1:E:576:MET:HG2   | 1.98                     | 0.45              |
| 1:E:897:ILE:HA   | 1:E:900:MET:HE2   | 1.98                     | 0.45              |
| 1:C:624:VAL:HG12 | 1:C:666:PHE:CD2   | 2.40                     | 0.45              |
| 1:C:768:CYS:O    | 1:C:769:LEU:C     | 2.60                     | 0.45              |
| 1:D:878:GLY:HA2  | 1:D:894:VAL:HG11  | 1.98                     | 0.45              |
| 1:A:1153:GLN:NE2 | 1:A:1154:LYS:HG2  | 2.32                     | 0.45              |
| 1:C:621:GLY:O    | 1:C:624:VAL:HG22  | 2.16                     | 0.45              |
| 1:D:786:ASN:OD1  | 1:D:790:TYR:HE2   | 2.00                     | 0.45              |
| 1:A:948:THR:O    | 1:A:952:LEU:HG    | 2.16                     | 0.44              |
| 1:E:684:MET:HA   | 1:E:710:PHE:CD1   | 2.52                     | 0.44              |
| 1:D:640:ARG:HD2  | 1:D:1113:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:899:PHE:O    | 1:D:903:THR:HG23  | 2.17                     | 0.44              |
| 1:D:1055:ASP:O   | 1:D:1059:LYS:HG2  | 2.17                     | 0.44              |
| 1:D:1058:TRP:CE3 | 1:D:1059:LYS:HD3  | 2.52                     | 0.44              |
| 1:A:927:MET:HE3  | 1:A:931:PHE:CE1   | 2.53                     | 0.44              |
| 1:A:1082:ILE:O   | 1:A:1085:LEU:HG   | 2.17                     | 0.44              |
| 1:A:432:ALA:CA   | 1:A:437:ARG:HE    | 2.28                     | 0.44              |
| 1:C:574:MET:HB3  | 1:C:578:PHE:CZ    | 2.53                     | 0.44              |
| 1:C:894:VAL:HA   | 1:C:897:ILE:HG22  | 1.98                     | 0.44              |
| 1:D:676:LEU:HD12 | 1:D:1066:ILE:HD11 | 2.00                     | 0.44              |
| 1:D:1137:ALA:O   | 1:D:1141:ARG:HG3  | 2.16                     | 0.44              |
| 1:E:959:PHE:HB3  | 1:E:960:PRO:HD3   | 2.00                     | 0.44              |
| 1:C:638:ALA:HA   | 1:C:641:LEU:HD12  | 2.00                     | 0.44              |
| 1:D:645:ARG:HH22 | 1:D:652:ALA:C     | 2.25                     | 0.44              |
| 1:D:797:PHE:CD2  | 1:D:899:PHE:HD1   | 2.35                     | 0.44              |
| 1:D:922:ILE:HG21 | 1:D:1047:PHE:CD1  | 2.43                     | 0.44              |
| 1:A:579:TRP:CD2  | 1:A:622:MET:HE1   | 2.52                     | 0.44              |
| 1:A:933:PHE:CZ   | 1:A:937:LEU:HD22  | 2.52                     | 0.44              |
| 1:E:1078:PRO:N   | 1:E:1079:PRO:HD2  | 2.33                     | 0.44              |
| 1:C:934:LEU:O    | 1:C:937:LEU:HG    | 2.18                     | 0.44              |
| 1:D:797:PHE:HD2  | 1:D:899:PHE:HD1   | 1.65                     | 0.44              |
| 1:A:959:PHE:CE1  | 3:A:1203:CLR:H111 | 2.47                     | 0.44              |
| 1:D:802:LEU:HB2  | 3:D:1201:CLR:H193 | 1.98                     | 0.44              |
| 1:D:882:ARG:O    | 1:D:882:ARG:NH1   | 2.41                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:914:LYS:HA    | 1:D:1058:TRP:CZ2  | 2.53                     | 0.44              |
| 1:A:426:GLU:HB3   | 1:A:459:ARG:HH22  | 1.82                     | 0.44              |
| 1:A:614:ASP:OD1   | 1:A:615:LEU:N     | 2.51                     | 0.44              |
| 1:A:656:GLN:HA    | 1:A:659:MET:HG2   | 1.98                     | 0.44              |
| 1:A:959:PHE:O     | 1:A:963:LEU:HD23  | 2.17                     | 0.44              |
| 1:A:1040:ILE:HG12 | 1:C:1037:ASN:OD1  | 2.17                     | 0.44              |
| 1:E:597:ARG:HH21  | 1:E:613:LYS:CD    | 2.30                     | 0.44              |
| 1:C:948:THR:O     | 1:C:952:LEU:HG    | 2.18                     | 0.44              |
| 1:C:1136:ARG:HA   | 1:C:1139:ASP:HB2  | 2.00                     | 0.44              |
| 1:D:579:TRP:HE1   | 1:D:589:ALA:CA    | 2.31                     | 0.44              |
| 1:D:922:ILE:O     | 1:D:926:MET:HG2   | 2.17                     | 0.44              |
| 1:D:1162:LEU:HA   | 1:D:1165:ILE:HG12 | 2.00                     | 0.44              |
| 1:A:618:LYS:O     | 1:A:622:MET:HG3   | 2.18                     | 0.44              |
| 1:E:994:SER:HB3   | 1:E:1000:TRP:CE2  | 2.53                     | 0.44              |
| 1:D:889:HIS:O     | 1:D:893:THR:HG23  | 2.18                     | 0.44              |
| 1:C:637:ARG:HD2   | 1:C:1124:TRP:CE2  | 2.52                     | 0.43              |
| 1:C:930:VAL:HG21  | 1:D:1034:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:963:LEU:HD13  | 1:A:967:PHE:CE2   | 2.51                     | 0.43              |
| 3:A:1202:CLR:H161 | 1:E:968:TYR:HB2   | 2.00                     | 0.43              |
| 1:E:772:TRP:HD1   | 1:E:773:PHE:CD1   | 2.36                     | 0.43              |
| 1:C:580:GLU:O     | 1:C:581:MET:HE2   | 2.19                     | 0.43              |
| 1:D:426:GLU:HB3   | 1:D:459:ARG:NH2   | 2.33                     | 0.43              |
| 1:A:640:ARG:HB2   | 1:A:1113:LEU:HD11 | 2.00                     | 0.43              |
| 1:E:945:GLY:O     | 1:E:948:THR:N     | 2.51                     | 0.43              |
| 1:E:952:LEU:HD12  | 1:E:954:PRO:HD3   | 2.00                     | 0.43              |
| 1:E:953:ARG:HG3   | 1:D:892:ARG:HH22  | 1.83                     | 0.43              |
| 1:C:655:LEU:HD12  | 1:C:1063:TYR:CE1  | 2.54                     | 0.43              |
| 1:C:969:ARG:HD2   | 1:C:979:PRO:HG3   | 2.00                     | 0.43              |
| 1:C:988:MET:HE1   | 1:C:1012:VAL:HG21 | 2.01                     | 0.43              |
| 1:C:1129:LYS:O    | 1:C:1133:LEU:HD23 | 2.18                     | 0.43              |
| 1:D:1039:LEU:HG   | 1:D:1043:PHE:CE2  | 2.53                     | 0.43              |
| 1:C:927:MET:HE3   | 1:C:931:PHE:CE1   | 2.53                     | 0.43              |
| 1:C:1115:LYS:C    | 1:C:1117:ALA:H    | 2.27                     | 0.43              |
| 1:A:1055:ASP:O    | 1:A:1059:LYS:HG2  | 2.19                     | 0.43              |
| 1:C:566:ALA:HB2   | 1:C:578:PHE:HE2   | 1.83                     | 0.43              |
| 1:D:681:TRP:HE3   | 1:D:686:SER:HA    | 1.83                     | 0.43              |
| 1:D:682:GLY:O     | 1:D:684:MET:HG2   | 2.19                     | 0.43              |
| 1:D:691:TRP:HA    | 1:D:694:VAL:HG12  | 2.01                     | 0.43              |
| 1:A:1043:PHE:HE2  | 1:C:1037:ASN:ND2  | 2.17                     | 0.43              |
| 1:E:432:ALA:HB2   | 1:E:437:ARG:HE    | 1.84                     | 0.43              |
| 1:E:937:LEU:HD12  | 1:E:938:GLY:N     | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1026:VAL:HG13 | 1:D:971:TYR:CE2   | 2.54                     | 0.43              |
| 1:D:702:LEU:O     | 1:D:705:THR:OG1   | 2.31                     | 0.43              |
| 3:D:1204:CLR:H193 | 3:D:1204:CLR:H111 | 1.90                     | 0.43              |
| 1:A:814:GLU:HG2   | 1:A:818:TYR:CZ    | 2.54                     | 0.43              |
| 3:A:1203:CLR:H272 | 1:E:795:LEU:HA    | 1.99                     | 0.43              |
| 1:E:934:LEU:O     | 1:E:937:LEU:HG    | 2.18                     | 0.43              |
| 1:C:772:TRP:HD1   | 1:C:773:PHE:CD1   | 2.37                     | 0.43              |
| 1:C:994:SER:HB3   | 1:C:1000:TRP:CE2  | 2.54                     | 0.43              |
| 1:A:1002:HIS:ND1  | 1:A:1010:THR:O    | 2.30                     | 0.43              |
| 1:E:943:ALA:O     | 1:D:900:MET:HE1   | 2.18                     | 0.43              |
| 1:D:1077:PRO:HA   | 1:D:1080:ILE:HB   | 2.01                     | 0.43              |
| 1:A:504:GLY:O     | 1:A:508:ARG:HG2   | 2.17                     | 0.43              |
| 1:A:1039:LEU:HG   | 1:A:1043:PHE:HE2  | 1.79                     | 0.43              |
| 1:E:1040:LEU:HD21 | 1:E:1044:PHE:CE2  | 2.54                     | 0.43              |
| 1:C:646:CYS:C     | 1:C:648:LEU:H     | 2.27                     | 0.43              |
| 1:C:985:VAL:HB    | 1:C:1017:ASN:ND2  | 2.34                     | 0.43              |
| 3:C:1202:CLR:H231 | 3:C:1202:CLR:H272 | 1.86                     | 0.43              |
| 1:D:626:LEU:HD12  | 1:D:629:GLU:OE2   | 2.19                     | 0.43              |
| 1:D:916:LEU:O     | 1:D:920:ILE:HG12  | 2.19                     | 0.43              |
| 1:A:704:TYR:OH    | 1:A:768:CYS:HA    | 2.19                     | 0.43              |
| 1:A:916:LEU:O     | 1:A:920:ILE:HG12  | 2.19                     | 0.43              |
| 1:E:912:VAL:HG12  | 1:E:1066:LEU:HD13 | 2.01                     | 0.43              |
| 1:C:768:CYS:SG    | 1:C:769:LEU:N     | 2.91                     | 0.43              |
| 1:C:917:GLY:HA3   | 1:C:1058:TRP:NE1  | 2.33                     | 0.43              |
| 1:D:669:GLN:NE2   | 1:D:670:ASP:OD1   | 2.52                     | 0.43              |
| 1:A:637:ARG:HG3   | 1:A:640:ARG:HE    | 1.83                     | 0.42              |
| 1:A:805:PHE:O     | 1:A:888:TYR:OH    | 2.30                     | 0.42              |
| 1:A:1033:ILE:HG13 | 1:E:975:PHE:HZ    | 1.84                     | 0.42              |
| 3:A:1205:CLR:H183 | 3:A:1205:CLR:C21  | 2.45                     | 0.42              |
| 1:E:805:PHE:O     | 1:E:888:TYR:OH    | 2.29                     | 0.42              |
| 1:E:1042:ALA:O    | 1:E:1045:SER:OG   | 2.31                     | 0.42              |
| 1:C:1119:ARG:NH1  | 1:C:1122:LEU:HD22 | 2.34                     | 0.42              |
| 1:D:1160:LYS:O    | 1:D:1164:HIS:ND1  | 2.52                     | 0.42              |
| 1:A:952:LEU:HD12  | 1:A:954:PRO:HD3   | 2.01                     | 0.42              |
| 1:A:1141:ARG:HH22 | 1:A:1150:ARG:CZ   | 2.32                     | 0.42              |
| 1:A:1150:ARG:O    | 1:A:1154:LYS:HG2  | 2.18                     | 0.42              |
| 1:E:933:PHE:CG    | 1:E:1040:LEU:HD12 | 2.54                     | 0.42              |
| 1:E:1017:ASN:O    | 1:E:1022:VAL:HG23 | 2.18                     | 0.42              |
| 1:C:968:TYR:CZ    | 1:C:972:LEU:HD11  | 2.54                     | 0.42              |
| 1:D:669:GLN:NE2   | 1:D:671:GLY:H     | 2.17                     | 0.42              |
| 1:D:1069:PHE:CD1  | 1:D:1072:ARG:HD2  | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1122:LEU:O    | 1:D:1125:GLU:HG3  | 2.18                     | 0.42              |
| 1:A:1029:LEU:HD12 | 1:A:1033:ILE:HD12 | 2.02                     | 0.42              |
| 3:A:1204:CLR:H212 | 3:A:1204:CLR:H121 | 2.00                     | 0.42              |
| 1:E:577:TYR:O     | 1:E:580:GLU:HG2   | 2.20                     | 0.42              |
| 1:E:620:GLU:O     | 1:E:624:VAL:HG13  | 2.19                     | 0.42              |
| 1:D:629:GLU:HA    | 1:D:632:ARG:HE    | 1.84                     | 0.42              |
| 1:A:579:TRP:NE1   | 1:A:585:ALA:HB1   | 2.32                     | 0.42              |
| 1:E:632:ARG:NH1   | 1:E:632:ARG:HB2   | 2.34                     | 0.42              |
| 1:C:648:LEU:C     | 1:C:650:GLY:H     | 2.23                     | 0.42              |
| 1:D:614:ASP:C     | 1:D:618:LYS:HZ2   | 2.27                     | 0.42              |
| 1:D:700:PRO:HG2   | 1:D:701:PRO:HD3   | 2.01                     | 0.42              |
| 1:C:805:PHE:HD2   | 1:C:892:ARG:NH1   | 2.16                     | 0.42              |
| 1:D:656:GLN:HA    | 1:D:659:MET:HG2   | 2.01                     | 0.42              |
| 1:D:784:MET:HE2   | 1:D:784:MET:HA    | 2.00                     | 0.42              |
| 1:D:955:ARG:HG2   | 1:D:1011:CYS:HB3  | 2.02                     | 0.42              |
| 1:D:957:SER:HB2   | 1:D:962:ILE:HD11  | 2.01                     | 0.42              |
| 3:D:1202:CLR:H121 | 3:D:1202:CLR:C21  | 2.48                     | 0.42              |
| 1:A:594:LEU:HD11  | 1:A:660:GLN:HB3   | 2.00                     | 0.42              |
| 1:A:911:THR:HG22  | 1:A:920:ILE:HG21  | 2.02                     | 0.42              |
| 1:E:655:LEU:HB3   | 1:E:1064:TYR:OH   | 2.19                     | 0.42              |
| 1:C:809:PRO:HA    | 1:C:882:ARG:HH22  | 1.85                     | 0.42              |
| 1:D:969:ARG:HB3   | 1:D:970:PRO:HD3   | 2.01                     | 0.42              |
| 1:D:990:HIS:HA    | 1:D:1001:ALA:HA   | 2.01                     | 0.42              |
| 1:D:1022:LEU:O    | 1:D:1026:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:899:PHE:CE2   | 1:C:946:VAL:HG11  | 2.54                     | 0.42              |
| 1:A:956:ASP:OD2   | 1:A:1010:THR:N    | 2.49                     | 0.42              |
| 1:A:1147:ARG:NH2  | 1:C:1149:LYS:HA   | 2.35                     | 0.42              |
| 1:C:590:LEU:HD13  | 1:C:654:CYS:HB3   | 2.01                     | 0.42              |
| 1:C:622:MET:HE2   | 1:C:622:MET:HB2   | 1.89                     | 0.42              |
| 1:C:658:ALA:HB1   | 1:C:663:ALA:HB3   | 2.00                     | 0.42              |
| 1:C:672:VAL:HG22  | 1:C:676:LEU:HD23  | 2.02                     | 0.42              |
| 1:C:920:ILE:HG12  | 1:D:936:PHE:CZ    | 2.48                     | 0.42              |
| 1:C:1036:VAL:O    | 1:C:1040:ILE:HG23 | 2.19                     | 0.42              |
| 1:C:1089:LEU:HD22 | 1:C:1093:CYS:SG   | 2.59                     | 0.42              |
| 1:D:572:ALA:HB2   | 1:D:615:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:437:ARG:HB2   | 1:A:440:PHE:CD2   | 2.54                     | 0.42              |
| 3:A:1203:CLR:H121 | 3:A:1203:CLR:C21  | 2.49                     | 0.42              |
| 1:C:1041:ALA:O    | 1:C:1044:SER:OG   | 2.33                     | 0.42              |
| 1:C:1072:ARG:HA   | 1:C:1072:ARG:NE   | 2.35                     | 0.42              |
| 1:E:946:VAL:HG13  | 1:D:802:LEU:HD11  | 2.01                     | 0.42              |
| 1:C:471:SER:O     | 1:C:475:ASN:ND2   | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:572:ALA:HB3   | 1:C:573:GLN:OE1   | 2.19                     | 0.42              |
| 1:C:889:HIS:O     | 1:C:893:THR:HG23  | 2.19                     | 0.42              |
| 1:C:900:MET:HE1   | 1:D:943:ALA:C     | 2.45                     | 0.42              |
| 1:D:655:LEU:HB3   | 1:D:1063:TYR:OH   | 2.20                     | 0.42              |
| 1:A:917:GLY:HA3   | 1:A:1058:TRP:NE1  | 2.35                     | 0.42              |
| 1:A:1090:ARG:HH22 | 1:A:1097:ARG:NH1  | 2.18                     | 0.42              |
| 3:A:1203:CLR:H271 | 1:E:794:LEU:HB2   | 2.01                     | 0.42              |
| 1:C:671:GLY:O     | 1:C:675:LEU:HD23  | 2.20                     | 0.42              |
| 1:D:626:LEU:O     | 1:D:629:GLU:HG3   | 2.20                     | 0.42              |
| 1:D:1135:ALA:HA   | 1:D:1138:ARG:CZ   | 2.50                     | 0.42              |
| 1:A:597:ARG:HH12  | 1:A:616:ALA:HB1   | 1.85                     | 0.41              |
| 1:A:631:TYR:OH    | 1:A:635:GLU:OE2   | 2.36                     | 0.41              |
| 1:A:887:LEU:HD22  | 1:A:890:LEU:HD22  | 2.02                     | 0.41              |
| 1:E:922:ILE:HG21  | 1:E:1048:PHE:HD1  | 1.85                     | 0.41              |
| 1:E:1022:VAL:HG13 | 1:D:968:TYR:CE1   | 2.55                     | 0.41              |
| 1:C:944:TYR:O     | 1:C:948:THR:HG23  | 2.20                     | 0.41              |
| 1:C:1082:ILE:O    | 1:C:1085:LEU:HG   | 2.20                     | 0.41              |
| 1:D:964:ARG:HD3   | 1:D:1007:GLN:HG2  | 2.02                     | 0.41              |
| 1:A:1033:ILE:HD13 | 1:E:933:PHE:CE2   | 2.55                     | 0.41              |
| 1:E:805:PHE:HE2   | 1:E:892:ARG:HB2   | 1.84                     | 0.41              |
| 1:C:459:ARG:HA    | 1:C:462:GLN:CD    | 2.46                     | 0.41              |
| 1:C:900:MET:HE3   | 1:D:947:ALA:CB    | 2.47                     | 0.41              |
| 1:D:605:ASP:CG    | 1:D:608:GLU:HB3   | 2.45                     | 0.41              |
| 1:D:669:GLN:HB3   | 1:D:672:VAL:HG12  | 2.02                     | 0.41              |
| 1:D:862:ASP:OD2   | 1:D:865:ASN:ND2   | 2.53                     | 0.41              |
| 1:D:875:PHE:HB2   | 1:D:902:PHE:HZ    | 1.85                     | 0.41              |
| 1:E:676:LEU:HD12  | 1:E:1067:ILE:HD11 | 2.02                     | 0.41              |
| 1:E:1063:ARG:HA   | 1:E:1066:LEU:HG   | 2.02                     | 0.41              |
| 1:D:623:GLY:O     | 1:D:627:PHE:N     | 2.52                     | 0.41              |
| 1:A:1065:LEU:O    | 1:A:1068:GLU:HG3  | 2.21                     | 0.41              |
| 1:E:820:TRP:CH2   | 1:E:1079:PRO:HD3  | 2.56                     | 0.41              |
| 1:E:1131:GLU:O    | 1:E:1135:LEU:HD23 | 2.20                     | 0.41              |
| 1:C:637:ARG:HD2   | 1:C:1124:TRP:CD2  | 2.55                     | 0.41              |
| 1:C:798:SER:O     | 1:C:802:LEU:HG    | 2.20                     | 0.41              |
| 1:C:1122:LEU:O    | 1:C:1126:SER:N    | 2.46                     | 0.41              |
| 1:D:585:ALA:HB2   | 1:D:1129:LYS:HZ2  | 1.86                     | 0.41              |
| 1:D:783:PHE:CD1   | 1:D:783:PHE:C     | 2.98                     | 0.41              |
| 1:A:889:HIS:O     | 1:A:892:ARG:HG2   | 2.19                     | 0.41              |
| 1:E:684:MET:O     | 1:E:684:MET:HG2   | 2.20                     | 0.41              |
| 1:C:691:TRP:HA    | 1:C:694:VAL:HG12  | 2.03                     | 0.41              |
| 1:C:937:LEU:HD12  | 1:C:938:GLY:N     | 2.34                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C:1153:GLN:HA   | 1:C:1156:ASP:OD2   | 2.20                     | 0.41              |
| 1:D:450:SER:C     | 1:D:452:GLY:H      | 2.28                     | 0.41              |
| 1:D:680:TRP:HD1   | 1:D:779:PRO:HB2    | 1.85                     | 0.41              |
| 1:A:596:LEU:HD22  | 1:A:612:ARG:HG3    | 2.03                     | 0.41              |
| 1:E:962:ILE:CG2   | 3:D:1201:CLR:H12   | 2.34                     | 0.41              |
| 1:C:795:LEU:N     | 3:C:1202:CLR:C27   | 2.84                     | 0.41              |
| 1:C:803:VAL:CG2   | 3:C:1202:CLR:C2    | 2.70                     | 0.41              |
| 1:C:891:GLY:HA2   | 1:C:894:VAL:HG12   | 2.03                     | 0.41              |
| 1:C:906:LEU:HA    | 1:C:909:ILE:HD12   | 2.01                     | 0.41              |
| 1:C:1029:LEU:HD12 | 1:C:1033:ILE:HD12  | 2.01                     | 0.41              |
| 1:C:1082:ILE:HA   | 1:C:1085:LEU:HG    | 2.02                     | 0.41              |
| 1:D:1138:ARG:O    | 1:D:1142:GLU:OE1   | 2.38                     | 0.41              |
| 1:E:608:GLU:HA    | 1:E:611:ARG:HG2    | 2.03                     | 0.41              |
| 1:C:587:SER:H     | 1:C:590:LEU:HD12   | 1.86                     | 0.41              |
| 1:C:922:ILE:HG21  | 1:C:1047:PHE:CE1   | 2.56                     | 0.41              |
| 1:D:483:SER:OG    | 1:D:508:ARG:NH1    | 2.53                     | 0.41              |
| 1:D:559:TRP:O     | 1:D:563:LEU:HB2    | 2.21                     | 0.41              |
| 1:A:608:GLU:OE1   | 1:A:611:ARG:HD3    | 2.20                     | 0.41              |
| 1:A:782:ILE:HD12  | 1:A:1074:ALA:HA    | 2.03                     | 0.41              |
| 1:A:793:PHE:HB2   | 1:A:820:TRP:CZ2    | 2.56                     | 0.41              |
| 1:A:881:CYS:HB3   | 1:A:887:LEU:O      | 2.21                     | 0.41              |
| 1:A:943:ALA:HB2   | 1:E:903:THR:HG21   | 2.03                     | 0.41              |
| 3:A:1203:CLR:C27  | 1:E:794:LEU:CB     | 2.99                     | 0.41              |
| 3:A:1204:CLR:H191 | 3:A:1204:CLR:H8    | 1.87                     | 0.41              |
| 1:E:790:TYR:CD2   | 1:E:909:ILE:HD13   | 2.56                     | 0.41              |
| 1:E:1127:SER:HA   | 1:E:1130:LYS:HG2   | 2.02                     | 0.41              |
| 1:C:450:SER:C     | 1:C:452:GLY:H      | 2.28                     | 0.41              |
| 1:C:627:PHE:CE1   | 1:C:642:LEU:HD21   | 2.56                     | 0.41              |
| 1:D:474:ARG:NH2   | 1:D:477:LEU:HB3    | 2.36                     | 0.41              |
| 1:D:566:ALA:HB1   | 1:D:571:ARG:HB2    | 2.03                     | 0.41              |
| 1:D:864:TRP:CD1   | 2:D:1203:A1H0C:C23 | 3.03                     | 0.41              |
| 1:D:1129:LYS:O    | 1:D:1133:LEU:HD23  | 2.20                     | 0.41              |
| 1:C:637:ARG:HE    | 1:C:640:ARG:NH2    | 2.19                     | 0.41              |
| 1:C:1133:LEU:HD13 | 1:C:1136:ARG:NH2   | 2.35                     | 0.41              |
| 1:D:594:LEU:HA    | 1:D:661:ALA:CB     | 2.51                     | 0.41              |
| 1:A:436:ASP:OD1   | 1:A:574:MET:HE1    | 2.20                     | 0.41              |
| 1:A:591:GLY:HA3   | 1:A:649:TRP:CD2    | 2.55                     | 0.41              |
| 1:A:1041:ALA:HB1  | 1:E:1045:SER:HA    | 2.02                     | 0.41              |
| 1:E:819:PHE:HA    | 1:E:822:PHE:CD2    | 2.56                     | 0.41              |
| 1:E:889:HIS:O     | 1:E:893:THR:HG23   | 2.20                     | 0.41              |
| 1:C:767:ARG:O     | 1:C:771:ARG:CB     | 2.69                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:C:790:TYR:CE2   | 1:C:909:ILE:HD13   | 2.56                     | 0.41              |
| 1:C:1162:LEU:HD13 | 1:C:1165:ILE:HD11  | 2.03                     | 0.41              |
| 1:D:559:TRP:CD1   | 1:D:583:SER:H      | 2.39                     | 0.41              |
| 1:D:876:LEU:HA    | 1:D:879:VAL:HG22   | 2.01                     | 0.41              |
| 1:D:891:GLY:HA2   | 1:D:894:VAL:HG12   | 2.02                     | 0.41              |
| 1:A:928:LYS:H     | 1:A:928:LYS:HG2    | 1.57                     | 0.40              |
| 3:A:1202:CLR:H121 | 3:A:1202:CLR:C21   | 2.50                     | 0.40              |
| 1:E:437:ARG:HG3   | 1:E:437:ARG:O      | 2.21                     | 0.40              |
| 1:C:614:ASP:OD2   | 1:C:614:ASP:N      | 2.53                     | 0.40              |
| 1:C:615:LEU:O     | 1:C:619:PHE:HD2    | 2.03                     | 0.40              |
| 1:C:797:PHE:HA    | 1:C:817:LEU:HD11   | 2.02                     | 0.40              |
| 1:C:862:ASP:O     | 1:C:865:ASN:N      | 2.54                     | 0.40              |
| 1:D:1136:ARG:O    | 1:D:1140:LYS:HE2   | 2.22                     | 0.40              |
| 1:A:559:TRP:CD1   | 1:A:582:GLY:HA2    | 2.57                     | 0.40              |
| 3:A:1204:CLR:H193 | 3:A:1204:CLR:H111  | 1.86                     | 0.40              |
| 1:E:1037:VAL:O    | 1:E:1041:ILE:HG13  | 2.21                     | 0.40              |
| 1:C:451:LEU:HA    | 1:C:454:PHE:HB3    | 2.02                     | 0.40              |
| 1:D:864:TRP:HD1   | 2:D:1203:A1H0C:C23 | 2.34                     | 0.40              |
| 1:A:676:LEU:HD13  | 1:A:676:LEU:HA     | 1.95                     | 0.40              |
| 1:A:825:LEU:HD13  | 1:A:872:LEU:HD13   | 2.04                     | 0.40              |
| 1:C:653:THR:HB    | 1:C:656:GLN:OE1    | 2.21                     | 0.40              |
| 1:C:855:ARG:O     | 1:C:858:LEU:HG     | 2.21                     | 0.40              |
| 1:D:615:LEU:HD23  | 1:D:618:LYS:HD2    | 2.03                     | 0.40              |
| 1:A:1126:SER:O    | 1:A:1129:LYS:HG2   | 2.21                     | 0.40              |
| 3:C:1202:CLR:H193 | 3:C:1202:CLR:H111  | 1.88                     | 0.40              |
| 1:D:432:ALA:CA    | 1:D:437:ARG:HE     | 2.34                     | 0.40              |
| 1:D:803:VAL:HG13  | 3:D:1201:CLR:O1    | 2.21                     | 0.40              |
| 1:D:967:PHE:C     | 1:D:970:PRO:HD2    | 2.46                     | 0.40              |
| 1:A:973:GLN:NE2   | 1:A:979:PRO:HD2    | 2.36                     | 0.40              |
| 1:E:942:VAL:CG2   | 3:D:1201:CLR:C21   | 2.99                     | 0.40              |
| 1:C:941:LEU:HD23  | 3:D:1204:CLR:H262  | 2.03                     | 0.40              |
| 1:D:627:PHE:CZ    | 1:D:642:LEU:HD21   | 2.56                     | 0.40              |
| 1:D:637:ARG:HE    | 1:D:640:ARG:NH2    | 2.19                     | 0.40              |
| 1:D:766:ARG:HD2   | 1:D:766:ARG:HA     | 1.93                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 594/749 (79%)   | 574 (97%)  | 19 (3%)  | 1 (0%)   | 43          | 77 |
| 1   | C     | 593/749 (79%)   | 551 (93%)  | 37 (6%)  | 5 (1%)   | 16          | 52 |
| 1   | D     | 594/749 (79%)   | 553 (93%)  | 38 (6%)  | 3 (0%)   | 24          | 62 |
| 1   | E     | 593/749 (79%)   | 573 (97%)  | 19 (3%)  | 1 (0%)   | 43          | 77 |
| All | All   | 2374/2996 (79%) | 2251 (95%) | 113 (5%) | 10 (0%)  | 31          | 66 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 586 | VAL  |
| 1   | C     | 587 | SER  |
| 1   | C     | 649 | TRP  |
| 1   | C     | 769 | LEU  |
| 1   | D     | 578 | PHE  |
| 1   | D     | 579 | TRP  |
| 1   | C     | 768 | CYS  |
| 1   | A     | 708 | ILE  |
| 1   | E     | 708 | ILE  |
| 1   | D     | 708 | ILE  |

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 525/626 (84%) | 525 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | C     | 524/626 (84%)   | 524 (100%)  | 0        | 100         | 100 |
| 1   | D     | 525/626 (84%)   | 525 (100%)  | 0        | 100         | 100 |
| 1   | E     | 524/626 (84%)   | 523 (100%)  | 1 (0%)   | 87          | 85  |
| All | All   | 2098/2504 (84%) | 2097 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 864 | TRP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 915  | GLN  |
| 1   | A     | 1070 | HIS  |
| 1   | A     | 1153 | GLN  |
| 1   | E     | 915  | GLN  |
| 1   | E     | 973  | GLN  |
| 1   | E     | 1014 | GLN  |
| 1   | E     | 1033 | ASN  |
| 1   | E     | 1038 | ASN  |
| 1   | E     | 1154 | GLN  |
| 1   | E     | 1162 | GLN  |
| 1   | C     | 505  | HIS  |
| 1   | C     | 570  | ASN  |
| 1   | C     | 831  | GLN  |
| 1   | C     | 865  | ASN  |
| 1   | C     | 973  | GLN  |
| 1   | C     | 980  | GLN  |
| 1   | C     | 1014 | GLN  |
| 1   | C     | 1161 | GLN  |
| 1   | D     | 462  | GLN  |
| 1   | D     | 889  | HIS  |
| 1   | D     | 908  | HIS  |
| 1   | D     | 973  | GLN  |
| 1   | D     | 977  | GLN  |
| 1   | D     | 1014 | GLN  |
| 1   | D     | 1070 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

| Mol | Type  | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |       |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | A1H0C | D     | 1203 | -    | 27,27,27     | 1.53 | 4 (14%)  | 37,37,37    | 1.57 | 3 (8%)   |
| 3   | CLR   | C     | 1202 | -    | 31,31,31     | 0.86 | 2 (6%)   | 48,48,48    | 1.45 | 8 (16%)  |
| 3   | CLR   | D     | 1202 | -    | 31,31,31     | 0.86 | 1 (3%)   | 48,48,48    | 1.40 | 7 (14%)  |
| 3   | CLR   | A     | 1202 | -    | 31,31,31     | 0.83 | 1 (3%)   | 48,48,48    | 1.61 | 12 (25%) |
| 2   | A1H0C | E     | 1201 | -    | 27,27,27     | 1.53 | 4 (14%)  | 37,37,37    | 1.58 | 3 (8%)   |
| 3   | CLR   | A     | 1203 | -    | 31,31,31     | 0.84 | 1 (3%)   | 48,48,48    | 1.40 | 8 (16%)  |
| 3   | CLR   | A     | 1204 | -    | 31,31,31     | 0.94 | 2 (6%)   | 48,48,48    | 1.47 | 10 (20%) |
| 3   | CLR   | D     | 1201 | -    | 31,31,31     | 0.42 | 0        | 48,48,48    | 1.40 | 9 (18%)  |
| 3   | CLR   | D     | 1204 | -    | 31,31,31     | 0.84 | 1 (3%)   | 48,48,48    | 1.54 | 9 (18%)  |
| 3   | CLR   | A     | 1205 | -    | 31,31,31     | 0.84 | 1 (3%)   | 48,48,48    | 1.61 | 12 (25%) |
| 2   | A1H0C | A     | 1201 | -    | 27,27,27     | 1.53 | 4 (14%)  | 37,37,37    | 1.57 | 3 (8%)   |
| 2   | A1H0C | C     | 1201 | -    | 27,27,27     | 1.53 | 4 (14%)  | 37,37,37    | 1.57 | 3 (8%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

| Mol | Type  | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|-------|-------|------|------|---------|------------|---------|
| 2   | A1H0C | D     | 1203 | -    | -       | 4/13/13/13 | 0/3/3/3 |
| 3   | CLR   | C     | 1202 | -    | -       | 1/10/68/68 | 0/4/4/4 |
| 3   | CLR   | D     | 1202 | -    | -       | 4/10/68/68 | 0/4/4/4 |
| 3   | CLR   | A     | 1202 | -    | -       | 1/10/68/68 | 0/4/4/4 |
| 2   | A1H0C | E     | 1201 | -    | -       | 4/13/13/13 | 0/3/3/3 |
| 3   | CLR   | A     | 1203 | -    | -       | 4/10/68/68 | 0/4/4/4 |
| 3   | CLR   | A     | 1204 | -    | -       | 3/10/68/68 | 0/4/4/4 |
| 3   | CLR   | D     | 1201 | -    | -       | 3/10/68/68 | 0/4/4/4 |
| 3   | CLR   | D     | 1204 | -    | -       | 1/10/68/68 | 0/4/4/4 |
| 3   | CLR   | A     | 1205 | -    | -       | 3/10/68/68 | 0/4/4/4 |
| 2   | A1H0C | A     | 1201 | -    | -       | 4/13/13/13 | 0/3/3/3 |
| 2   | A1H0C | C     | 1201 | -    | -       | 4/13/13/13 | 0/3/3/3 |

All (25) bond length outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|-------|-------------|----------|
| 2   | D     | 1203 | A1H0C | C02-N15 | 4.87  | 1.46        | 1.35     |
| 2   | C     | 1201 | A1H0C | C02-N15 | 4.86  | 1.46        | 1.35     |
| 2   | E     | 1201 | A1H0C | C02-N15 | 4.84  | 1.46        | 1.35     |
| 2   | A     | 1201 | A1H0C | C02-N15 | 4.82  | 1.46        | 1.35     |
| 2   | D     | 1203 | A1H0C | C14-C09 | -3.05 | 1.37        | 1.43     |
| 2   | E     | 1201 | A1H0C | C14-C09 | -3.04 | 1.37        | 1.43     |
| 2   | A     | 1201 | A1H0C | C14-C09 | -3.04 | 1.37        | 1.43     |
| 2   | C     | 1201 | A1H0C | C14-C09 | -3.04 | 1.37        | 1.43     |
| 3   | A     | 1205 | CLR   | C10-C9  | -2.45 | 1.52        | 1.56     |
| 2   | D     | 1203 | A1H0C | O01-C02 | -2.32 | 1.18        | 1.23     |
| 2   | E     | 1201 | A1H0C | O01-C02 | -2.31 | 1.18        | 1.23     |
| 2   | A     | 1201 | A1H0C | O01-C02 | -2.30 | 1.18        | 1.23     |
| 2   | C     | 1201 | A1H0C | O01-C02 | -2.29 | 1.18        | 1.23     |
| 3   | C     | 1202 | CLR   | C10-C9  | -2.23 | 1.52        | 1.56     |
| 3   | A     | 1204 | CLR   | C10-C9  | -2.23 | 1.52        | 1.56     |
| 3   | A     | 1203 | CLR   | C10-C9  | -2.17 | 1.52        | 1.56     |
| 2   | E     | 1201 | A1H0C | C16-N15 | 2.16  | 1.46        | 1.41     |
| 2   | C     | 1201 | A1H0C | C16-N15 | 2.15  | 1.46        | 1.41     |
| 2   | A     | 1201 | A1H0C | C16-N15 | 2.14  | 1.46        | 1.41     |
| 3   | A     | 1204 | CLR   | C13-C14 | -2.10 | 1.51        | 1.55     |
| 2   | D     | 1203 | A1H0C | C16-N15 | 2.10  | 1.45        | 1.41     |
| 3   | D     | 1202 | CLR   | C13-C14 | -2.08 | 1.51        | 1.55     |
| 3   | A     | 1202 | CLR   | C13-C14 | -2.05 | 1.51        | 1.55     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 1204 | CLR  | C13-C14 | -2.03 | 1.51        | 1.55     |
| 3   | C     | 1202 | CLR  | C13-C14 | -2.00 | 1.51        | 1.55     |

All (87) bond angle outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 2   | C     | 1201 | A1H0C | C03-C02-N15 | 5.80  | 127.19      | 115.62   |
| 2   | E     | 1201 | A1H0C | C03-C02-N15 | 5.78  | 127.16      | 115.62   |
| 2   | A     | 1201 | A1H0C | C03-C02-N15 | 5.77  | 127.13      | 115.62   |
| 2   | D     | 1203 | A1H0C | C03-C02-N15 | 5.75  | 127.09      | 115.62   |
| 3   | A     | 1205 | CLR   | C4-C5-C10   | 4.21  | 121.81      | 116.42   |
| 3   | D     | 1202 | CLR   | C13-C17-C20 | -4.16 | 113.07      | 119.50   |
| 2   | C     | 1201 | A1H0C | O01-C02-N15 | -4.13 | 116.23      | 123.64   |
| 2   | E     | 1201 | A1H0C | O01-C02-N15 | -4.12 | 116.26      | 123.64   |
| 2   | D     | 1203 | A1H0C | O01-C02-N15 | -4.10 | 116.29      | 123.64   |
| 2   | A     | 1201 | A1H0C | O01-C02-N15 | -4.10 | 116.30      | 123.64   |
| 3   | D     | 1202 | CLR   | C17-C13-C14 | 4.00  | 104.69      | 100.10   |
| 3   | A     | 1205 | CLR   | C13-C17-C20 | -4.00 | 113.33      | 119.50   |
| 3   | A     | 1202 | CLR   | C13-C17-C20 | -3.92 | 113.45      | 119.50   |
| 3   | C     | 1202 | CLR   | C10-C9-C8   | -3.82 | 107.13      | 112.71   |
| 3   | D     | 1201 | CLR   | C15-C14-C13 | 3.78  | 108.29      | 103.84   |
| 3   | D     | 1201 | CLR   | C17-C13-C14 | 3.68  | 104.33      | 100.10   |
| 3   | A     | 1204 | CLR   | C10-C9-C8   | -3.68 | 107.33      | 112.71   |
| 3   | A     | 1202 | CLR   | C17-C13-C14 | 3.60  | 104.23      | 100.10   |
| 3   | D     | 1204 | CLR   | C13-C17-C20 | -3.56 | 114.00      | 119.50   |
| 3   | A     | 1203 | CLR   | C13-C17-C20 | -3.52 | 114.05      | 119.50   |
| 3   | A     | 1203 | CLR   | C4-C5-C10   | 3.48  | 120.88      | 116.42   |
| 3   | A     | 1202 | CLR   | C13-C14-C8  | -3.46 | 109.50      | 114.41   |
| 3   | A     | 1202 | CLR   | C10-C9-C8   | -3.45 | 107.67      | 112.71   |
| 3   | D     | 1204 | CLR   | C10-C9-C8   | -3.41 | 107.72      | 112.71   |
| 3   | D     | 1204 | CLR   | C17-C13-C14 | 3.41  | 104.01      | 100.10   |
| 3   | D     | 1204 | CLR   | C13-C14-C8  | -3.35 | 109.66      | 114.41   |
| 3   | D     | 1204 | CLR   | C8-C7-C6    | -3.32 | 108.16      | 112.76   |
| 3   | A     | 1204 | CLR   | C17-C13-C14 | 3.29  | 103.88      | 100.10   |
| 3   | A     | 1202 | CLR   | C8-C7-C6    | -3.26 | 108.24      | 112.76   |
| 3   | A     | 1203 | CLR   | C10-C9-C8   | -3.12 | 108.16      | 112.71   |
| 3   | C     | 1202 | CLR   | C11-C12-C13 | -3.11 | 107.49      | 112.74   |
| 3   | A     | 1204 | CLR   | C13-C17-C20 | -2.97 | 114.91      | 119.50   |
| 3   | D     | 1201 | CLR   | C12-C13-C14 | -2.95 | 102.83      | 107.25   |
| 3   | A     | 1203 | CLR   | C13-C14-C8  | -2.93 | 110.25      | 114.41   |
| 3   | A     | 1203 | CLR   | C17-C13-C14 | 2.92  | 103.45      | 100.10   |
| 3   | A     | 1205 | CLR   | C11-C12-C13 | -2.84 | 107.95      | 112.74   |

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| Mol | Chain | Res  | Type  | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|-------|-------------|----------|
| 3   | C     | 1202 | CLR   | C13-C17-C20 | -2.83 | 115.12      | 119.50   |
| 3   | A     | 1204 | CLR   | C4-C5-C10   | 2.83  | 120.05      | 116.42   |
| 3   | A     | 1204 | CLR   | C13-C14-C8  | -2.79 | 110.46      | 114.41   |
| 3   | D     | 1202 | CLR   | C13-C14-C8  | -2.78 | 110.46      | 114.41   |
| 3   | D     | 1202 | CLR   | C10-C9-C8   | -2.76 | 108.68      | 112.71   |
| 3   | D     | 1202 | CLR   | C11-C12-C13 | -2.75 | 108.10      | 112.74   |
| 3   | A     | 1205 | CLR   | C1-C10-C5   | 2.73  | 113.46      | 108.74   |
| 3   | C     | 1202 | CLR   | C11-C9-C8   | 2.70  | 115.55      | 111.78   |
| 2   | D     | 1203 | A1H0C | O04-C03-C02 | -2.64 | 103.54      | 110.80   |
| 3   | A     | 1205 | CLR   | C17-C13-C14 | 2.64  | 103.13      | 100.10   |
| 2   | E     | 1201 | A1H0C | O04-C03-C02 | -2.63 | 103.56      | 110.80   |
| 2   | A     | 1201 | A1H0C | O04-C03-C02 | -2.63 | 103.56      | 110.80   |
| 2   | C     | 1201 | A1H0C | O04-C03-C02 | -2.63 | 103.58      | 110.80   |
| 3   | A     | 1204 | CLR   | C11-C12-C13 | -2.60 | 108.35      | 112.74   |
| 3   | C     | 1202 | CLR   | C8-C7-C6    | -2.58 | 109.19      | 112.76   |
| 3   | A     | 1203 | CLR   | C4-C5-C6    | -2.53 | 117.14      | 120.57   |
| 3   | A     | 1202 | CLR   | C11-C12-C13 | -2.51 | 108.50      | 112.74   |
| 3   | A     | 1202 | CLR   | C11-C9-C8   | 2.51  | 115.28      | 111.78   |
| 3   | D     | 1201 | CLR   | C10-C9-C8   | -2.47 | 109.11      | 112.71   |
| 3   | A     | 1205 | CLR   | C18-C13-C12 | -2.47 | 106.97      | 110.61   |
| 3   | C     | 1202 | CLR   | C14-C8-C9   | 2.46  | 112.30      | 109.09   |
| 3   | A     | 1205 | CLR   | C10-C9-C8   | -2.44 | 109.14      | 112.71   |
| 3   | D     | 1204 | CLR   | C11-C9-C8   | 2.43  | 115.17      | 111.78   |
| 3   | D     | 1204 | CLR   | C11-C12-C13 | -2.42 | 108.65      | 112.74   |
| 3   | A     | 1205 | CLR   | C13-C14-C8  | -2.42 | 110.98      | 114.41   |
| 3   | A     | 1204 | CLR   | C11-C9-C8   | 2.41  | 115.15      | 111.78   |
| 3   | A     | 1203 | CLR   | C11-C12-C13 | -2.41 | 108.67      | 112.74   |
| 3   | A     | 1205 | CLR   | C9-C10-C5   | -2.37 | 106.18      | 109.65   |
| 3   | A     | 1202 | CLR   | C4-C5-C10   | 2.37  | 119.46      | 116.42   |
| 3   | C     | 1202 | CLR   | C7-C8-C9    | -2.36 | 106.99      | 109.72   |
| 3   | A     | 1203 | CLR   | C11-C9-C8   | 2.35  | 115.05      | 111.78   |
| 3   | A     | 1202 | CLR   | C4-C5-C6    | -2.33 | 117.41      | 120.57   |
| 3   | D     | 1202 | CLR   | C1-C10-C9   | 2.28  | 111.76      | 108.74   |
| 3   | C     | 1202 | CLR   | C17-C13-C14 | 2.28  | 102.72      | 100.10   |
| 3   | A     | 1205 | CLR   | C7-C8-C9    | 2.21  | 112.28      | 109.72   |
| 3   | A     | 1202 | CLR   | C7-C8-C9    | -2.17 | 107.21      | 109.72   |
| 3   | A     | 1202 | CLR   | C14-C8-C9   | 2.17  | 111.92      | 109.09   |
| 3   | D     | 1201 | CLR   | C12-C11-C9  | 2.17  | 116.83      | 113.14   |
| 3   | A     | 1204 | CLR   | C19-C10-C9  | -2.12 | 109.28      | 111.66   |
| 3   | D     | 1202 | CLR   | C4-C5-C10   | 2.11  | 119.12      | 116.42   |
| 3   | A     | 1202 | CLR   | C21-C20-C17 | -2.11 | 109.72      | 112.88   |
| 3   | D     | 1204 | CLR   | C4-C5-C10   | 2.09  | 119.10      | 116.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 1201 | CLR  | C2-C3-C4    | -2.09 | 107.36      | 110.29   |
| 3   | D     | 1204 | CLR  | C4-C5-C6    | -2.08 | 117.75      | 120.57   |
| 3   | A     | 1204 | CLR  | C11-C9-C10  | -2.08 | 110.52      | 113.08   |
| 3   | A     | 1205 | CLR  | C4-C5-C6    | -2.07 | 117.76      | 120.57   |
| 3   | D     | 1201 | CLR  | C15-C16-C17 | 2.07  | 109.19      | 105.14   |
| 3   | D     | 1201 | CLR  | C1-C2-C3    | -2.07 | 107.75      | 110.48   |
| 3   | D     | 1201 | CLR  | C11-C9-C8   | 2.05  | 114.64      | 111.78   |
| 3   | A     | 1205 | CLR  | C14-C8-C9   | -2.05 | 106.41      | 109.09   |
| 3   | A     | 1204 | CLR  | C4-C5-C6    | -2.05 | 117.80      | 120.57   |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 2   | A     | 1201 | A1H0C | C03-C02-N15-C16 |
| 2   | E     | 1201 | A1H0C | C03-C02-N15-C16 |
| 2   | C     | 1201 | A1H0C | C03-C02-N15-C16 |
| 2   | D     | 1203 | A1H0C | C03-C02-N15-C16 |
| 2   | A     | 1201 | A1H0C | O01-C02-N15-C16 |
| 2   | E     | 1201 | A1H0C | O01-C02-N15-C16 |
| 2   | C     | 1201 | A1H0C | O01-C02-N15-C16 |
| 2   | D     | 1203 | A1H0C | O01-C02-N15-C16 |
| 3   | A     | 1203 | CLR   | C21-C20-C22-C23 |
| 3   | A     | 1204 | CLR   | C21-C20-C22-C23 |
| 3   | A     | 1204 | CLR   | C17-C20-C22-C23 |
| 3   | A     | 1203 | CLR   | C17-C20-C22-C23 |
| 3   | D     | 1202 | CLR   | C17-C20-C22-C23 |
| 3   | D     | 1202 | CLR   | C20-C22-C23-C24 |
| 3   | A     | 1205 | CLR   | C20-C22-C23-C24 |
| 3   | D     | 1201 | CLR   | C17-C20-C22-C23 |
| 3   | A     | 1205 | CLR   | C21-C20-C22-C23 |
| 3   | A     | 1203 | CLR   | C23-C24-C25-C26 |
| 3   | A     | 1205 | CLR   | C17-C20-C22-C23 |
| 3   | C     | 1202 | CLR   | C22-C23-C24-C25 |
| 3   | D     | 1201 | CLR   | C21-C20-C22-C23 |
| 3   | D     | 1202 | CLR   | C21-C20-C22-C23 |
| 3   | A     | 1203 | CLR   | C23-C24-C25-C27 |
| 3   | D     | 1201 | CLR   | C22-C23-C24-C25 |
| 3   | A     | 1204 | CLR   | C22-C23-C24-C25 |
| 3   | A     | 1202 | CLR   | C23-C24-C25-C27 |
| 3   | D     | 1204 | CLR   | C23-C24-C25-C27 |
| 2   | A     | 1201 | A1H0C | N15-C02-C03-O04 |

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| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 2   | E     | 1201 | A1H0C | N15-C02-C03-O04 |
| 2   | C     | 1201 | A1H0C | N15-C02-C03-O04 |
| 2   | D     | 1203 | A1H0C | N15-C02-C03-O04 |
| 3   | D     | 1202 | CLR   | C22-C23-C24-C25 |
| 2   | A     | 1201 | A1H0C | O01-C02-C03-O04 |
| 2   | C     | 1201 | A1H0C | O01-C02-C03-O04 |
| 2   | D     | 1203 | A1H0C | O01-C02-C03-O04 |
| 2   | E     | 1201 | A1H0C | O01-C02-C03-O04 |

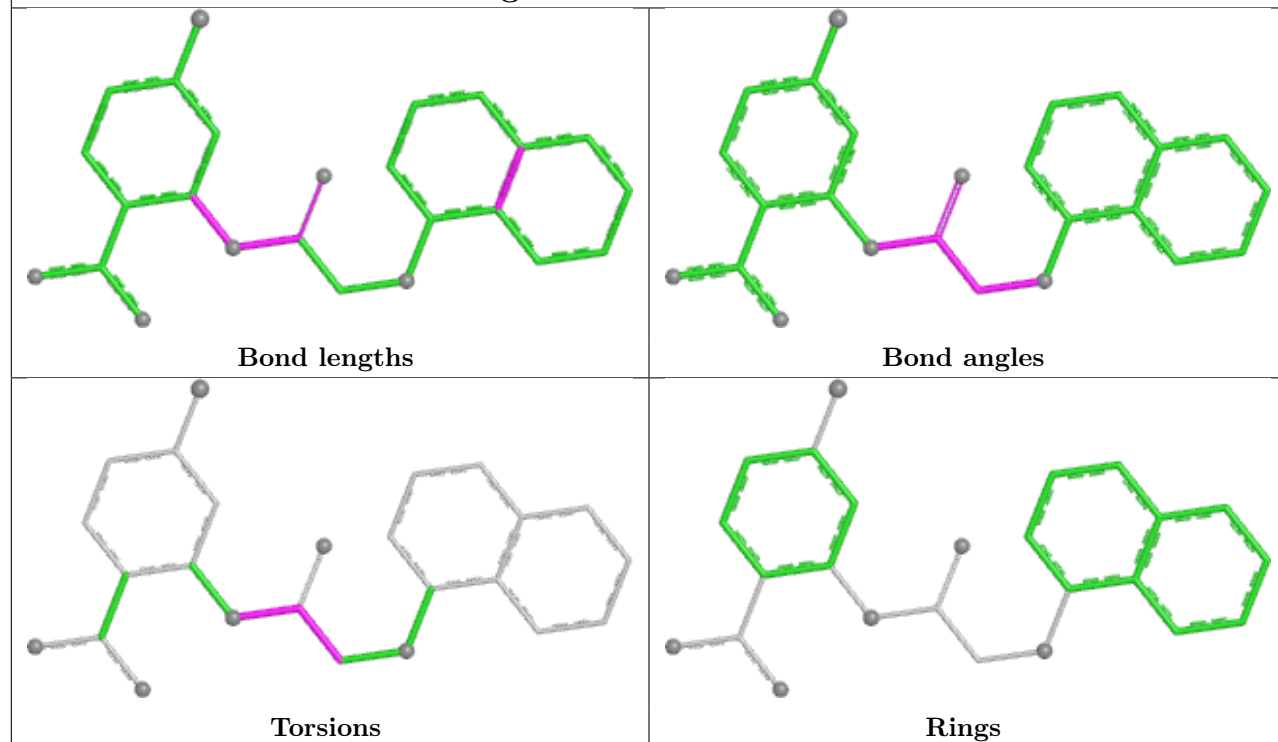
There are no ring outliers.

12 monomers are involved in 194 short contacts:

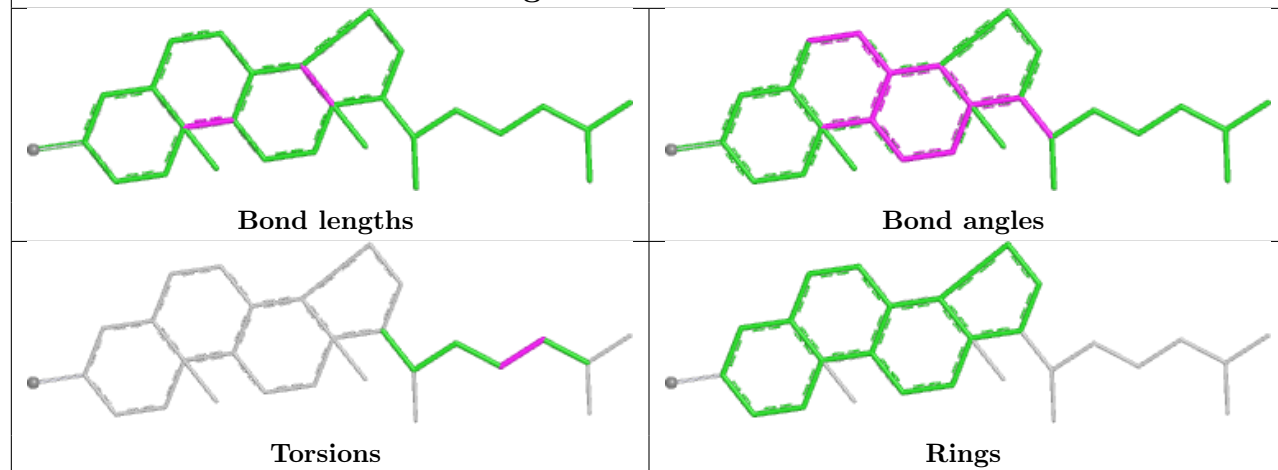
| Mol | Chain | Res  | Type  | Clashes | Symm-Clashes |
|-----|-------|------|-------|---------|--------------|
| 2   | D     | 1203 | A1H0C | 5       | 0            |
| 3   | C     | 1202 | CLR   | 36      | 0            |
| 3   | D     | 1202 | CLR   | 13      | 0            |
| 3   | A     | 1202 | CLR   | 4       | 0            |
| 2   | E     | 1201 | A1H0C | 5       | 0            |
| 3   | A     | 1203 | CLR   | 23      | 0            |
| 3   | A     | 1204 | CLR   | 11      | 0            |
| 3   | D     | 1201 | CLR   | 58      | 0            |
| 3   | D     | 1204 | CLR   | 7       | 0            |
| 3   | A     | 1205 | CLR   | 29      | 0            |
| 2   | A     | 1201 | A1H0C | 2       | 0            |
| 2   | C     | 1201 | A1H0C | 1       | 0            |

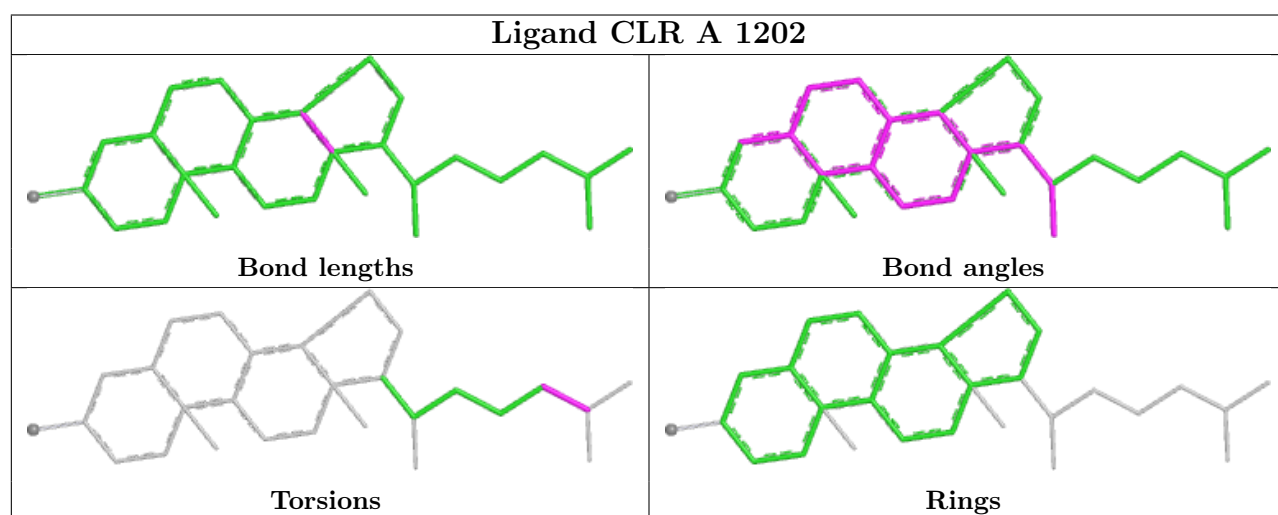
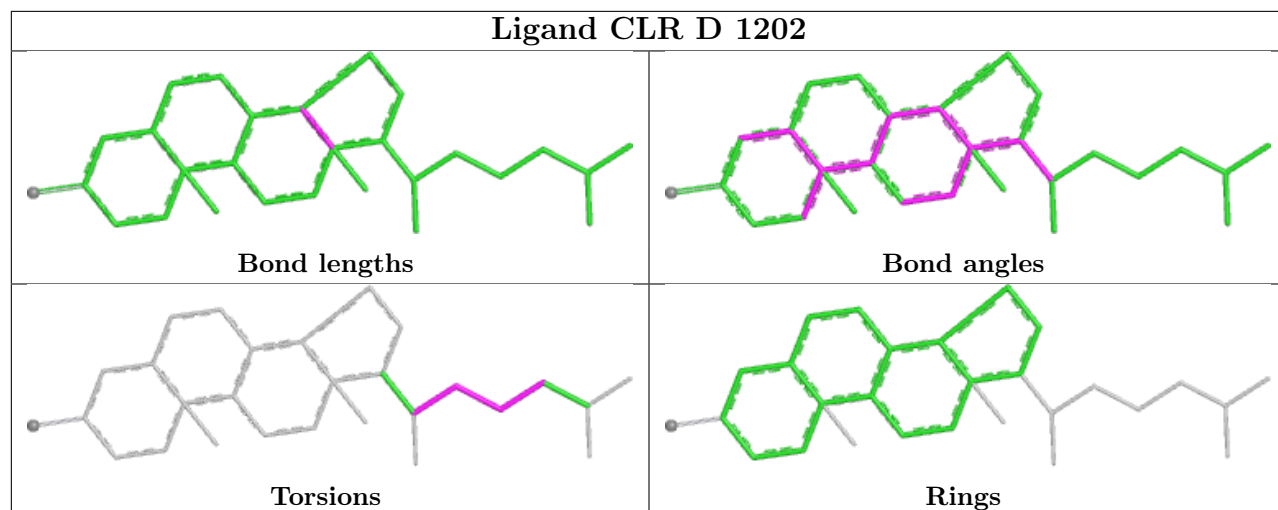
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand A1H0C D 1203

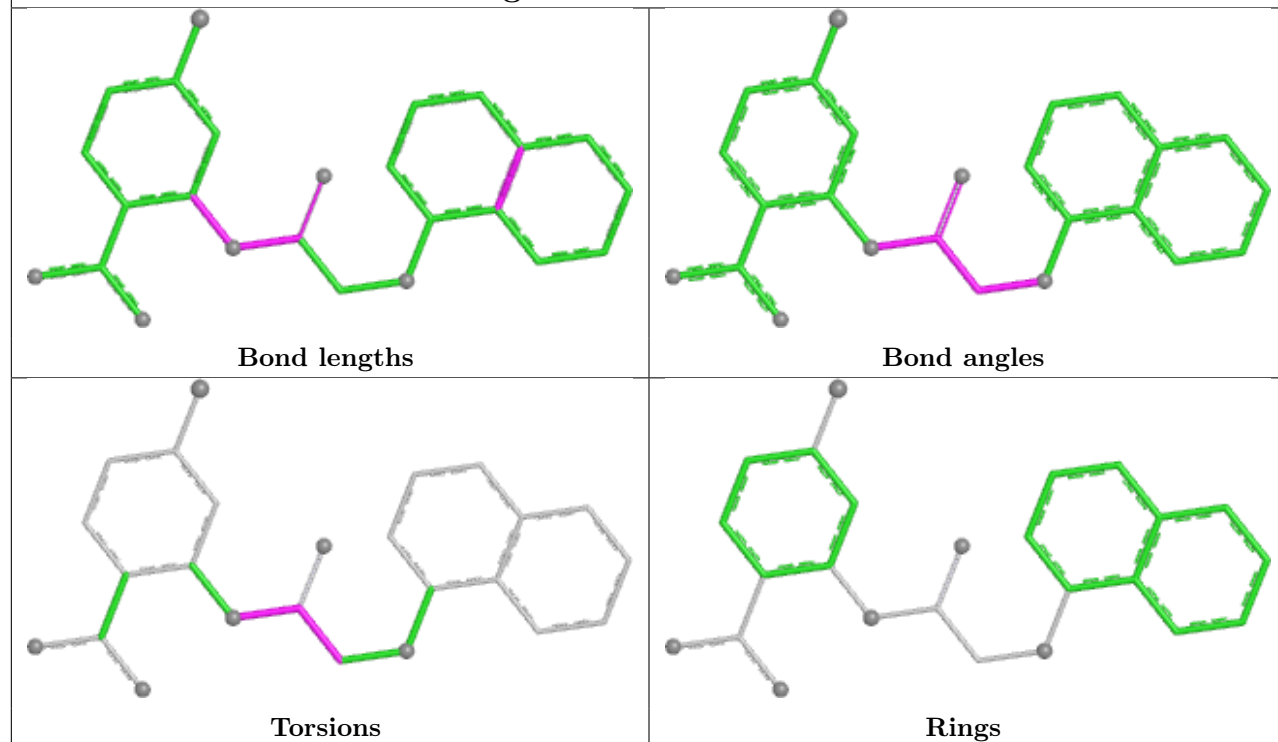


## Ligand CLR C 1202

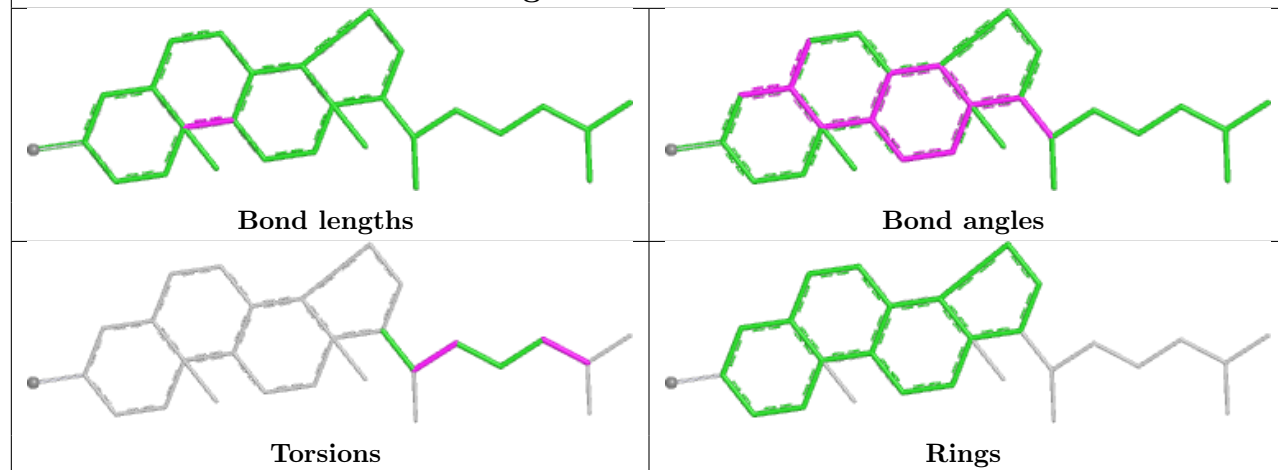


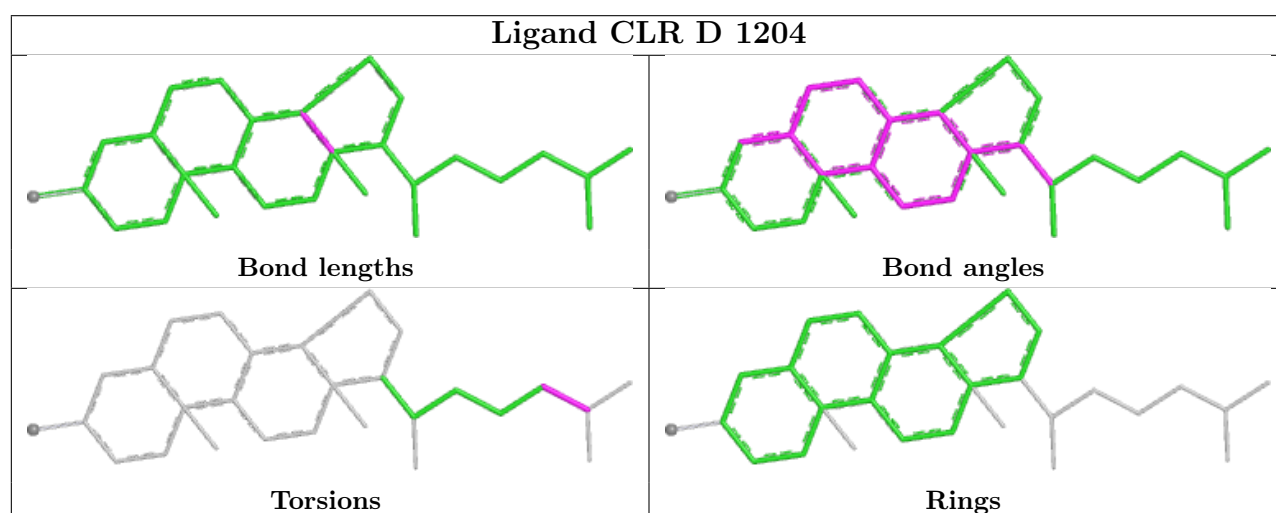
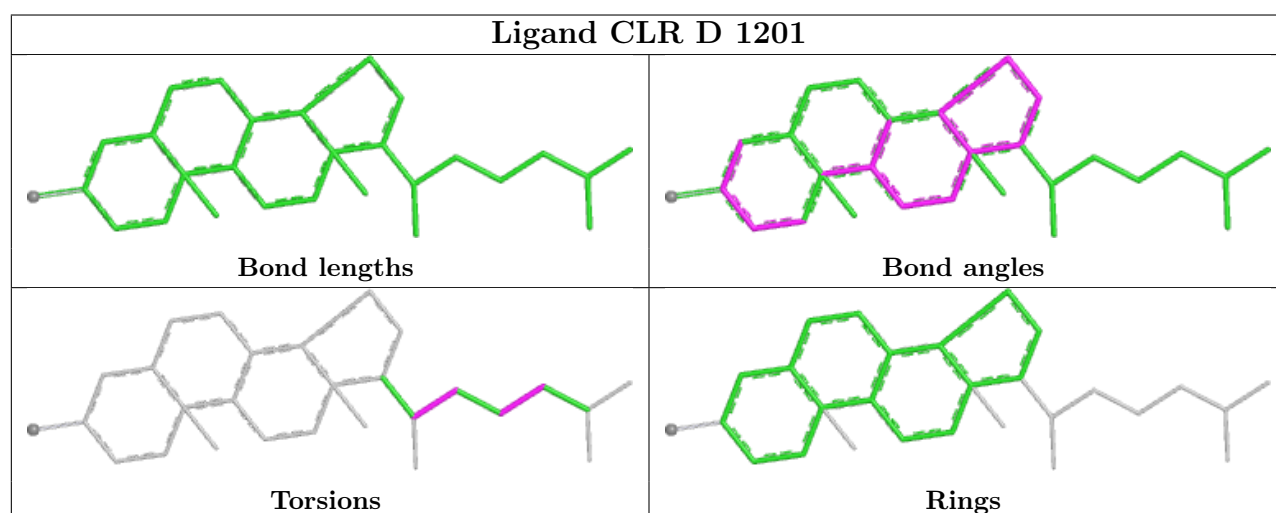
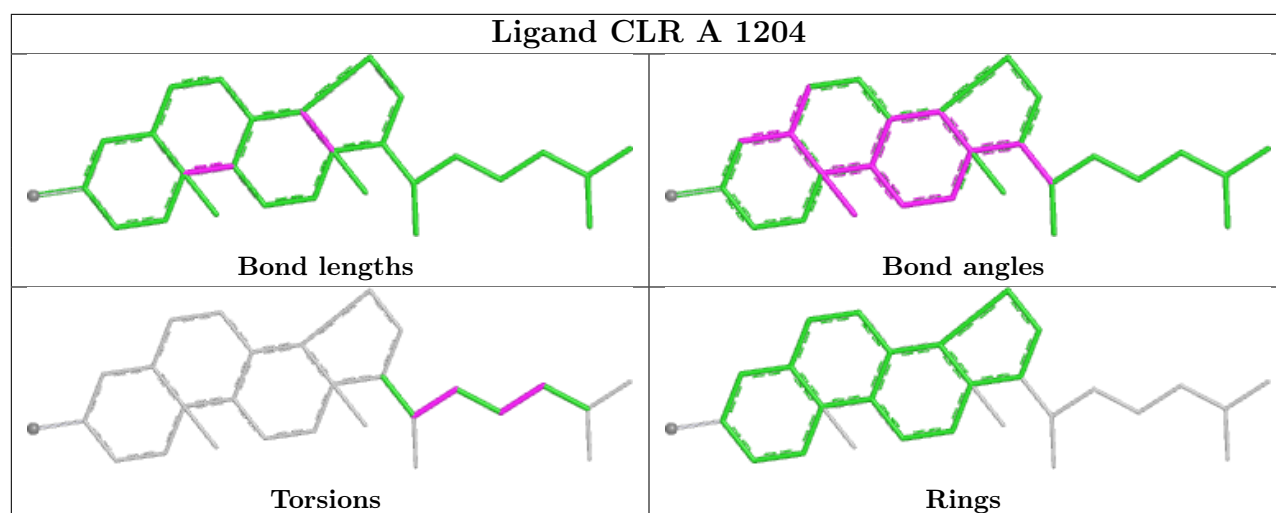


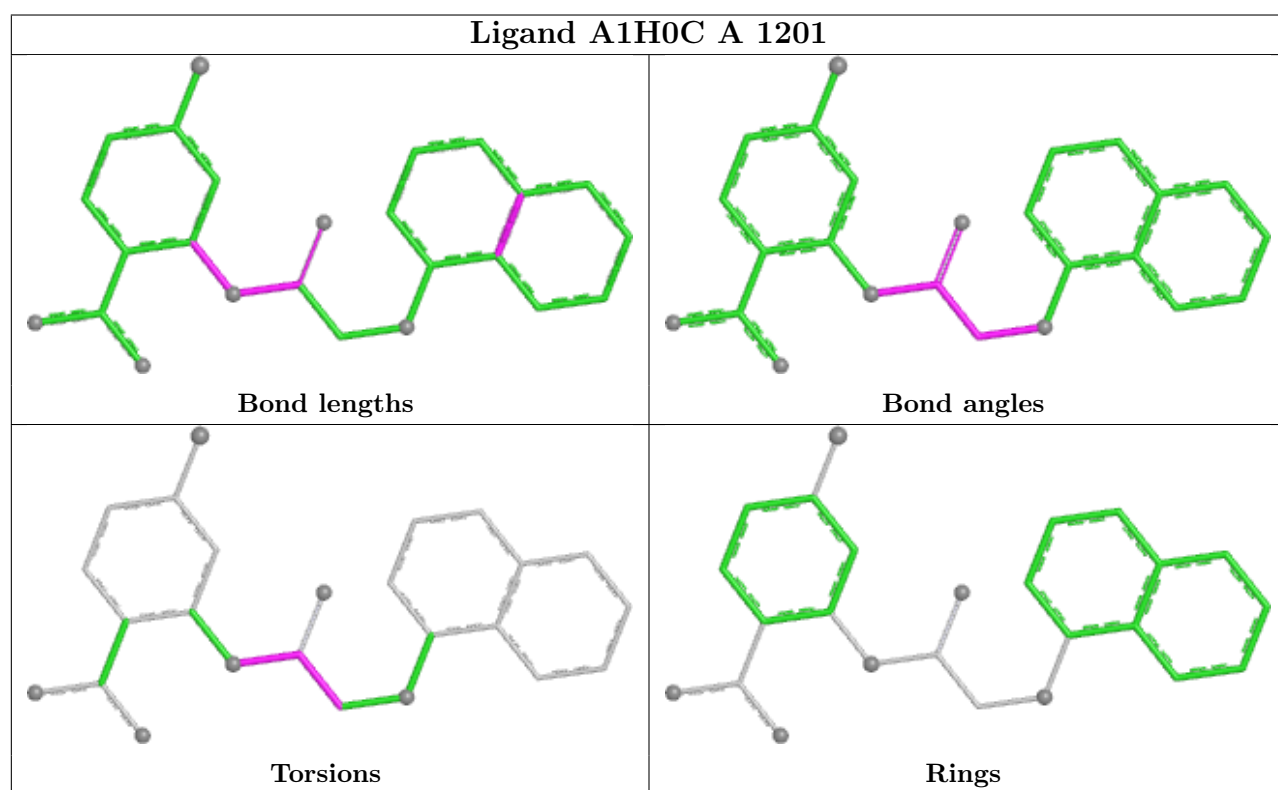
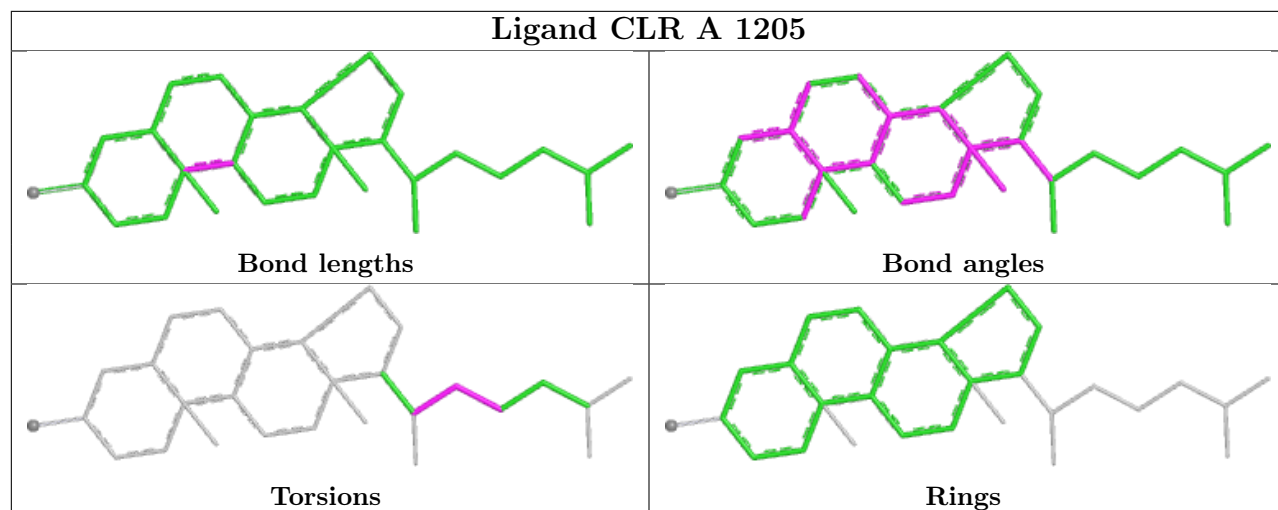
## Ligand A1H0C E 1201

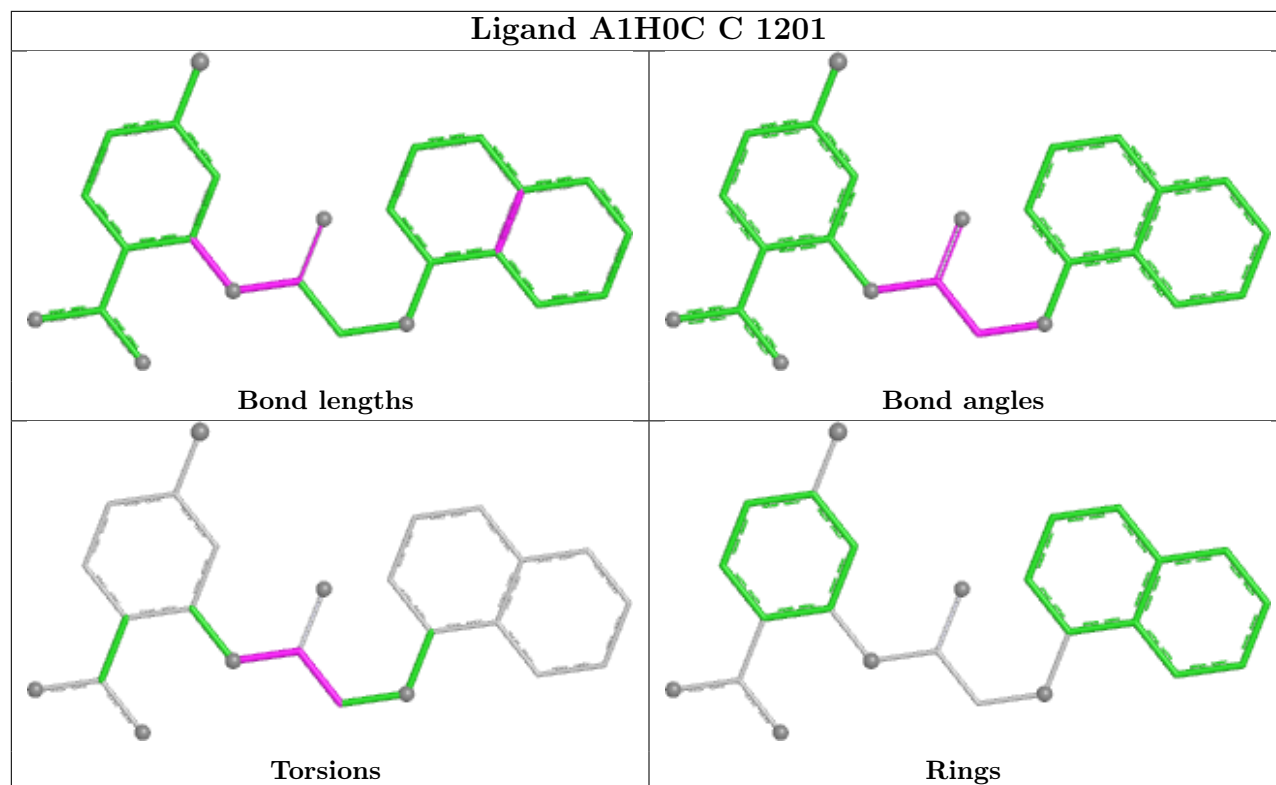


## Ligand CLR A 1203









## 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.

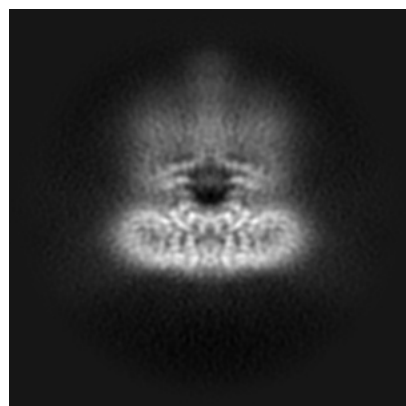
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19069. These allow visual inspection of the internal detail of the map and identification of artifacts.

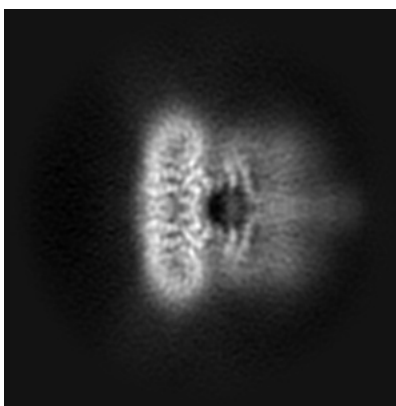
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

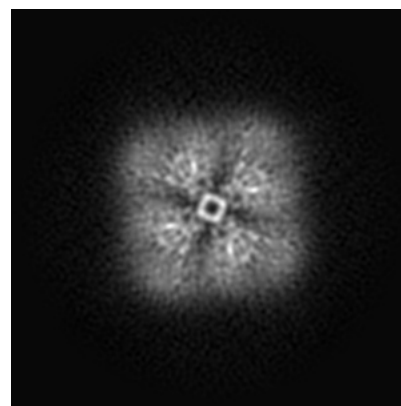
#### 6.1.1 Primary map



X

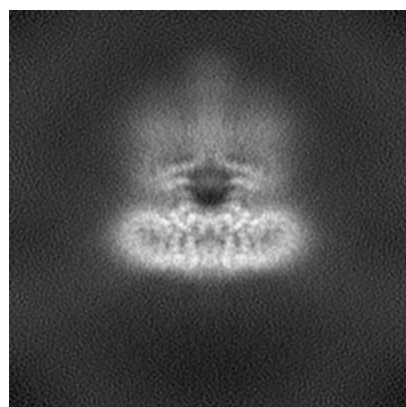


Y

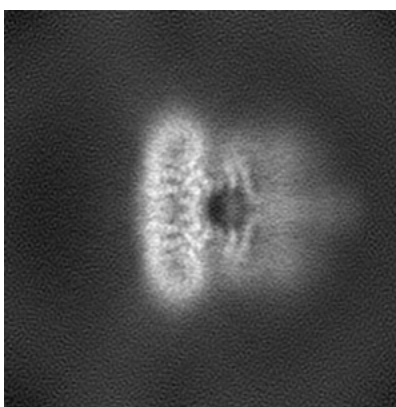


Z

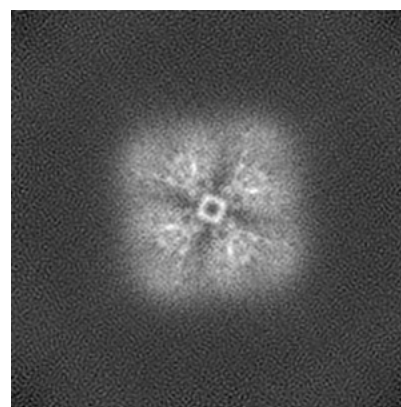
#### 6.1.2 Raw map



X



Y

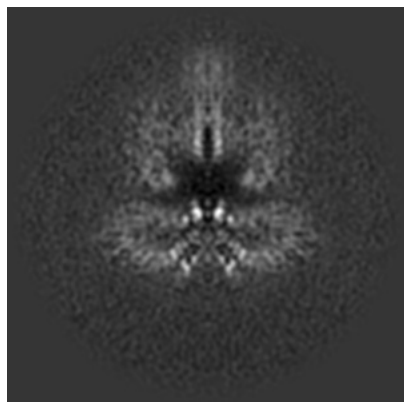


Z

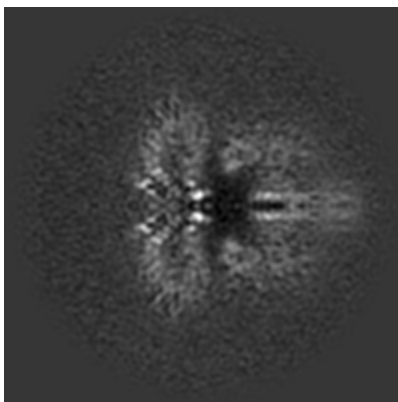
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

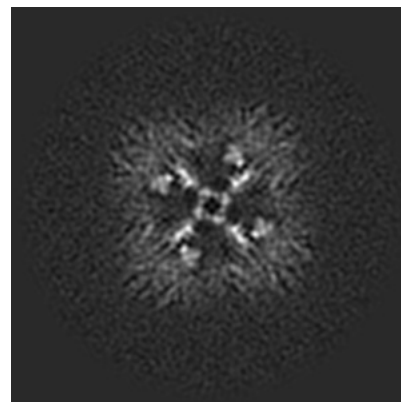
### 6.2.1 Primary map



X Index: 100

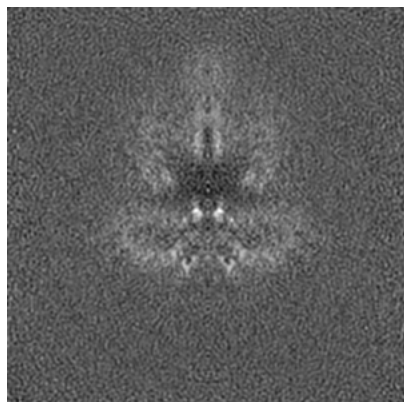


Y Index: 100

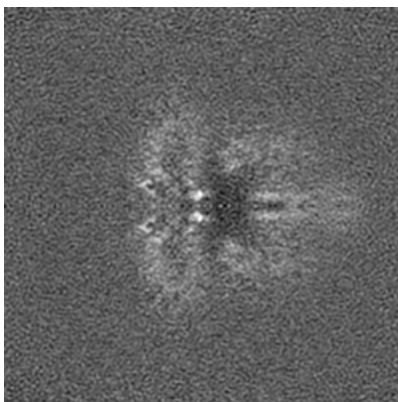


Z Index: 100

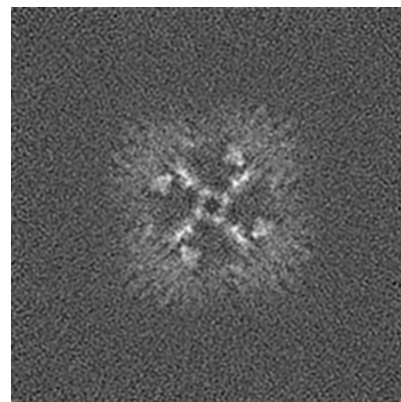
### 6.2.2 Raw map



X Index: 100



Y Index: 100

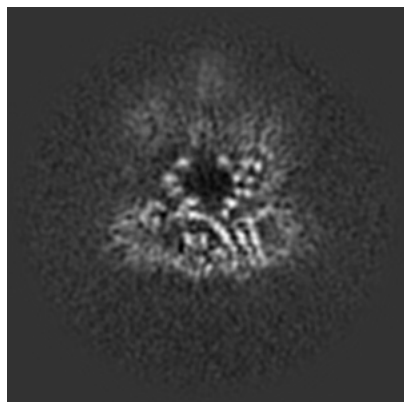


Z Index: 100

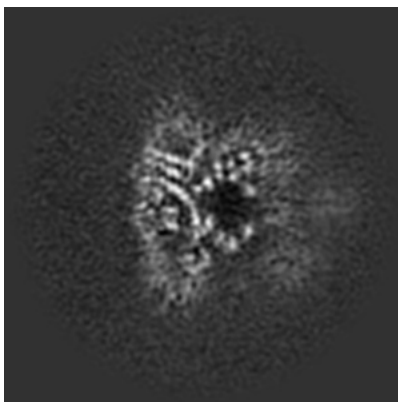
The images above show central slices of the map in three orthogonal directions.

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

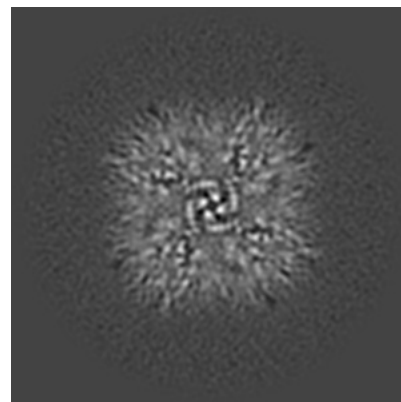
### 6.3.1 Primary map



X Index: 90

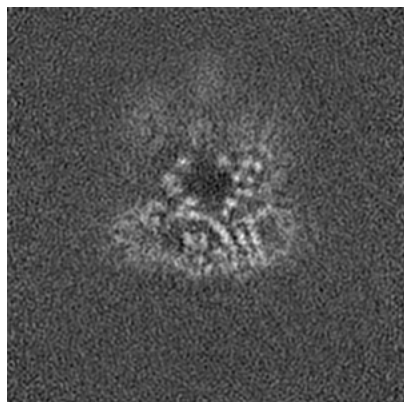


Y Index: 110

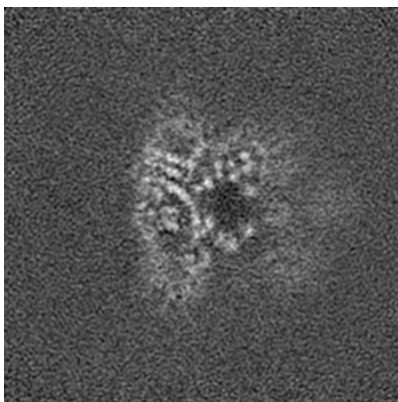


Z Index: 94

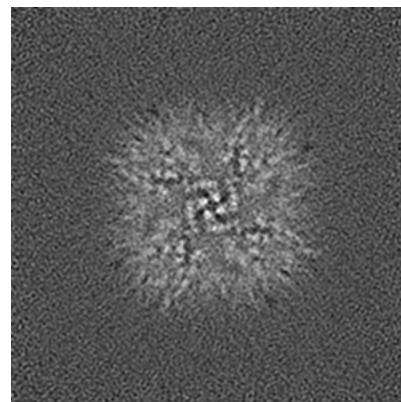
### 6.3.2 Raw map



X Index: 90



Y Index: 110

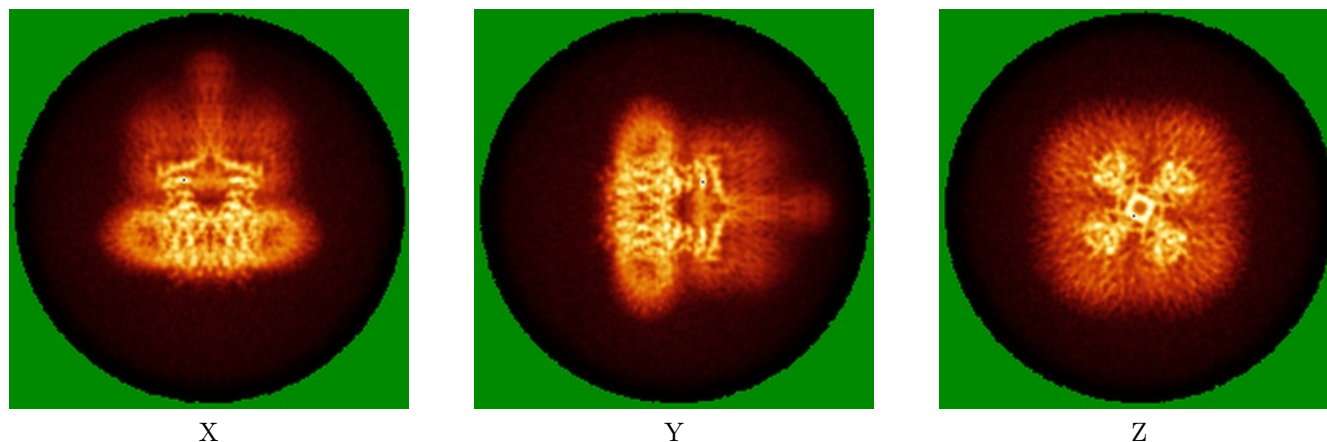


Z Index: 94

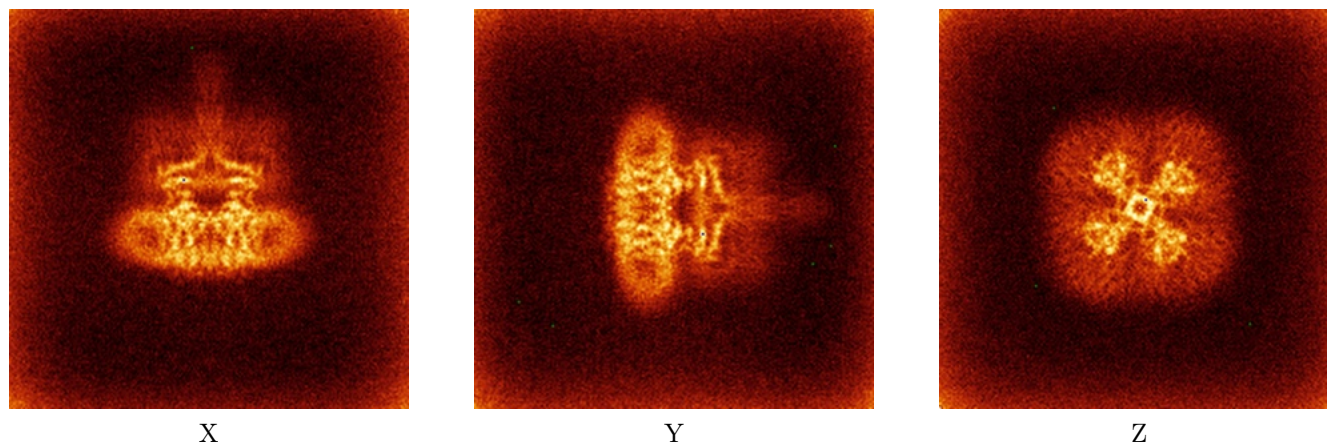
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



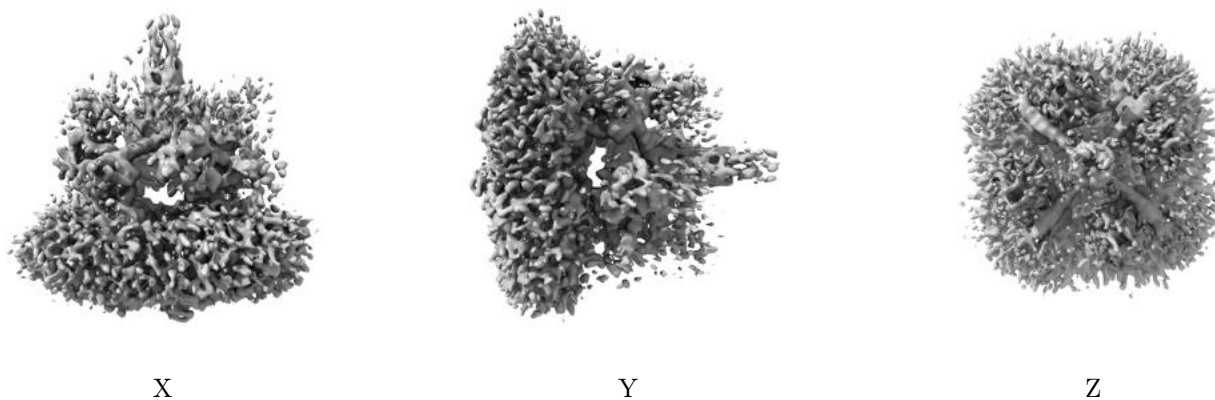
### 6.4.2 Raw map



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

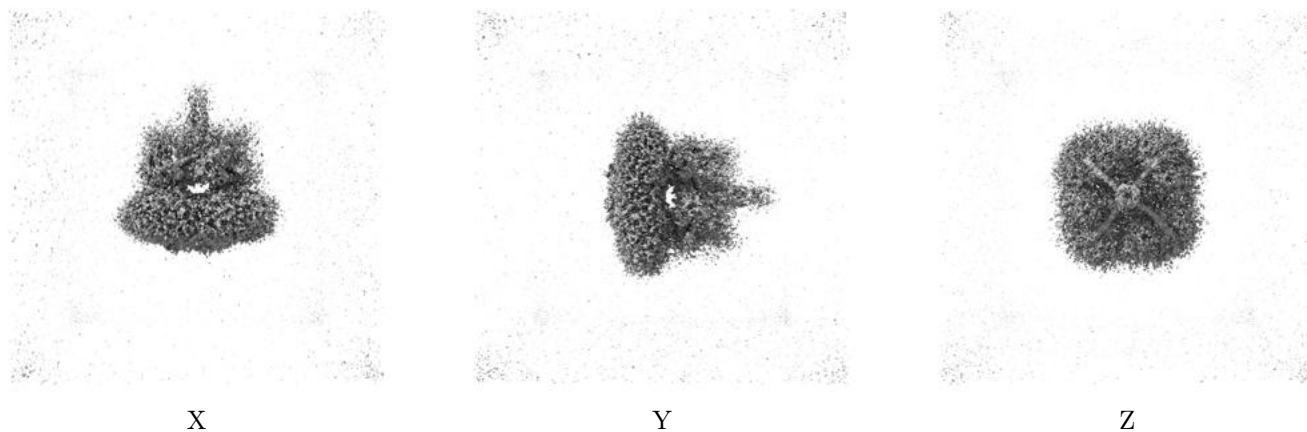
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

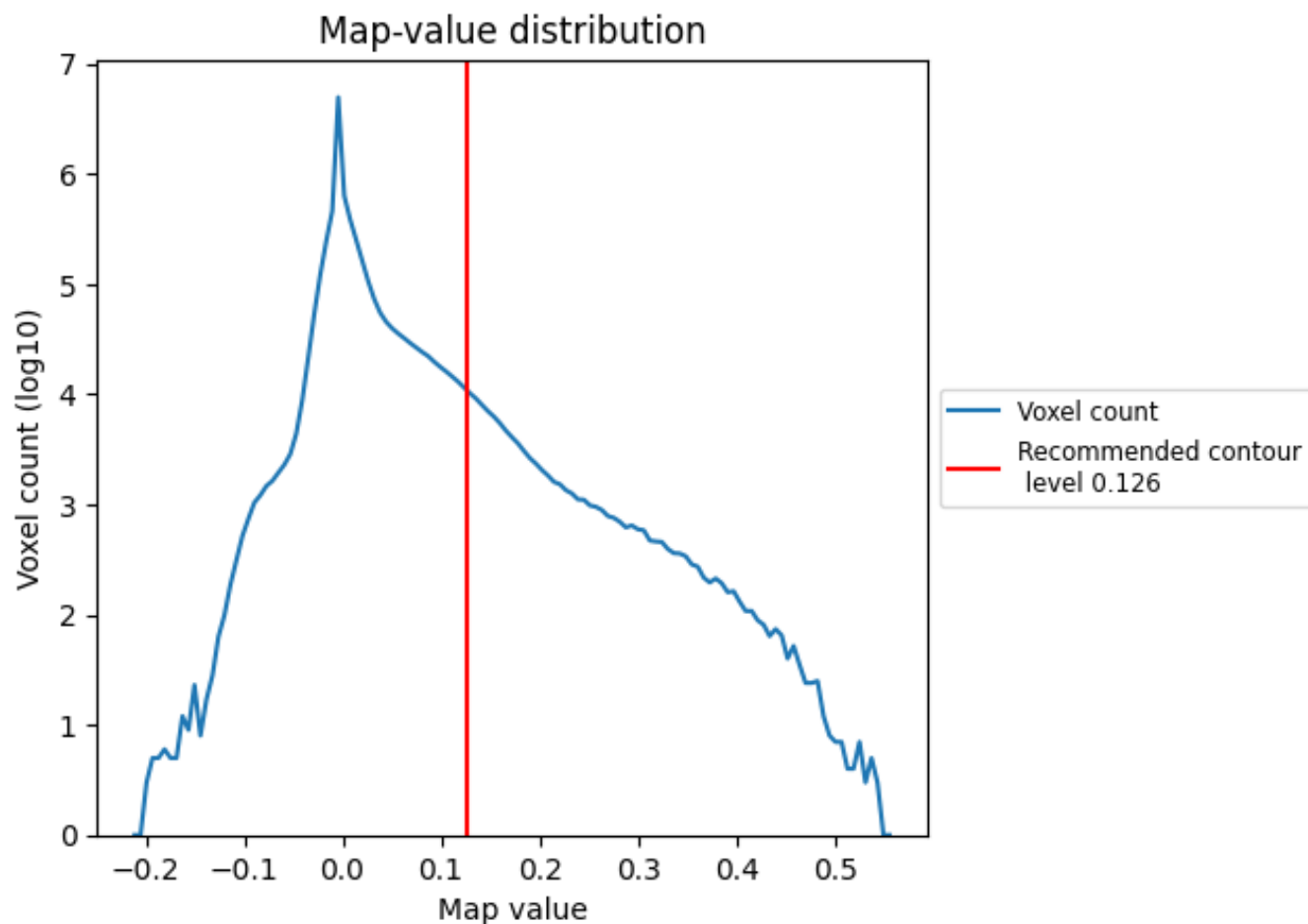
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

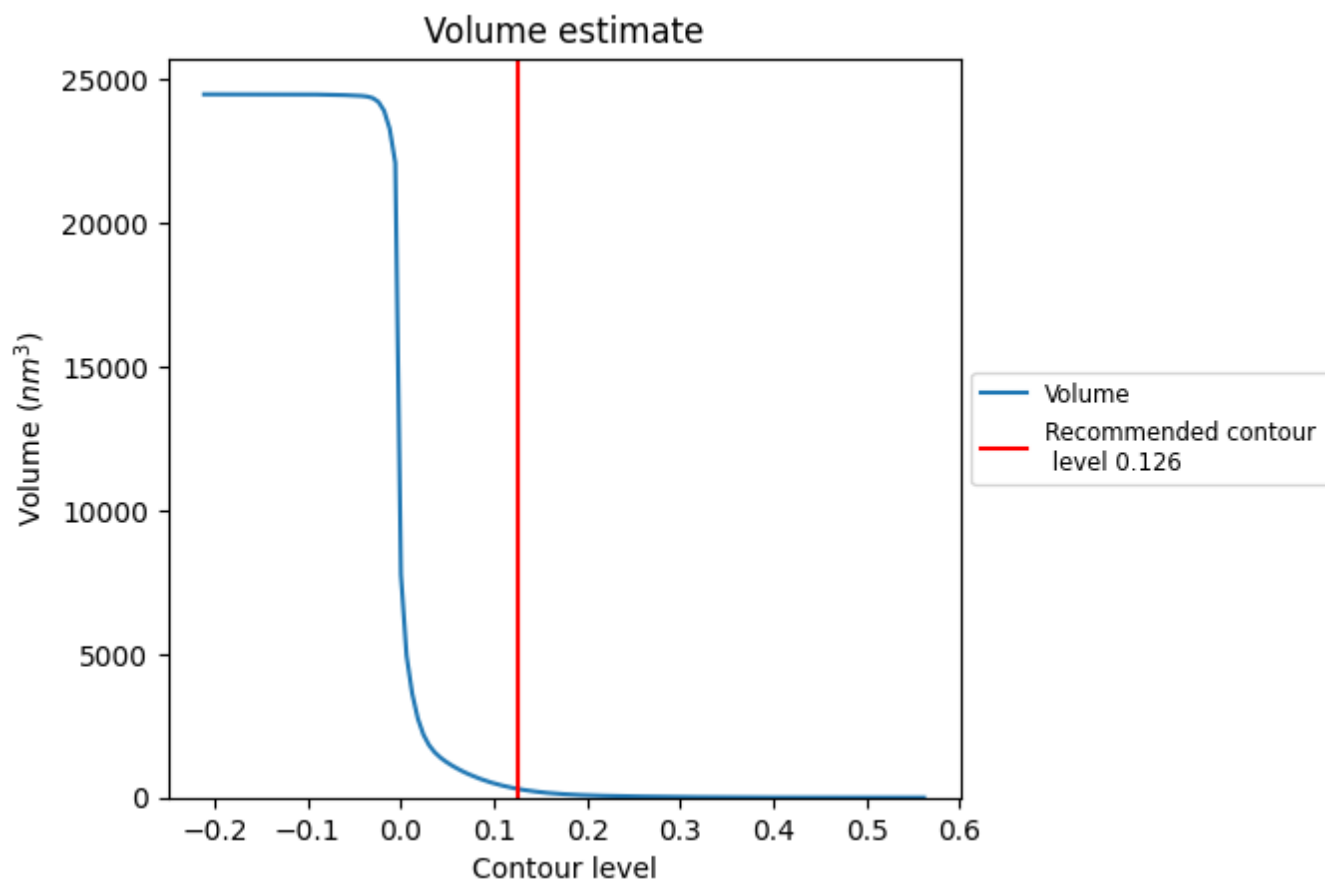
This section contains the results of statistical analysis of the map.

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



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

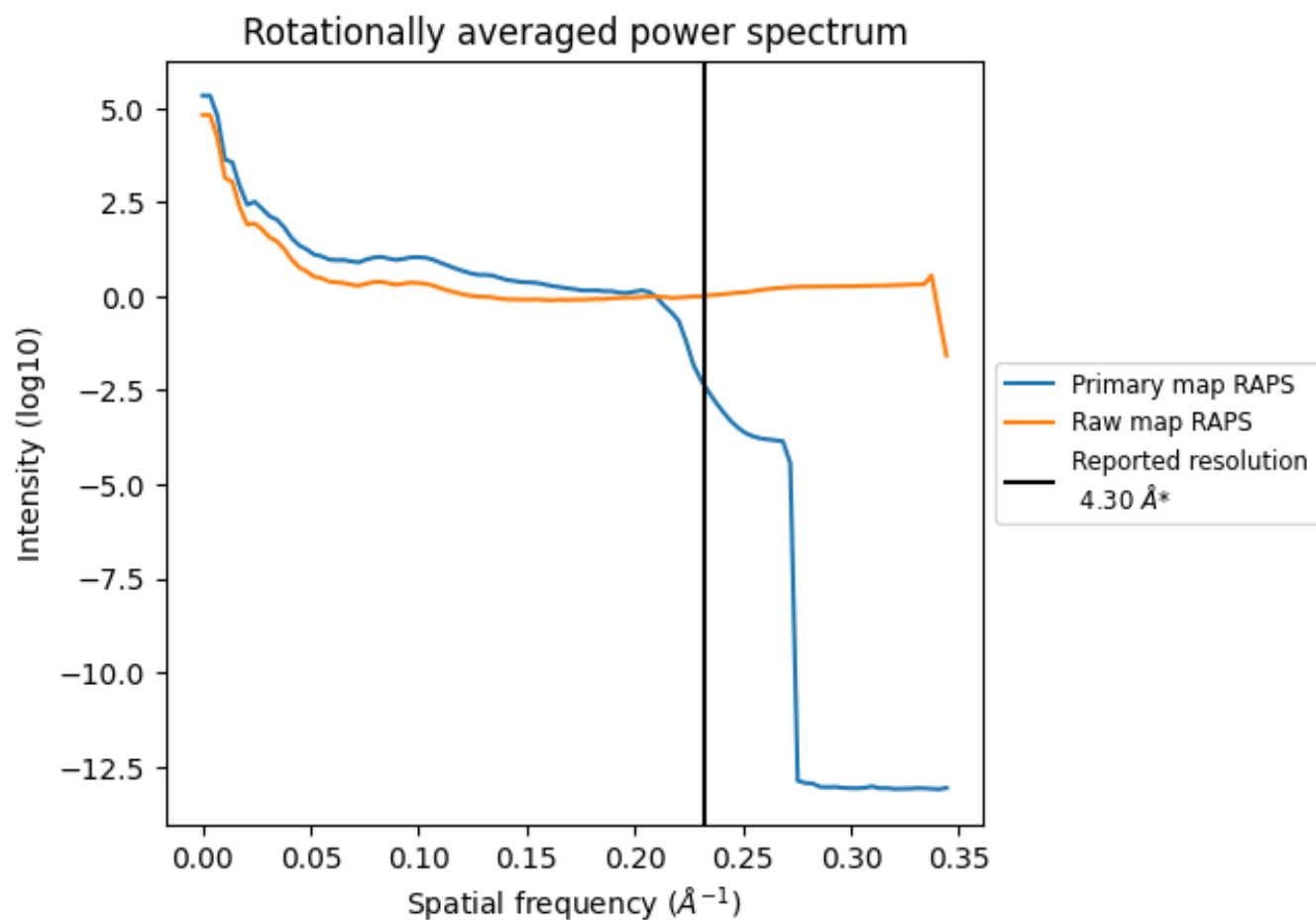
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm<sup>3</sup>; this corresponds to an approximate mass of 271 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 ⓘ

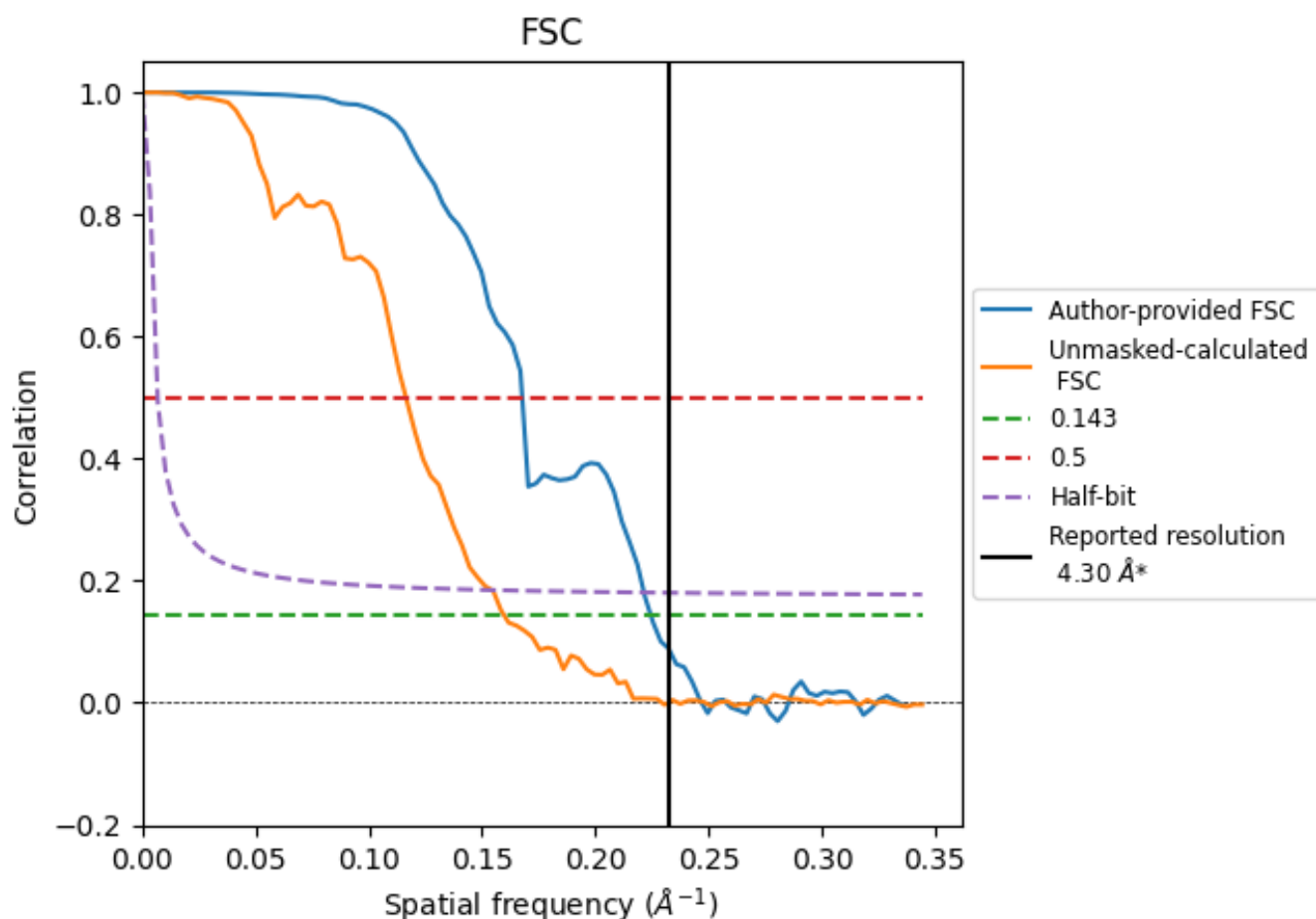


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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  $0.233 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

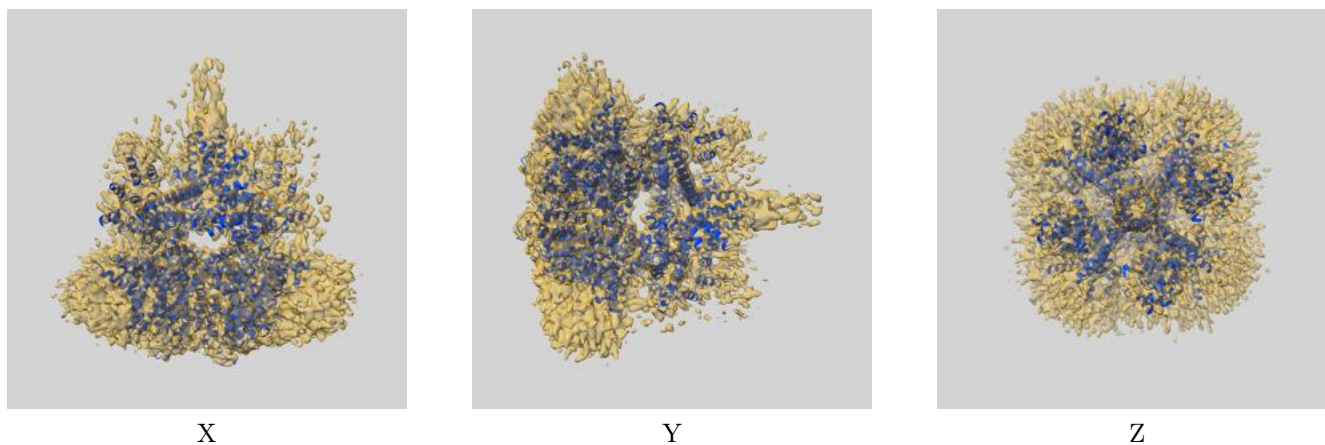
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.30                               | -    | -        |
| Author-provided FSC curve | 4.45                               | 5.96 | 4.51     |
| Unmasked-calculated*      | 6.25                               | 8.58 | 6.48     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.25 differs from the reported value 4.3 by more than 10 %

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

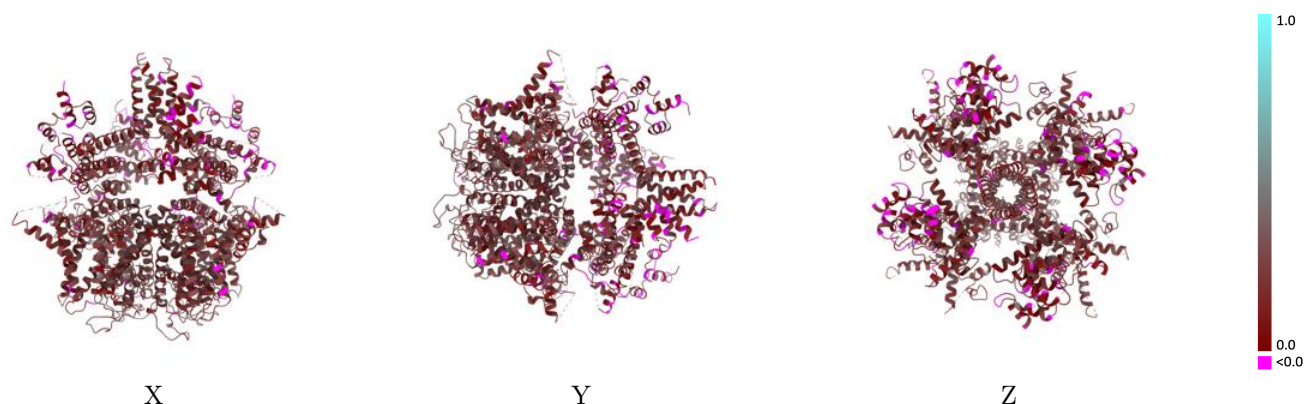
This section contains information regarding the fit between EMDB map EMD-19069 and PDB model 8RD9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



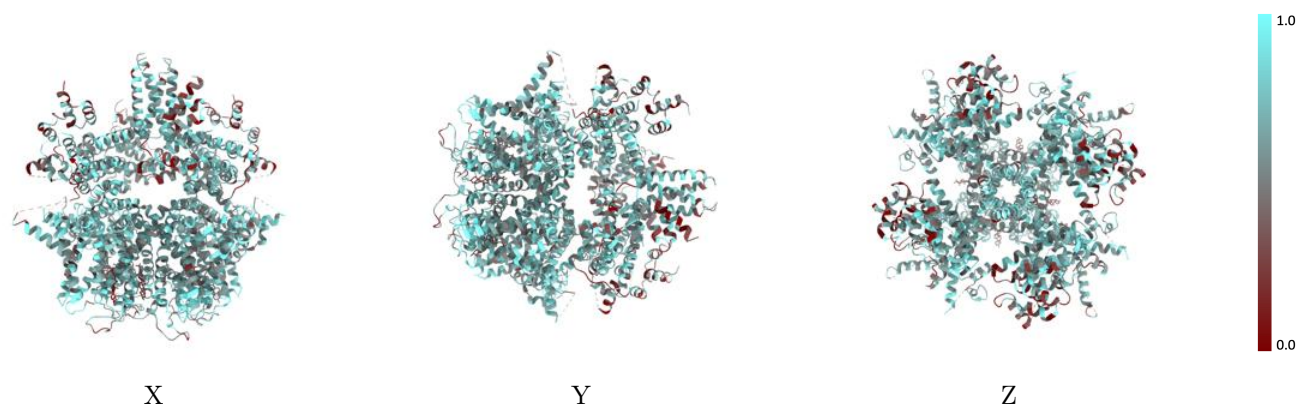
The images above show the 3D surface view of the map at the recommended contour level 0.126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



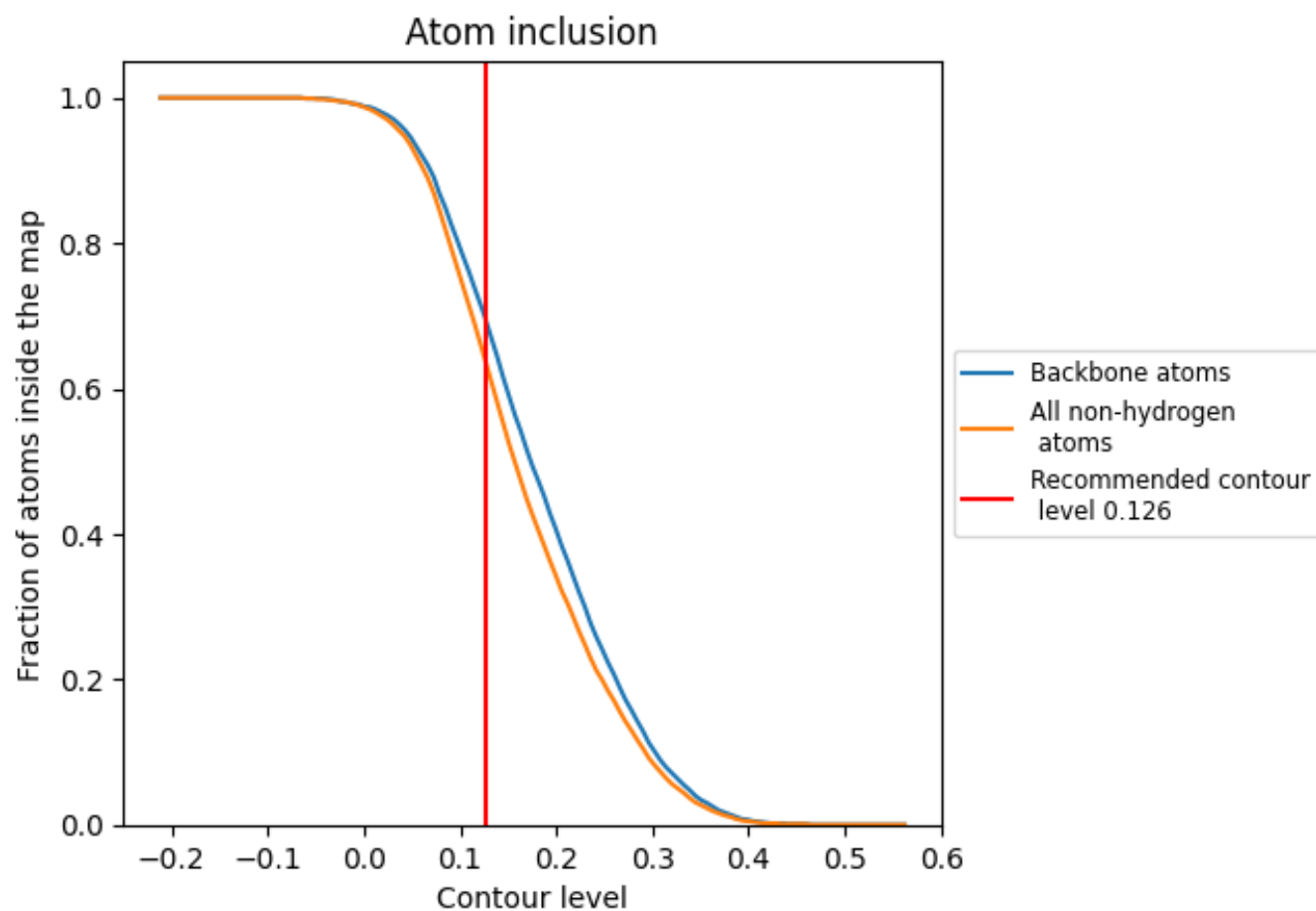
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.126).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 64% 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 (0.126) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6400 | <div></div> 0.2000 |
| A     | <div></div> 0.6360 | <div></div> 0.2010 |
| C     | <div></div> 0.6500 | <div></div> 0.1980 |
| D     | <div></div> 0.6430 | <div></div> 0.1990 |
| E     | <div></div> 0.6440 | <div></div> 0.2030 |

