



## Full wwPDB EM Validation Report ⓘ

May 5, 2025 – 12:21 AM EDT

PDB ID : 8SHG / pdb\_00008shg  
EMDB ID : EMD-40487  
Title : CCT G beta 5 complex closed state 9  
Authors : Wang, S.; Sass, M.; Willardson, B.M.; Shen, P.S.  
Deposited on : 2023-04-14  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

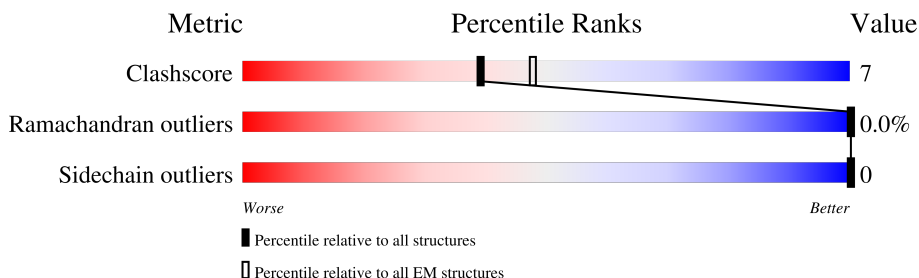
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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





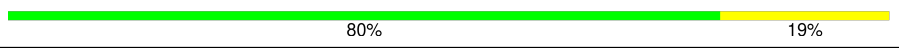



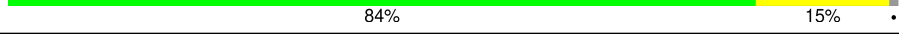
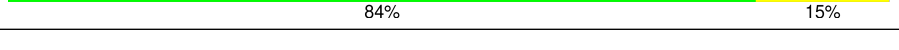
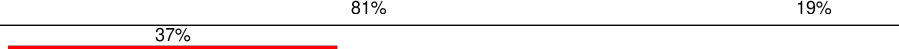
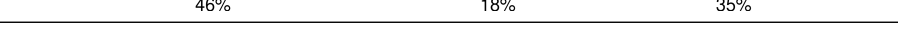
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

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   | N     | 395    |                  |
| 2   | A     | 536    |                  |
| 2   | a     | 536    |                  |
| 3   | B     | 526    |                  |
| 3   | b     | 526    |                  |
| 4   | D     | 520    |                  |
| 4   | d     | 520    |                  |
| 5   | E     | 540    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 5   | e     | 540    |  |
| 6   | G     | 528    |  |
| 6   | g     | 528    |  |
| 7   | H     | 528    |  |
| 7   | h     | 528    |  |
| 8   | Q     | 538    |  |
| 8   | q     | 538    |  |
| 9   | Z     | 527    |  |
| 9   | z     | 527    |  |
| 10  | P     | 301    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | AF3  | B     | 603 | -         | -        | X       | -                |
| 13  | AF3  | D     | 603 | -         | -        | X       | -                |
| 13  | AF3  | G     | 603 | -         | -        | X       | -                |
| 13  | AF3  | H     | 603 | -         | -        | X       | -                |
| 13  | AF3  | Q     | 603 | -         | -        | X       | -                |
| 13  | AF3  | a     | 603 | -         | -        | X       | -                |
| 13  | AF3  | g     | 603 | -         | -        | X       | -                |
| 13  | AF3  | q     | 603 | -         | -        | X       | -                |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 67663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Guanine nucleotide-binding protein subunit beta-5.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1   | N     | 130      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 985   | 608 | 169 | 198 | 10 |         |       |

- Molecule 2 is a protein called T-complex protein 1 subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | A     | 536      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4069  | 2548 | 711 | 787 | 23 |         |       |
| 2   | a     | 532      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4041  | 2533 | 707 | 778 | 23 |         |       |

- Molecule 3 is a protein called T-complex protein 1 subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | B     | 526      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3952  | 2473 | 696 | 764 | 19 |         |       |
| 3   | b     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3943  | 2467 | 694 | 763 | 19 |         |       |

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 520      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3923  | 2453 | 683 | 764 | 23 |         |       |
| 4   | d     | 520      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3917  | 2450 | 680 | 764 | 23 |         |       |

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 535      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4121  | 2581 | 718 | 791 | 31 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | e     | 540      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 4169  | 2610 | 724 | 804 | 31 |         |       |

- Molecule 6 is a protein called T-complex protein 1 subunit gamma.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | G     | 526      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4089  | 2548 | 726 | 785 | 30 |         |       |
| 6   | g     | 526      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4088  | 2548 | 725 | 785 | 30 |         |       |

- Molecule 7 is a protein called T-complex protein 1 subunit eta, N-terminally processed.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | H     | 528      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4054  | 2561 | 699 | 769 | 25 |         |       |
| 7   | h     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4032  | 2548 | 696 | 763 | 25 |         |       |

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | Q     | 538      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4086  | 2579 | 696 | 784 | 27 |         |       |
| 8   | q     | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4053  | 2558 | 690 | 778 | 27 |         |       |

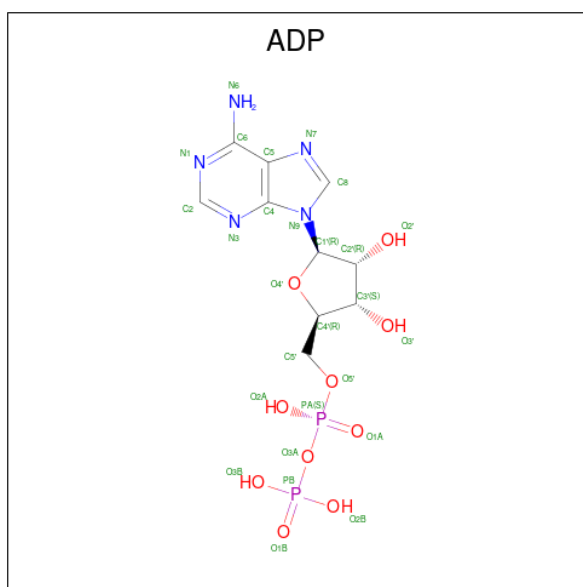
- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | Z     | 525      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4022  | 2528 | 704 | 769 | 21 |         |       |
| 9   | z     | 527      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4033  | 2534 | 706 | 772 | 21 |         |       |

- Molecule 10 is a protein called Phosducin-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10  | P     | 195      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1555  | 979 | 266 | 297 | 13 |         |       |

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 11  | A     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | B     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | D     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | E     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | G     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | H     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | Q     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | Z     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | a     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | b     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | d     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | e     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | g     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 11  | h     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |

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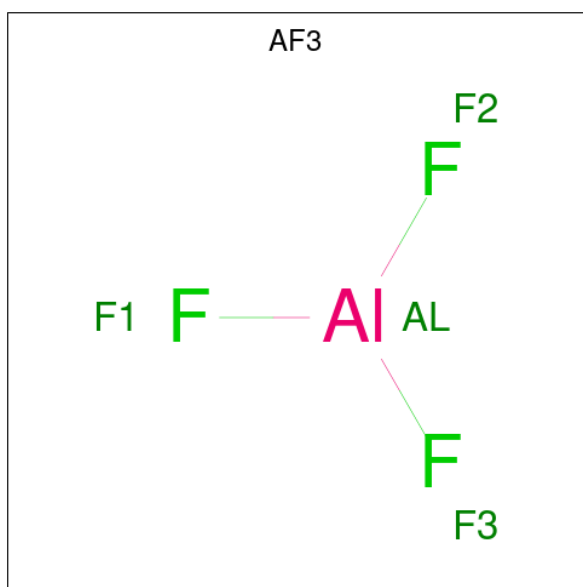
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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 11  | q     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 11  | z     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 12  | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | B     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | G     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | H     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | Q     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | Z     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | a     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | b     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | d     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | e     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | g     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | h     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | q     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | z     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 13 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 13  | A     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | B     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | D     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | E     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | G     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | H     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | Q     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | Z     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | a     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | b     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | d     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | e     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | g     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | h     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 13  | q     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 13  | z     | 1        | Total | Al | F | 0       |
|     |       |          | 4     | 1  | 3 |         |

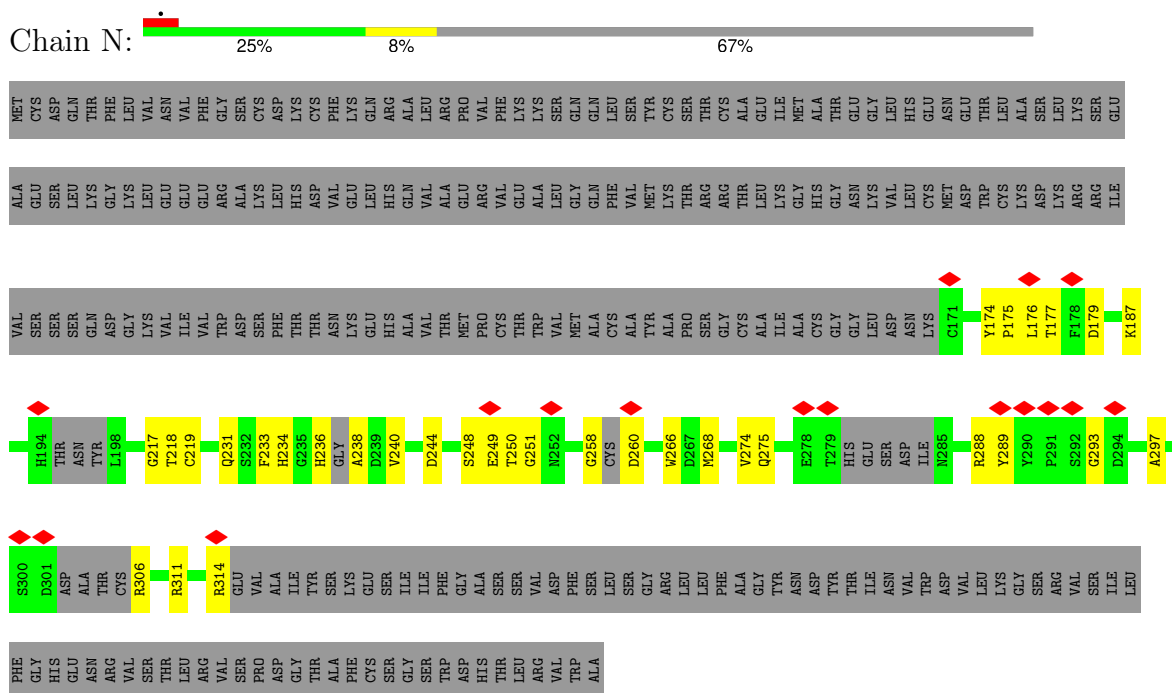
- Molecule 14 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 14  | A     | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 14  | B     | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 14  | D     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | E     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | G     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | H     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | Q     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | Z     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | a     | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |
| 14  | b     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | d     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | e     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | g     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | h     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | q     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 14  | z     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

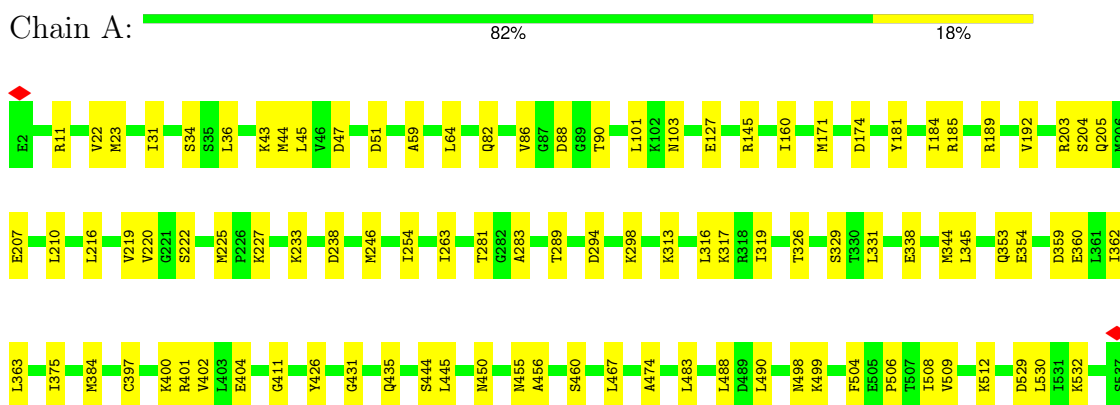
### 3 Residue-property plots

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


- Molecule 1: Guanine nucleotide-binding protein subunit beta-5

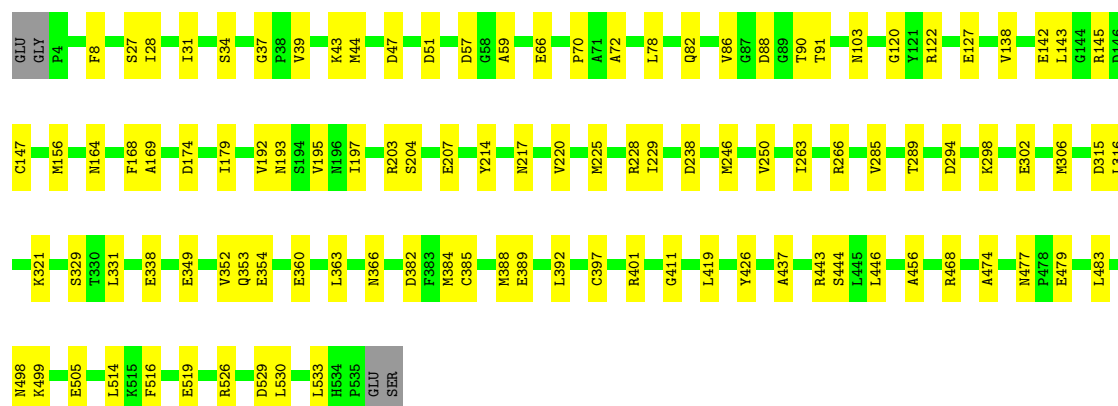


- Molecule 2: T-complex protein 1 subunit alpha




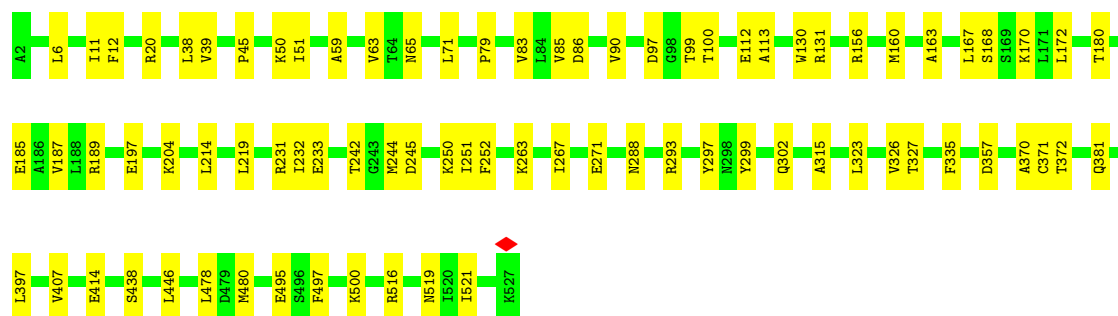
- Molecule 2: T-complex protein 1 subunit alpha

Chain a:  80% 20%




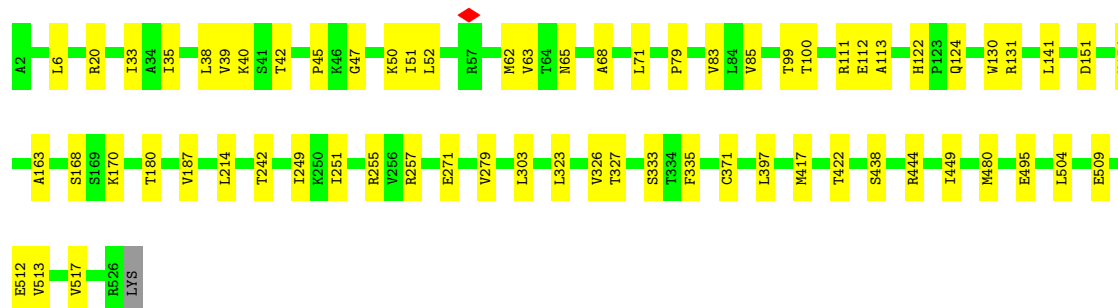
- Molecule 3: T-complex protein 1 subunit beta

Chain B:  85% 15%




- Molecule 3: T-complex protein 1 subunit beta

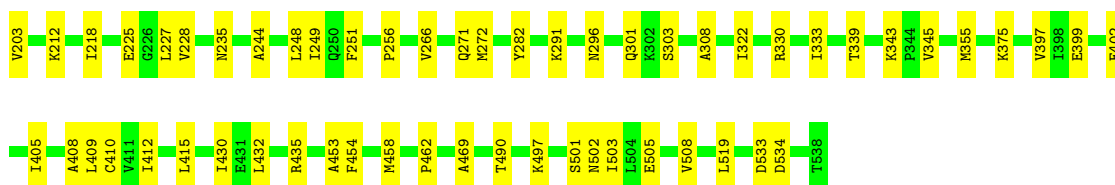
Chain b:  87% 13%



- Molecule 4: T-complex protein 1 subunit delta

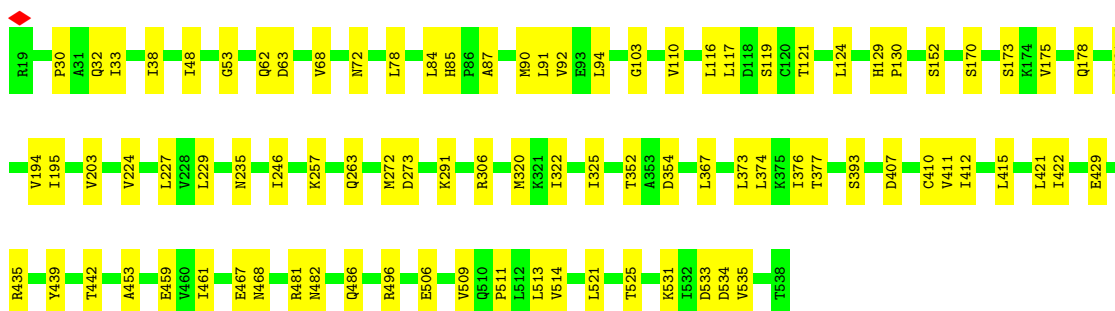
Chain D:  83% 17%





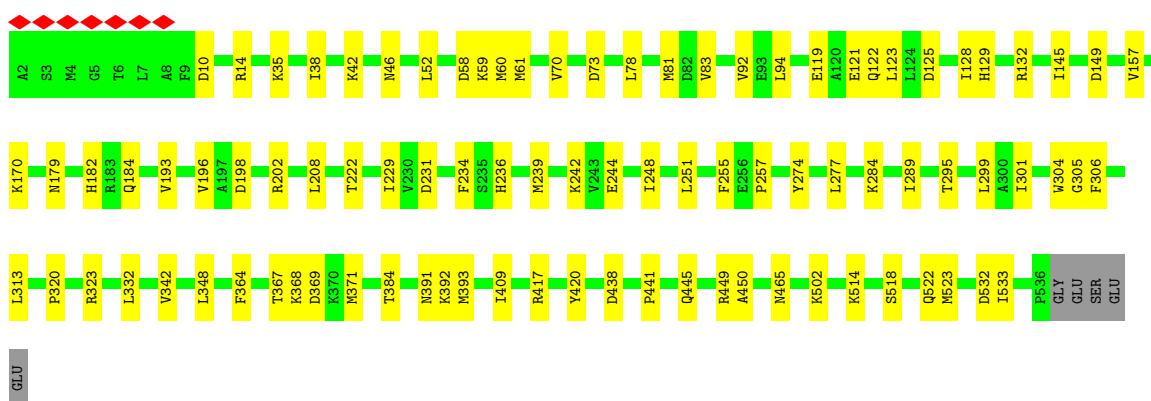
• Molecule 4: T-complex protein 1 subunit delta

Chain d: 83% 17%



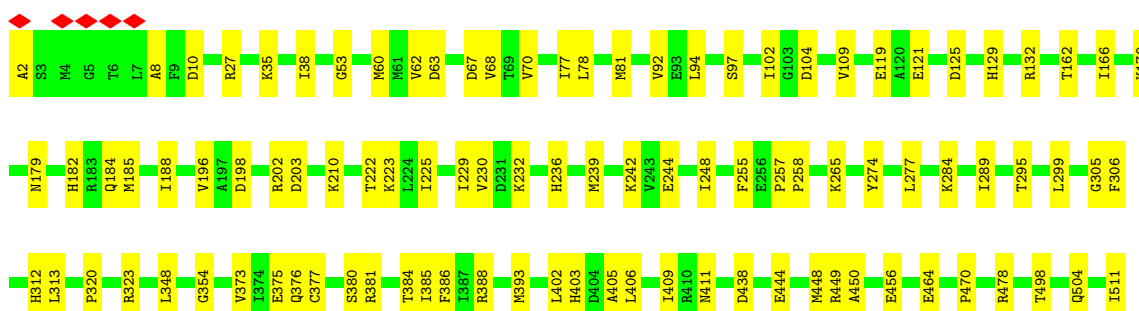
• Molecule 5: T-complex protein 1 subunit epsilon

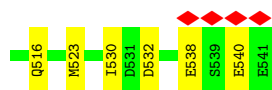
Chain E: 82% 17%



• Molecule 5: T-complex protein 1 subunit epsilon

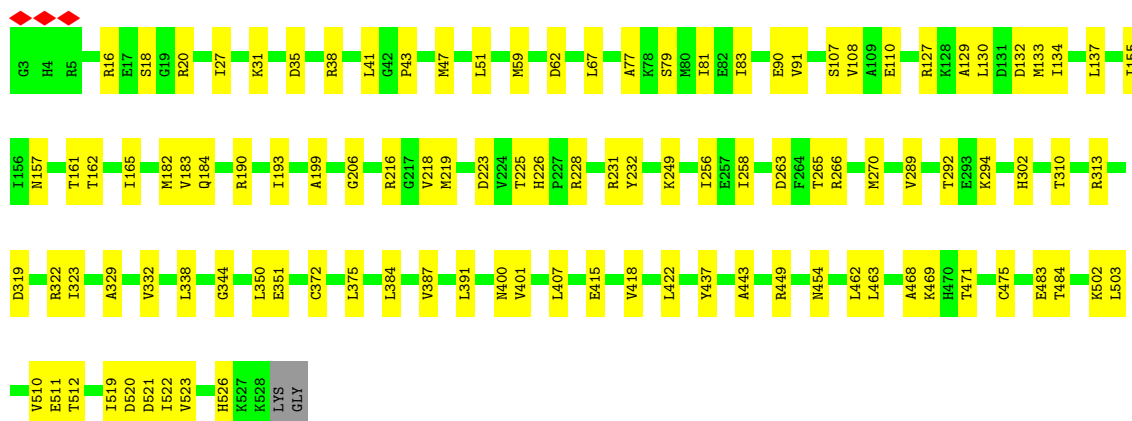
Chain e: 81% 19%





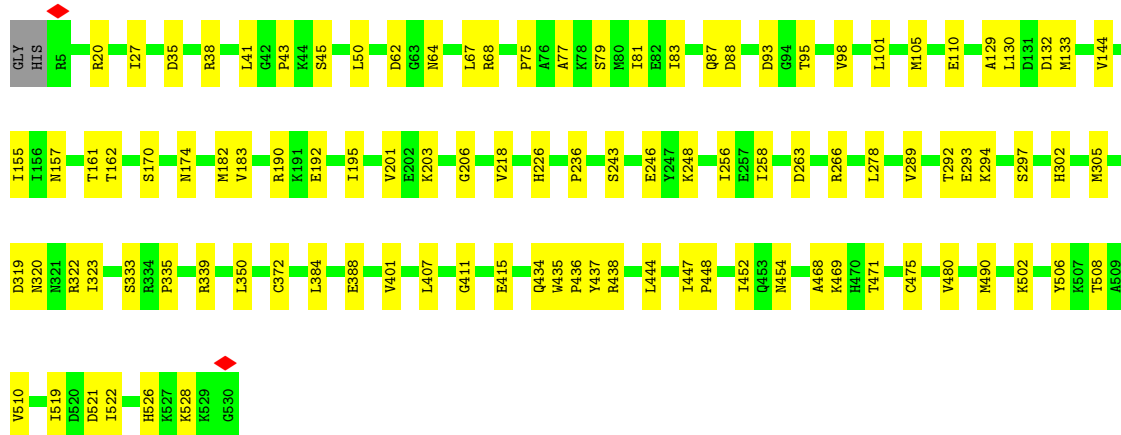
- Molecule 6: T-complex protein 1 subunit gamma

Chain G: 79% 20%



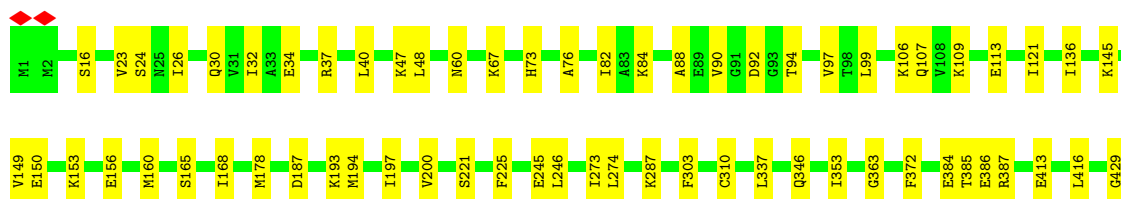
- Molecule 6: T-complex protein 1 subunit gamma

Chain g: 80% 19%



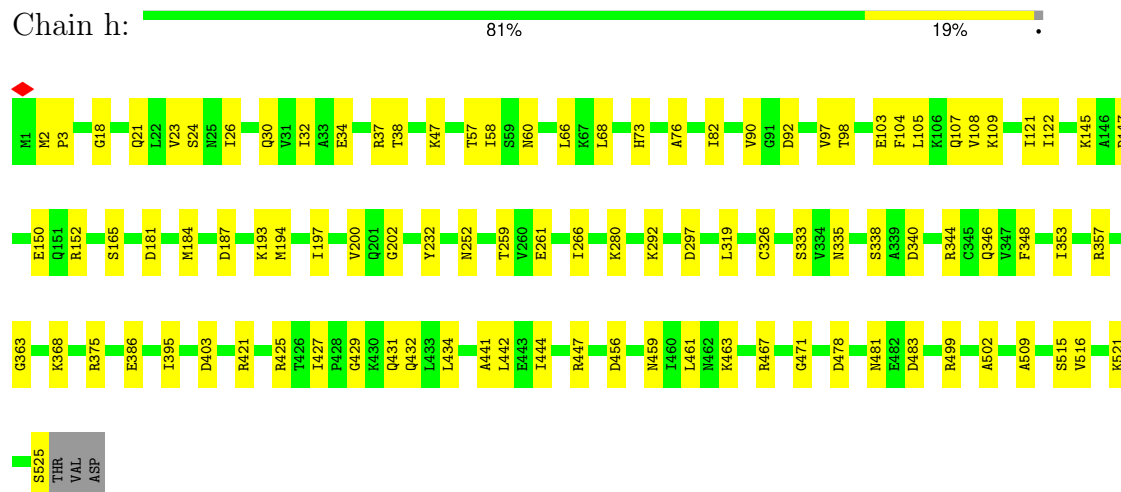
- Molecule 7: T-complex protein 1 subunit eta, N-terminally processed

Chain H: 84% 16%

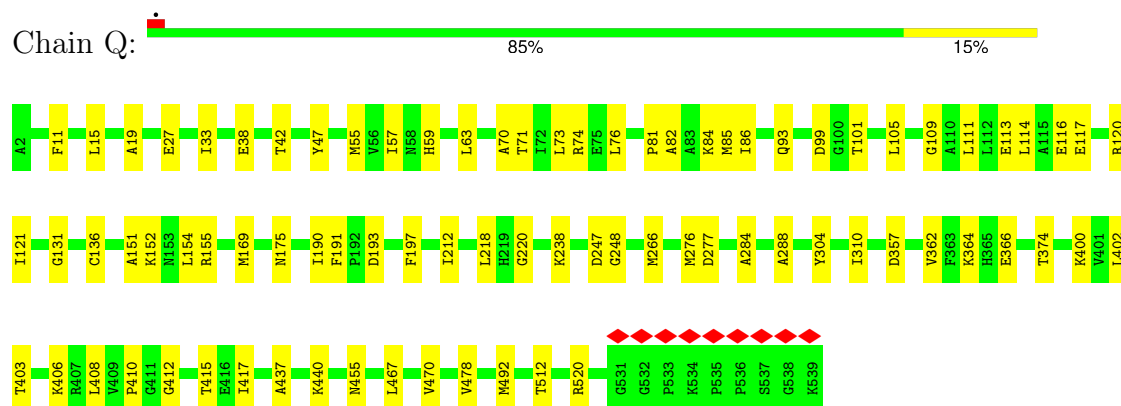




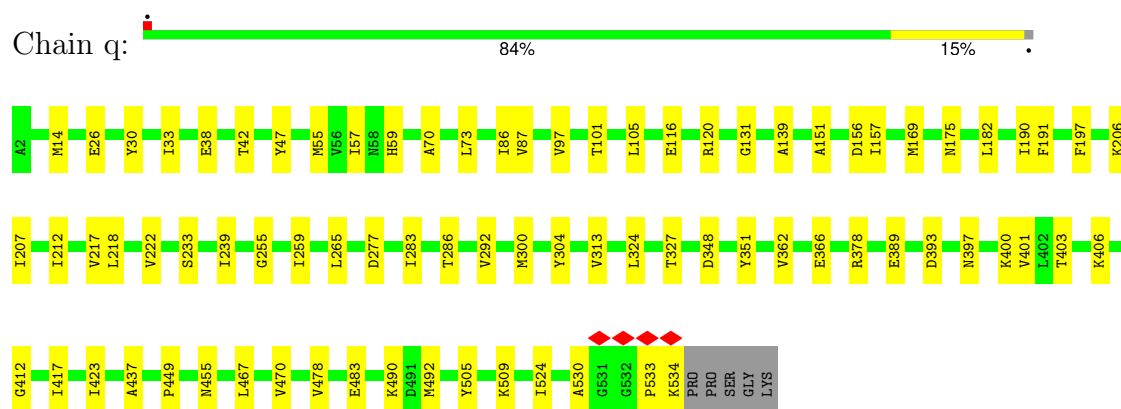
- Molecule 7: T-complex protein 1 subunit eta, N-terminally processed




- Molecule 8: T-complex protein 1 subunit theta

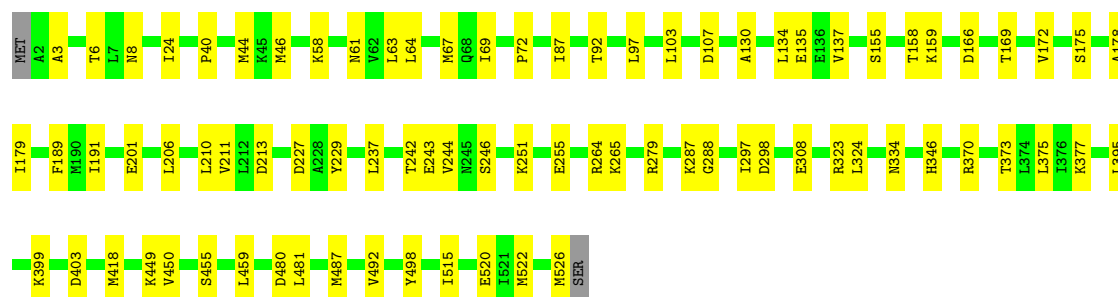


- Molecule 8: T-complex protein 1 subunit theta




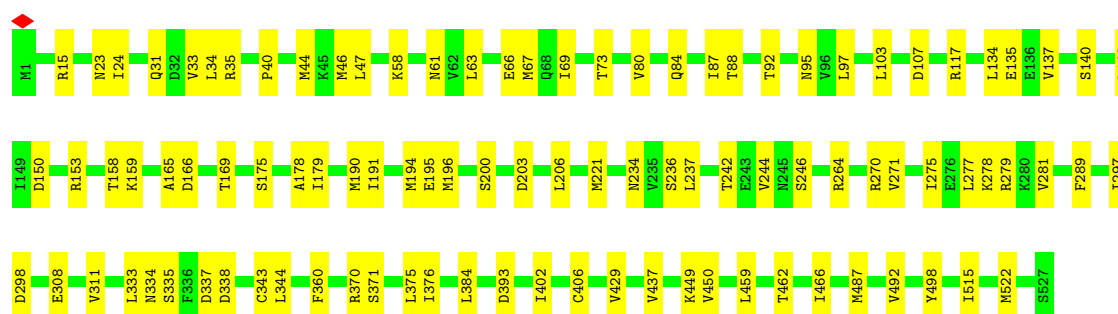
- Molecule 9: T-complex protein 1 subunit zeta

Chain Z:  84% 15%



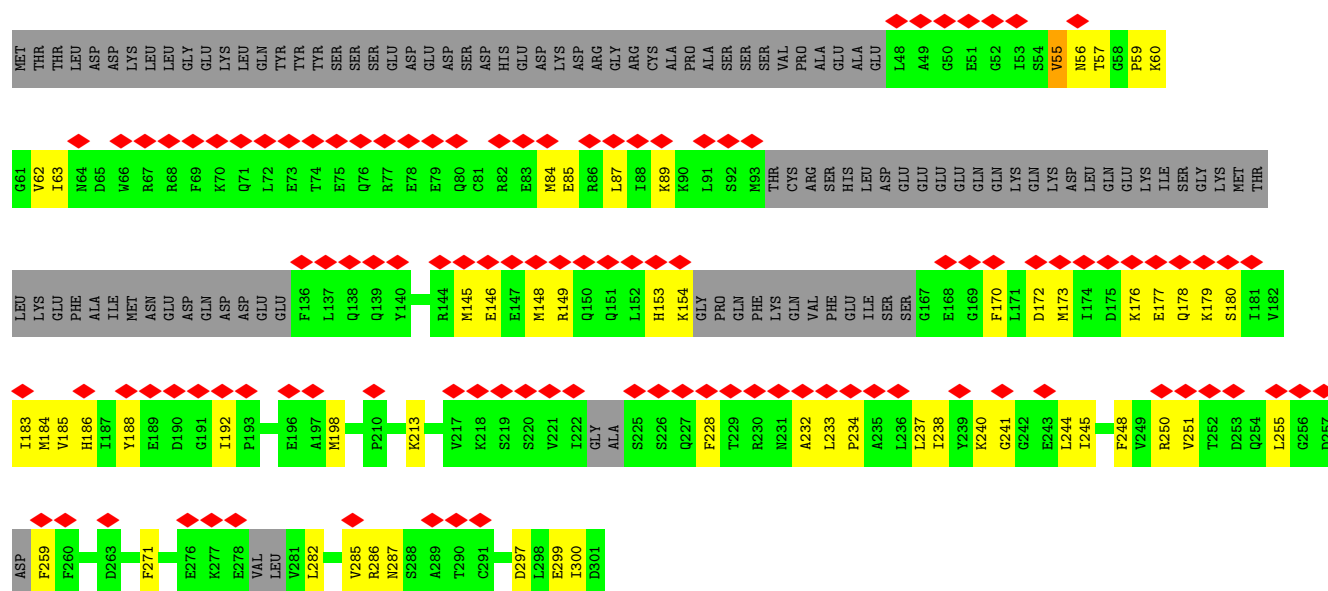
• Molecule 9: T-complex protein 1 subunit zeta

Chain z:  81% 19%



• Molecule 10: Phosducin-like protein

Chain P:  37% 46% 18% 35%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 120668                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40.42                                   | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 1200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 1.003                                   | Depositor |
| Minimum map value                    | -0.319                                  | Depositor |
| Average map value                    | 0.004                                   | Depositor |
| Map value standard deviation         | 0.044                                   | Depositor |
| Recommended contour level            | 0.126                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 317.4, 317.4, 317.4                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.058, 1.058, 1.058                     | 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: MG, AF3, ADP

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   | N     | 0.12         | 0/999   | 0.34        | 0/1341         |
| 2   | A     | 0.12         | 0/4109  | 0.26        | 0/5548         |
| 2   | a     | 0.12         | 0/4081  | 0.26        | 0/5510         |
| 3   | B     | 0.12         | 0/3995  | 0.25        | 0/5386         |
| 3   | b     | 0.12         | 0/3986  | 0.23        | 0/5375         |
| 4   | D     | 0.12         | 0/3955  | 0.24        | 0/5338         |
| 4   | d     | 0.12         | 0/3949  | 0.25        | 0/5331         |
| 5   | E     | 0.13         | 0/4171  | 0.27        | 0/5619         |
| 5   | e     | 0.12         | 0/4220  | 0.25        | 0/5684         |
| 6   | G     | 0.12         | 0/4136  | 0.26        | 0/5579         |
| 6   | g     | 0.12         | 0/4134  | 0.25        | 0/5575         |
| 7   | H     | 0.13         | 0/4111  | 0.25        | 0/5550         |
| 7   | h     | 0.12         | 0/4089  | 0.25        | 0/5519         |
| 8   | Q     | 0.11         | 0/4147  | 0.24        | 0/5606         |
| 8   | q     | 0.11         | 0/4112  | 0.26        | 1/5558 (0.0%)  |
| 9   | Z     | 0.12         | 0/4069  | 0.23        | 0/5486         |
| 9   | z     | 0.12         | 0/4080  | 0.25        | 0/5501         |
| 10  | P     | 0.10         | 0/1573  | 0.32        | 0/2101         |
| All | All   | 0.12         | 0/67916 | 0.25        | 1/91607 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | q     | 530 | ALA  | CB-CA-C | -5.08 | 110.32      | 117.23   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | N     | 985   | 0        | 924      | 27      | 0            |
| 2   | A     | 4069  | 0        | 4224     | 63      | 0            |
| 2   | a     | 4041  | 0        | 4205     | 71      | 0            |
| 3   | B     | 3952  | 0        | 4070     | 58      | 0            |
| 3   | b     | 3943  | 0        | 4057     | 49      | 0            |
| 4   | D     | 3923  | 0        | 4131     | 56      | 0            |
| 4   | d     | 3917  | 0        | 4120     | 66      | 0            |
| 5   | E     | 4121  | 0        | 4238     | 67      | 0            |
| 5   | e     | 4169  | 0        | 4272     | 70      | 0            |
| 6   | G     | 4089  | 0        | 4224     | 72      | 0            |
| 6   | g     | 4088  | 0        | 4230     | 67      | 0            |
| 7   | H     | 4054  | 0        | 4160     | 54      | 0            |
| 7   | h     | 4032  | 0        | 4140     | 67      | 0            |
| 8   | Q     | 4086  | 0        | 4160     | 56      | 0            |
| 8   | q     | 4053  | 0        | 4125     | 48      | 0            |
| 9   | Z     | 4022  | 0        | 4161     | 52      | 0            |
| 9   | z     | 4033  | 0        | 4171     | 60      | 0            |
| 10  | P     | 1555  | 0        | 1549     | 43      | 0            |
| 11  | A     | 27    | 0        | 12       | 1       | 0            |
| 11  | B     | 27    | 0        | 12       | 4       | 0            |
| 11  | D     | 27    | 0        | 12       | 1       | 0            |
| 11  | E     | 27    | 0        | 12       | 0       | 0            |
| 11  | G     | 27    | 0        | 12       | 2       | 0            |
| 11  | H     | 27    | 0        | 12       | 2       | 0            |
| 11  | Q     | 27    | 0        | 12       | 3       | 0            |
| 11  | Z     | 27    | 0        | 12       | 1       | 0            |
| 11  | a     | 27    | 0        | 12       | 4       | 0            |
| 11  | b     | 27    | 0        | 12       | 3       | 0            |
| 11  | d     | 27    | 0        | 12       | 3       | 0            |
| 11  | e     | 27    | 0        | 12       | 1       | 0            |
| 11  | g     | 27    | 0        | 12       | 3       | 0            |
| 11  | h     | 27    | 0        | 12       | 1       | 0            |
| 11  | q     | 27    | 0        | 12       | 2       | 0            |
| 11  | z     | 27    | 0        | 12       | 1       | 0            |
| 12  | A     | 1     | 0        | 0        | 0       | 0            |
| 12  | B     | 1     | 0        | 0        | 0       | 0            |
| 12  | D     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12  | E     | 1     | 0        | 0        | 0       | 0            |
| 12  | G     | 1     | 0        | 0        | 0       | 0            |
| 12  | H     | 1     | 0        | 0        | 0       | 0            |
| 12  | Q     | 1     | 0        | 0        | 0       | 0            |
| 12  | Z     | 1     | 0        | 0        | 0       | 0            |
| 12  | a     | 1     | 0        | 0        | 0       | 0            |
| 12  | b     | 1     | 0        | 0        | 0       | 0            |
| 12  | d     | 1     | 0        | 0        | 0       | 0            |
| 12  | e     | 1     | 0        | 0        | 0       | 0            |
| 12  | g     | 1     | 0        | 0        | 0       | 0            |
| 12  | h     | 1     | 0        | 0        | 0       | 0            |
| 12  | q     | 1     | 0        | 0        | 0       | 0            |
| 12  | z     | 1     | 0        | 0        | 0       | 0            |
| 13  | A     | 4     | 0        | 0        | 1       | 0            |
| 13  | B     | 4     | 0        | 0        | 4       | 0            |
| 13  | D     | 4     | 0        | 0        | 2       | 0            |
| 13  | E     | 4     | 0        | 0        | 1       | 0            |
| 13  | G     | 4     | 0        | 0        | 3       | 0            |
| 13  | H     | 4     | 0        | 0        | 2       | 0            |
| 13  | Q     | 4     | 0        | 0        | 2       | 0            |
| 13  | Z     | 4     | 0        | 0        | 1       | 0            |
| 13  | a     | 4     | 0        | 0        | 2       | 0            |
| 13  | b     | 4     | 0        | 0        | 0       | 0            |
| 13  | d     | 4     | 0        | 0        | 1       | 0            |
| 13  | e     | 4     | 0        | 0        | 0       | 0            |
| 13  | g     | 4     | 0        | 0        | 3       | 0            |
| 13  | h     | 4     | 0        | 0        | 1       | 0            |
| 13  | q     | 4     | 0        | 0        | 2       | 0            |
| 13  | z     | 4     | 0        | 0        | 1       | 0            |
| 14  | A     | 2     | 0        | 0        | 0       | 0            |
| 14  | B     | 2     | 0        | 0        | 0       | 0            |
| 14  | D     | 1     | 0        | 0        | 0       | 0            |
| 14  | E     | 1     | 0        | 0        | 0       | 0            |
| 14  | G     | 1     | 0        | 0        | 0       | 0            |
| 14  | H     | 1     | 0        | 0        | 0       | 0            |
| 14  | Q     | 1     | 0        | 0        | 0       | 0            |
| 14  | Z     | 1     | 0        | 0        | 0       | 0            |
| 14  | a     | 2     | 0        | 0        | 0       | 0            |
| 14  | b     | 1     | 0        | 0        | 0       | 0            |
| 14  | d     | 1     | 0        | 0        | 0       | 0            |
| 14  | e     | 1     | 0        | 0        | 0       | 0            |
| 14  | g     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | h     | 1     | 0        | 0        | 0       | 0            |
| 14  | q     | 1     | 0        | 0        | 0       | 0            |
| 14  | z     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 67663 | 0        | 69353    | 956     | 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 7.

All (956) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:79:PRO:HB2   | 5:E:60:MET:HE2   | 1.53                     | 0.90              |
| 8:Q:85:MET:HE3   | 9:Z:46:MET:HE3   | 1.57                     | 0.85              |
| 2:a:217:ASN:HD22 | 10:P:287:ASN:HB2 | 1.47                     | 0.79              |
| 10:P:186:HIS:HE1 | 10:P:198:MET:HE3 | 1.48                     | 0.78              |
| 6:G:292:THR:HG22 | 6:G:294:LYS:H    | 1.51                     | 0.76              |
| 6:g:27:ILE:HD13  | 6:g:110:GLU:HB2  | 1.69                     | 0.75              |
| 3:B:219:LEU:HB2  | 3:B:372:THR:HG21 | 1.68                     | 0.75              |
| 7:H:346:GLN:HB2  | 7:H:363:GLY:HA3  | 1.70                     | 0.74              |
| 6:g:133:MET:HE3  | 6:g:444:LEU:HD11 | 1.70                     | 0.73              |
| 2:A:474:ALA:HB2  | 2:A:483:LEU:HB2  | 1.70                     | 0.73              |
| 6:g:289:VAL:HG21 | 6:g:350:LEU:HD13 | 1.69                     | 0.73              |
| 9:Z:189:PHE:O    | 9:Z:323:ARG:NH1  | 2.22                     | 0.73              |
| 1:N:311:ARG:HG2  | 5:E:304:TRP:HZ2  | 1.54                     | 0.72              |
| 4:D:78:LEU:HB3   | 4:D:92:VAL:HG22  | 1.71                     | 0.72              |
| 5:E:236:HIS:H    | 5:E:239:MET:HE2  | 1.54                     | 0.72              |
| 6:G:132:ASP:OD2  | 6:G:437:TYR:OH   | 2.07                     | 0.72              |
| 2:a:44:MET:HE2   | 6:g:519:ILE:HG21 | 1.72                     | 0.72              |
| 3:b:112:GLU:HB3  | 3:b:438:SER:HB3  | 1.72                     | 0.72              |
| 9:z:242:THR:HG22 | 9:z:244:VAL:H    | 1.55                     | 0.71              |
| 5:e:38:ILE:HG21  | 5:e:121:GLU:HB2  | 1.73                     | 0.71              |
| 3:b:39:VAL:HG22  | 3:b:100:THR:HG23 | 1.72                     | 0.70              |
| 7:h:82:ILE:HG21  | 7:h:509:ALA:HB2  | 1.72                     | 0.70              |
| 2:A:354:GLU:HG3  | 2:A:363:LEU:HD12 | 1.73                     | 0.70              |
| 3:B:39:VAL:HG22  | 3:B:100:THR:HG23 | 1.73                     | 0.70              |
| 6:G:16:ARG:HG3   | 6:G:523:VAL:HG22 | 1.73                     | 0.70              |
| 6:g:64:ASN:ND2   | 6:g:88:ASP:OD2   | 2.25                     | 0.70              |
| 6:g:218:VAL:HG21 | 6:g:323:ILE:HG12 | 1.73                     | 0.70              |
| 9:z:264:ARG:NH2  | 9:z:298:ASP:OD2  | 2.25                     | 0.69              |
| 4:D:235:ASN:ND2  | 4:D:322:ILE:O    | 2.25                     | 0.69              |
| 5:E:60:MET:HG3   | 5:E:70:VAL:HG22  | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:198:ASP:HB3  | 5:E:202:ARG:HB2  | 1.74                     | 0.69              |
| 5:E:231:ASP:HA   | 5:E:371:MET:HG2  | 1.74                     | 0.69              |
| 6:g:302:HIS:HB2  | 9:z:334:ASN:HB2  | 1.75                     | 0.69              |
| 4:D:212:LYS:HD3  | 4:D:402:GLU:HG2  | 1.75                     | 0.69              |
| 6:g:35:ASP:OD1   | 6:g:38:ARG:NH1   | 2.25                     | 0.69              |
| 2:a:285:VAL:HA   | 2:a:306:MET:HB2  | 1.73                     | 0.69              |
| 7:h:346:GLN:HB2  | 7:h:363:GLY:HA3  | 1.75                     | 0.68              |
| 2:a:474:ALA:HB2  | 2:a:483:LEU:HB2  | 1.74                     | 0.68              |
| 3:B:63:VAL:HG22  | 3:B:381:GLN:HB3  | 1.76                     | 0.68              |
| 6:G:35:ASP:OD1   | 6:G:38:ARG:NH1   | 2.27                     | 0.68              |
| 5:e:305:GLY:HA2  | 5:e:323:ARG:HB2  | 1.75                     | 0.68              |
| 10:P:179:LYS:HB3 | 10:P:241:GLY:HA2 | 1.75                     | 0.67              |
| 4:d:30:PRO:HB3   | 4:d:533:ASP:HB2  | 1.77                     | 0.67              |
| 7:H:82:ILE:HG21  | 7:H:509:ALA:HB2  | 1.77                     | 0.67              |
| 7:h:32:ILE:HG13  | 7:h:76:ALA:HB1   | 1.75                     | 0.66              |
| 10:P:55:VAL:HG22 | 10:P:56:ASN:H    | 1.59                     | 0.66              |
| 1:N:249:GLU:HB2  | 3:B:252:PHE:HZ   | 1.61                     | 0.66              |
| 2:a:203:ARG:HD3  | 2:a:207:GLU:HG2  | 1.77                     | 0.66              |
| 7:h:38:THR:OG1   | 7:h:47:LYS:NZ    | 2.28                     | 0.66              |
| 4:d:78:LEU:HB3   | 4:d:92:VAL:HG22  | 1.77                     | 0.66              |
| 7:h:2:MET:HE3    | 7:h:3:PRO:HD2    | 1.77                     | 0.66              |
| 8:q:175:ASN:HD21 | 8:q:212:ILE:HD11 | 1.61                     | 0.66              |
| 10:P:186:HIS:CE1 | 10:P:198:MET:HE3 | 2.30                     | 0.66              |
| 7:h:23:VAL:HG13  | 7:h:109:LYS:HE3  | 1.78                     | 0.66              |
| 4:D:75:ALA:HB2   | 4:D:106:THR:HG21 | 1.78                     | 0.65              |
| 5:e:230:VAL:HG12 | 5:e:232:LYS:H    | 1.61                     | 0.65              |
| 6:g:246:GLU:HG3  | 6:g:248:LYS:HE3  | 1.78                     | 0.65              |
| 9:Z:242:THR:HG22 | 9:Z:244:VAL:H    | 1.61                     | 0.65              |
| 3:B:50:LYS:HD3   | 4:D:534:ASP:HB3  | 1.77                     | 0.65              |
| 7:h:292:LYS:HG3  | 7:h:319:LEU:HD12 | 1.76                     | 0.65              |
| 2:A:353:GLN:O    | 6:G:190:ARG:NH1  | 2.30                     | 0.65              |
| 8:Q:169:MET:SD   | 11:Q:601:ADP:N6  | 2.64                     | 0.65              |
| 4:d:103:GLY:HA3  | 4:d:410:CYS:HB3  | 1.78                     | 0.65              |
| 3:B:112:GLU:HB3  | 3:B:438:SER:HB3  | 1.78                     | 0.65              |
| 5:e:60:MET:HG3   | 5:e:70:VAL:HG22  | 1.78                     | 0.65              |
| 7:h:60:ASN:ND2   | 7:h:165:SER:O    | 2.30                     | 0.64              |
| 7:H:32:ILE:HG13  | 7:H:76:ALA:HB1   | 1.78                     | 0.64              |
| 1:N:274:VAL:HG23 | 1:N:275:GLN:HG2  | 1.78                     | 0.64              |
| 4:D:119:SER:HB3  | 4:D:453:ALA:HB1  | 1.80                     | 0.64              |
| 6:g:292:THR:HG22 | 6:g:294:LYS:H    | 1.62                     | 0.64              |
| 3:b:251:ILE:HG13 | 5:e:277:LEU:HD11 | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:g:469:LYS:NZ   | 6:g:475:CYS:SG   | 2.70                     | 0.64              |
| 4:d:119:SER:HB2  | 4:d:453:ALA:HB1  | 1.80                     | 0.64              |
| 7:H:429:GLY:HA2  | 7:H:432:GLN:HB3  | 1.80                     | 0.63              |
| 4:D:30:PRO:HB3   | 4:D:533:ASP:HB2  | 1.80                     | 0.63              |
| 6:g:41:LEU:O     | 6:g:454:ASN:ND2  | 2.29                     | 0.63              |
| 2:A:34:SER:OG    | 2:A:43:LYS:NZ    | 2.32                     | 0.63              |
| 8:Q:412:GLY:HA3  | 8:Q:492:MET:HE1  | 1.81                     | 0.63              |
| 6:g:130:LEU:HB2  | 6:g:510:VAL:HG11 | 1.81                     | 0.63              |
| 3:B:478:LEU:HB3  | 3:B:480:MET:HE3  | 1.81                     | 0.62              |
| 3:B:45:PRO:HG2   | 3:B:480:MET:HG3  | 1.81                     | 0.62              |
| 2:A:467:LEU:HD11 | 2:A:488:LEU:HG   | 1.81                     | 0.62              |
| 9:z:84:GLN:OE1   | 9:z:88:THR:OG1   | 2.17                     | 0.62              |
| 3:b:131:ARG:NH2  | 5:e:179:ASN:OD1  | 2.33                     | 0.61              |
| 4:D:502:ASN:ND2  | 4:D:505:GLU:OE1  | 2.33                     | 0.61              |
| 6:G:18:SER:OG    | 6:G:521:ASP:OD1  | 2.19                     | 0.61              |
| 2:a:229:ILE:HG13 | 2:a:306:MET:HE2  | 1.83                     | 0.61              |
| 2:a:145:ARG:NH2  | 2:a:174:ASP:OD1  | 2.34                     | 0.61              |
| 5:E:532:ASP:OD2  | 7:H:47:LYS:NZ    | 2.34                     | 0.61              |
| 5:e:198:ASP:HB3  | 5:e:202:ARG:HB2  | 1.81                     | 0.61              |
| 6:G:27:ILE:HD13  | 6:G:110:GLU:HB2  | 1.83                     | 0.60              |
| 2:a:59:ALA:HB2   | 2:a:90:THR:HG21  | 1.82                     | 0.60              |
| 11:B:601:ADP:O3A | 13:B:603:AF3:F1  | 2.09                     | 0.60              |
| 8:q:151:ALA:HB3  | 8:q:406:LYS:HE2  | 1.82                     | 0.60              |
| 10:P:84:MET:HE1  | 10:P:87:LEU:HD23 | 1.83                     | 0.60              |
| 3:b:122:HIS:HD2  | 3:b:124:GLN:HB2  | 1.66                     | 0.60              |
| 4:d:38:ILE:HG21  | 4:d:121:THR:HG1  | 1.67                     | 0.60              |
| 10:P:176:LYS:O   | 10:P:177:GLU:HG3 | 2.01                     | 0.60              |
| 6:G:302:HIS:HB2  | 9:Z:334:ASN:HB2  | 1.82                     | 0.60              |
| 8:Q:412:GLY:N    | 11:Q:601:ADP:O2' | 2.34                     | 0.60              |
| 2:a:246:MET:HE3  | 2:a:250:VAL:HG11 | 1.82                     | 0.60              |
| 6:G:469:LYS:NZ   | 6:G:475:CYS:SG   | 2.74                     | 0.60              |
| 6:g:155:ILE:HG21 | 6:g:401:VAL:HG21 | 1.82                     | 0.60              |
| 1:N:249:GLU:HB2  | 3:B:252:PHE:CZ   | 2.37                     | 0.60              |
| 3:b:38:LEU:O     | 3:b:50:LYS:NZ    | 2.33                     | 0.60              |
| 4:d:229:LEU:HB2  | 4:d:374:LEU:HD23 | 1.83                     | 0.60              |
| 8:q:222:VAL:HG22 | 8:q:362:VAL:HG22 | 1.84                     | 0.60              |
| 3:B:163:ALA:HB3  | 3:B:180:THR:HG23 | 1.84                     | 0.59              |
| 4:D:432:LEU:HD23 | 4:D:458:MET:HE2  | 1.84                     | 0.59              |
| 9:Z:264:ARG:NH2  | 9:Z:298:ASP:OD2  | 2.35                     | 0.59              |
| 5:e:78:LEU:HB3   | 5:e:92:VAL:HG22  | 1.82                     | 0.59              |
| 3:B:71:LEU:HB3   | 3:B:85:VAL:HG22  | 1.83                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:251:ILE:HG13  | 5:E:277:LEU:HD11 | 1.83                     | 0.59              |
| 7:H:499:ARG:NH2   | 11:H:601:ADP:O3' | 2.34                     | 0.59              |
| 5:E:78:LEU:HB3    | 5:E:92:VAL:HG22  | 1.85                     | 0.59              |
| 2:a:354:GLU:HG3   | 2:a:363:LEU:HD12 | 1.85                     | 0.59              |
| 8:Q:27:GLU:OE2    | 9:z:15:ARG:NH1   | 2.35                     | 0.59              |
| 8:q:33:ILE:HG21   | 8:q:116:GLU:HB2  | 1.85                     | 0.59              |
| 3:B:131:ARG:NH2   | 5:E:179:ASN:OD1  | 2.36                     | 0.59              |
| 7:h:447:ARG:HB2   | 7:h:461:LEU:HD11 | 1.84                     | 0.59              |
| 5:E:38:ILE:HG21   | 5:E:121:GLU:HB2  | 1.84                     | 0.59              |
| 5:E:42:LYS:O      | 5:E:46:ASN:ND2   | 2.35                     | 0.59              |
| 9:Z:24:ILE:HD13   | 9:Z:107:ASP:HB2  | 1.85                     | 0.59              |
| 1:N:311:ARG:NH2   | 7:H:245:GLU:OE1  | 2.35                     | 0.59              |
| 6:G:289:VAL:HG11  | 6:G:350:LEU:HD13 | 1.84                     | 0.59              |
| 2:a:103:ASN:ND2   | 2:a:444:SER:OG   | 2.21                     | 0.59              |
| 4:d:235:ASN:ND2   | 4:d:322:ILE:O    | 2.36                     | 0.59              |
| 7:H:26:ILE:O      | 7:H:30:GLN:HG2   | 2.03                     | 0.59              |
| 8:q:38:GLU:O      | 8:q:42:THR:HG23  | 2.03                     | 0.59              |
| 4:D:497:LYS:HE2   | 4:D:501:SER:HB3  | 1.85                     | 0.58              |
| 5:e:444:GLU:O     | 5:e:448:MET:HG2  | 2.03                     | 0.58              |
| 8:q:182:LEU:HD22  | 8:q:217:VAL:HG23 | 1.83                     | 0.58              |
| 5:E:184:GLN:NE2   | 5:E:222:THR:O    | 2.36                     | 0.58              |
| 7:H:524:ARG:NH1   | 8:Q:59:HIS:O     | 2.37                     | 0.58              |
| 10:P:228:PHE:HA   | 10:P:232:ALA:HB3 | 1.84                     | 0.58              |
| 10:P:233:LEU:HD23 | 10:P:234:PRO:HD3 | 1.84                     | 0.58              |
| 6:g:206:GLY:HA3   | 9:z:87:ILE:HG13  | 1.84                     | 0.58              |
| 11:g:601:ADP:O1B  | 13:g:603:AF3:F3  | 2.11                     | 0.58              |
| 7:h:252:ASN:ND2   | 8:q:255:GLY:O    | 2.31                     | 0.58              |
| 2:A:456:ALA:HB2   | 2:A:490:LEU:HD12 | 1.86                     | 0.58              |
| 3:B:38:LEU:O      | 3:B:50:LYS:NZ    | 2.29                     | 0.58              |
| 3:B:189:ARG:NH2   | 3:B:370:ALA:O    | 2.36                     | 0.58              |
| 6:G:266:ARG:HG3   | 6:G:270:MET:HE2  | 1.85                     | 0.58              |
| 4:d:195:ILE:HG21  | 4:d:203:VAL:HG22 | 1.85                     | 0.58              |
| 11:q:601:ADP:O1B  | 13:q:603:AF3:F2  | 2.11                     | 0.58              |
| 6:G:130:LEU:HB2   | 6:G:510:VAL:HG11 | 1.85                     | 0.58              |
| 10:P:178:GLN:HG2  | 10:P:180:SER:H   | 1.68                     | 0.58              |
| 8:Q:151:ALA:HB3   | 8:Q:406:LYS:HE2  | 1.84                     | 0.58              |
| 3:b:141:LEU:HD13  | 3:b:417:MET:HE3  | 1.85                     | 0.58              |
| 6:g:468:ALA:O     | 6:g:471:THR:OG1  | 2.22                     | 0.58              |
| 3:B:97:ASP:OD1    | 13:B:603:AF3:F1  | 2.11                     | 0.58              |
| 5:E:367:THR:HG23  | 5:E:369:ASP:H    | 1.69                     | 0.58              |
| 4:D:193:LYS:NZ    | 4:D:225:GLU:OE2  | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:420:TYR:OH   | 5:E:502:LYS:NZ   | 2.36                     | 0.57              |
| 9:Z:135:GLU:OE2  | 9:Z:498:TYR:OH   | 2.21                     | 0.57              |
| 9:Z:449:LYS:HB3  | 9:Z:459:LEU:HD23 | 1.87                     | 0.57              |
| 8:q:70:ALA:HB2   | 8:q:101:THR:HG21 | 1.86                     | 0.57              |
| 5:E:438:ASP:OD1  | 5:E:449:ARG:NH2  | 2.35                     | 0.57              |
| 2:a:8:PHE:HB2    | 4:d:84:LEU:HD11  | 1.84                     | 0.57              |
| 4:D:228:VAL:HG22 | 4:D:375:LYS:HG2  | 1.87                     | 0.57              |
| 6:g:170:SER:O    | 6:g:174:ASN:ND2  | 2.36                     | 0.57              |
| 2:A:23:MET:HE2   | 5:e:8:ALA:HA     | 1.85                     | 0.57              |
| 7:h:90:VAL:HG12  | 7:h:92:ASP:H     | 1.70                     | 0.57              |
| 9:z:135:GLU:OE2  | 9:z:498:TYR:OH   | 2.21                     | 0.57              |
| 4:d:72:ASN:ND2   | 4:d:173:SER:O    | 2.37                     | 0.57              |
| 9:Z:279:ARG:NH2  | 9:Z:308:GLU:OE2  | 2.35                     | 0.57              |
| 4:D:32:GLN:HB3   | 3:b:6:LEU:HD23   | 1.86                     | 0.57              |
| 4:D:430:ILE:HG12 | 4:D:462:PRO:HG2  | 1.86                     | 0.56              |
| 1:N:233:PHE:CZ   | 1:N:268:MET:HG2  | 2.41                     | 0.56              |
| 6:G:155:ILE:HG21 | 6:G:401:VAL:HG21 | 1.87                     | 0.56              |
| 6:G:206:GLY:HA3  | 9:Z:87:ILE:HG13  | 1.86                     | 0.56              |
| 7:h:193:LYS:HE3  | 7:h:194:MET:HE2  | 1.87                     | 0.56              |
| 5:E:248:ILE:HG12 | 5:E:299:LEU:HD23 | 1.87                     | 0.56              |
| 6:G:31:LYS:HD3   | 6:G:107:SER:HB2  | 1.87                     | 0.56              |
| 8:Q:70:ALA:HB2   | 8:Q:101:THR:HG21 | 1.87                     | 0.56              |
| 6:g:68:ARG:HD2   | 10:P:153:HIS:CE1 | 2.40                     | 0.56              |
| 8:q:14:MET:HB3   | 9:z:69:ILE:HG23  | 1.86                     | 0.56              |
| 9:z:281:VAL:HB   | 9:z:289:PHE:HZ   | 1.70                     | 0.56              |
| 3:b:257:ARG:HH21 | 4:d:263:GLN:HE21 | 1.52                     | 0.56              |
| 7:h:145:LYS:NZ   | 7:h:147:ASP:O    | 2.35                     | 0.56              |
| 7:h:333:SER:HB3  | 8:q:300:MET:HE1  | 1.88                     | 0.56              |
| 1:N:240:VAL:HA   | 1:N:258:GLY:HA3  | 1.87                     | 0.56              |
| 4:d:87:ALA:HA    | 4:d:90:MET:HE2   | 1.87                     | 0.56              |
| 7:h:187:ASP:HB3  | 7:h:368:LYS:HD2  | 1.88                     | 0.56              |
| 9:z:279:ARG:NH1  | 9:z:308:GLU:OE2  | 2.39                     | 0.56              |
| 9:z:40:PRO:HD3   | 9:z:158:THR:HG22 | 1.88                     | 0.56              |
| 2:A:145:ARG:NH2  | 2:A:174:ASP:OD1  | 2.39                     | 0.56              |
| 5:E:170:LYS:O    | 5:E:182:HIS:NE2  | 2.35                     | 0.56              |
| 6:g:129:ALA:O    | 6:g:133:MET:HG3  | 2.06                     | 0.56              |
| 9:z:150:ASP:OD1  | 9:z:153:ARG:NH2  | 2.39                     | 0.56              |
| 6:G:332:VAL:HG21 | 6:G:338:LEU:HD13 | 1.87                     | 0.56              |
| 6:G:415:GLU:OE2  | 6:G:502:LYS:NZ   | 2.27                     | 0.56              |
| 3:b:168:SER:OG   | 11:b:601:ADP:N7  | 2.37                     | 0.56              |
| 4:d:38:ILE:HG21  | 4:d:121:THR:OG1  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:h:463:LYS:NZ   | 7:h:483:ASP:OD1   | 2.32                     | 0.56              |
| 10:P:145:MET:HA  | 10:P:148:MET:HG2  | 1.87                     | 0.56              |
| 2:A:59:ALA:HB2   | 2:A:90:THR:HG21   | 1.87                     | 0.55              |
| 4:D:432:LEU:HD21 | 4:D:519:LEU:HD11  | 1.88                     | 0.55              |
| 2:a:477:ASN:ND2  | 2:a:479:GLU:OE2   | 2.40                     | 0.55              |
| 3:b:422:THR:OG1  | 3:b:444:ARG:NH2   | 2.39                     | 0.55              |
| 3:b:71:LEU:HB3   | 3:b:85:VAL:HG22   | 1.88                     | 0.55              |
| 3:B:156:ARG:NH2  | 3:B:185:GLU:OE2   | 2.37                     | 0.55              |
| 8:Q:175:ASN:HD21 | 8:Q:212:ILE:HD11  | 1.70                     | 0.55              |
| 8:Q:417:ILE:HG13 | 8:Q:467:LEU:HD13  | 1.89                     | 0.55              |
| 9:Z:63:LEU:O     | 9:Z:67:MET:HG3    | 2.06                     | 0.55              |
| 8:q:417:ILE:HD11 | 8:q:449:PRO:HG3   | 1.89                     | 0.55              |
| 7:H:88:ALA:HB1   | 8:Q:357:ASP:HB2   | 1.89                     | 0.55              |
| 6:g:87:GLN:NE2   | 6:g:93:ASP:O      | 2.36                     | 0.55              |
| 4:D:55:LYS:HG3   | 4:D:469:ALA:HA    | 1.88                     | 0.55              |
| 6:G:258:ILE:HG23 | 6:G:263:ASP:HB2   | 1.89                     | 0.55              |
| 5:e:27:ARG:NH2   | 5:e:532:ASP:OD2   | 2.37                     | 0.55              |
| 5:e:411:ASN:HB3  | 5:e:511:ILE:HD11  | 1.88                     | 0.55              |
| 5:e:538:GLU:HG3  | 5:e:540:GLU:HB3   | 1.89                     | 0.55              |
| 7:h:429:GLY:HA2  | 7:h:432:GLN:HB3   | 1.89                     | 0.55              |
| 9:z:103:LEU:HD21 | 9:z:515:ILE:HG21  | 1.88                     | 0.55              |
| 9:z:237:LEU:HB2  | 9:z:297:ILE:HG12  | 1.87                     | 0.55              |
| 10:P:172:ASP:OD1 | 10:P:173:MET:N    | 2.39                     | 0.55              |
| 2:A:411:GLY:O    | 2:A:498:ASN:ND2   | 2.39                     | 0.55              |
| 5:E:196:VAL:HG21 | 5:E:208:LEU:HB2   | 1.89                     | 0.55              |
| 2:a:43:LYS:HG2   | 6:g:521:ASP:HB3   | 1.89                     | 0.55              |
| 7:h:57:THR:HG21  | 7:h:68:LEU:HG     | 1.89                     | 0.55              |
| 9:z:194:MET:HE2  | 9:z:360:PHE:HE1   | 1.72                     | 0.55              |
| 10:P:59:PRO:HA   | 10:P:62:VAL:HG12  | 1.87                     | 0.55              |
| 10:P:85:GLU:HG3  | 10:P:244:LEU:HD12 | 1.88                     | 0.55              |
| 3:B:250:LYS:HB2  | 5:E:257:PRO:HG2   | 1.88                     | 0.55              |
| 6:G:183:VAL:HG21 | 6:G:199:ALA:HB2   | 1.89                     | 0.55              |
| 3:B:299:TYR:HD1  | 3:B:302:GLN:HE21  | 1.53                     | 0.55              |
| 6:G:218:VAL:HG21 | 6:G:323:ILE:HG12  | 1.88                     | 0.55              |
| 10:P:184:MET:HG2 | 10:P:238:ILE:HG12 | 1.88                     | 0.55              |
| 2:A:47:ASP:HB2   | 2:A:51:ASP:HB2    | 1.88                     | 0.55              |
| 5:e:438:ASP:OD1  | 5:e:449:ARG:NH2   | 2.39                     | 0.55              |
| 9:z:23:ASN:OD1   | 9:z:73:THR:OG1    | 2.25                     | 0.55              |
| 4:d:94:LEU:HD11  | 4:d:521:LEU:HB3   | 1.88                     | 0.55              |
| 8:q:417:ILE:HG13 | 8:q:467:LEU:HD13  | 1.89                     | 0.55              |
| 7:h:338:SER:OG   | 7:h:340:ASP:OD1   | 2.20                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:171:MET:HG3  | 2:A:210:LEU:HB2   | 1.88                     | 0.54              |
| 5:E:518:SER:O    | 5:E:522:GLN:HG2   | 2.07                     | 0.54              |
| 3:b:163:ALA:HB3  | 3:b:180:THR:HG23  | 1.89                     | 0.54              |
| 6:g:256:ILE:HB   | 9:z:246:SER:HA    | 1.89                     | 0.54              |
| 7:h:26:ILE:O     | 7:h:30:GLN:HG2    | 2.07                     | 0.54              |
| 7:H:455:PHE:CE1  | 7:H:482:GLU:HG2   | 2.42                     | 0.54              |
| 7:h:478:ASP:OD2  | 7:h:481:ASN:ND2   | 2.35                     | 0.54              |
| 4:D:303:SER:HB3  | 4:D:308:ALA:HB2   | 1.89                     | 0.54              |
| 5:e:236:HIS:HB2  | 5:e:239:MET:HE3   | 1.89                     | 0.54              |
| 4:D:38:ILE:HG21  | 4:D:121:THR:OG1   | 2.07                     | 0.54              |
| 5:E:229:ILE:HG22 | 5:E:384:THR:HG21  | 1.89                     | 0.54              |
| 2:a:526:ARG:HG3  | 4:d:175:VAL:HG23  | 1.89                     | 0.54              |
| 2:a:533:LEU:HD12 | 4:d:63:ASP:HA     | 1.90                     | 0.54              |
| 5:e:295:THR:HG21 | 5:e:348:LEU:HG    | 1.89                     | 0.54              |
| 9:z:221:MET:SD   | 9:z:311:VAL:HA    | 2.47                     | 0.54              |
| 9:Z:3:ALA:O      | 9:Z:6:THR:OG1     | 2.25                     | 0.54              |
| 2:a:289:THR:HG23 | 2:a:316:LEU:HD22  | 1.88                     | 0.54              |
| 8:q:190:ILE:HG22 | 8:q:191:PHE:H     | 1.73                     | 0.54              |
| 11:g:601:ADP:O1B | 13:g:603:AF3:F1   | 2.15                     | 0.54              |
| 9:z:462:THR:O    | 9:z:466:ILE:HG12  | 2.07                     | 0.54              |
| 6:G:47:MET:HE2   | 6:G:59:MET:HG2    | 1.89                     | 0.54              |
| 6:g:101:LEU:O    | 6:g:105:MET:HG3   | 2.07                     | 0.54              |
| 5:E:14:ARG:NH1   | 7:H:16:SER:OG     | 2.40                     | 0.54              |
| 6:G:182:MET:SD   | 6:G:372:CYS:HB3   | 2.47                     | 0.54              |
| 11:a:601:ADP:O2B | 13:a:603:AF3:F3   | 2.16                     | 0.54              |
| 4:d:173:SER:OG   | 11:d:601:ADP:O1A  | 2.26                     | 0.54              |
| 4:D:26:ASP:OD1   | 4:D:26:ASP:N      | 2.41                     | 0.53              |
| 7:H:156:GLU:O    | 7:H:160:MET:HG3   | 2.08                     | 0.53              |
| 7:H:168:ILE:HG21 | 7:H:385:THR:HG23  | 1.89                     | 0.53              |
| 8:Q:33:ILE:HG21  | 8:Q:116:GLU:HB2   | 1.90                     | 0.53              |
| 6:G:468:ALA:O    | 6:G:471:THR:OG1   | 2.23                     | 0.53              |
| 1:N:174:TYR:CD1  | 1:N:175:PRO:HD2   | 2.44                     | 0.53              |
| 3:B:51:ILE:HG12  | 3:B:63:VAL:HG12   | 1.90                     | 0.53              |
| 7:H:447:ARG:HB2  | 7:H:461:LEU:HD11  | 1.89                     | 0.53              |
| 3:b:51:ILE:HG12  | 3:b:63:VAL:HG22   | 1.89                     | 0.53              |
| 9:z:236:SER:O    | 9:z:270:ARG:NH2   | 2.41                     | 0.53              |
| 4:D:42:LYS:NZ    | 4:D:46:ASP:OD2    | 2.42                     | 0.53              |
| 5:E:364:PHE:HE2  | 5:E:371:MET:HB2   | 1.73                     | 0.53              |
| 2:a:142:GLU:HG2  | 2:a:143:LEU:HD22  | 1.90                     | 0.53              |
| 10:P:240:LYS:HB3 | 10:P:245:ILE:HG13 | 1.91                     | 0.53              |
| 3:B:83:VAL:HG22  | 5:E:393:MET:SD    | 2.48                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:72:ASN:ND2   | 4:D:173:SER:O    | 2.41                     | 0.53              |
| 6:G:83:ILE:HD13  | 6:G:512:THR:HG21 | 1.91                     | 0.53              |
| 6:g:50:LEU:HD13  | 9:z:522:MET:HB2  | 1.89                     | 0.53              |
| 2:A:450:ASN:ND2  | 2:A:460:SER:OG   | 2.37                     | 0.53              |
| 11:G:601:ADP:O2B | 13:G:603:AF3:F1  | 2.17                     | 0.53              |
| 2:a:446:LEU:HD11 | 2:a:468:ARG:HD2  | 1.91                     | 0.53              |
| 4:D:343:LYS:HB2  | 4:D:355:MET:HG3  | 1.90                     | 0.53              |
| 6:G:226:HIS:HD2  | 6:G:228:ARG:H    | 1.55                     | 0.53              |
| 6:G:449:ARG:HB2  | 6:G:463:LEU:HD11 | 1.91                     | 0.53              |
| 9:Z:40:PRO:HD3   | 9:Z:158:THR:HG22 | 1.90                     | 0.53              |
| 2:A:203:ARG:HD3  | 2:A:207:GLU:HG2  | 1.89                     | 0.53              |
| 6:G:62:ASP:OD1   | 13:G:603:AF3:F3  | 2.17                     | 0.53              |
| 7:H:178:MET:HE3  | 7:H:372:PHE:CE2  | 2.44                     | 0.53              |
| 8:Q:33:ILE:HD13  | 8:Q:116:GLU:HB2  | 1.91                     | 0.53              |
| 6:g:190:ARG:NH1  | 6:g:192:GLU:OE1  | 2.38                     | 0.53              |
| 8:Q:277:ASP:HB2  | 8:Q:304:TYR:CZ   | 2.44                     | 0.52              |
| 5:e:102:ILE:HG22 | 5:e:104:ASP:H    | 1.74                     | 0.52              |
| 6:g:132:ASP:OD2  | 6:g:437:TYR:OH   | 2.20                     | 0.52              |
| 7:h:145:LYS:HZ3  | 7:h:147:ASP:HB3  | 1.74                     | 0.52              |
| 9:z:47:LEU:HD13  | 9:z:66:GLU:HB2   | 1.90                     | 0.52              |
| 8:Q:190:ILE:HG22 | 8:Q:191:PHE:H    | 1.74                     | 0.52              |
| 5:e:119:GLU:HB3  | 5:e:450:ALA:HB1  | 1.91                     | 0.52              |
| 8:q:139:ALA:HB2  | 8:q:423:ILE:HD11 | 1.91                     | 0.52              |
| 2:A:222:SER:H    | 2:A:225:MET:HE2  | 1.74                     | 0.52              |
| 8:q:239:ILE:HD12 | 8:q:239:ILE:H    | 1.74                     | 0.52              |
| 11:z:601:ADP:O1B | 13:z:603:AF3:F3  | 2.17                     | 0.52              |
| 1:N:306:ARG:NH1  | 1:N:314:ARG:O    | 2.41                     | 0.52              |
| 6:G:90:GLU:HG3   | 6:G:91:VAL:HG13  | 1.91                     | 0.52              |
| 3:b:40:LYS:HD2   | 3:b:449:ILE:HD13 | 1.92                     | 0.52              |
| 7:h:103:GLU:HG2  | 7:h:444:ILE:HB   | 1.92                     | 0.52              |
| 9:z:335:SER:OG   | 9:z:337:ASP:OD1  | 2.24                     | 0.52              |
| 5:E:289:ILE:HG13 | 5:E:313:LEU:HB3  | 1.92                     | 0.52              |
| 6:G:289:VAL:HG12 | 6:G:310:THR:HB   | 1.92                     | 0.52              |
| 4:d:467:GLU:HG3  | 4:d:468:ASN:H    | 1.75                     | 0.52              |
| 4:d:496:ARG:NH1  | 4:d:506:GLU:OE2  | 2.42                     | 0.52              |
| 7:h:525:SER:HB2  | 8:q:59:HIS:HB2   | 1.91                     | 0.52              |
| 1:N:288:ARG:O    | 1:N:297:ALA:N    | 2.43                     | 0.52              |
| 5:e:239:MET:SD   | 5:e:320:PRO:HA   | 2.49                     | 0.52              |
| 3:B:519:ASN:HB3  | 5:E:59:LYS:HD3   | 1.91                     | 0.52              |
| 5:E:234:PHE:HB3  | 5:E:239:MET:HE3  | 1.92                     | 0.52              |
| 10:P:185:VAL:N   | 10:P:237:LEU:O   | 2.41                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:Q:109:GLY:O    | 8:Q:113:GLU:HG3   | 2.10                     | 0.52              |
| 9:Z:227:ASP:O    | 9:Z:288:GLY:N     | 2.42                     | 0.52              |
| 9:Z:251:LYS:NZ   | 9:Z:255:GLU:OE2   | 2.40                     | 0.52              |
| 11:Z:601:ADP:O2B | 13:Z:603:AF3:F1   | 2.17                     | 0.52              |
| 2:a:143:LEU:HB3  | 2:a:147:CYS:HB2   | 1.92                     | 0.52              |
| 6:g:203:LYS:HB2  | 6:g:384:LEU:HD13  | 1.91                     | 0.52              |
| 3:b:83:VAL:HG22  | 5:e:393:MET:SD    | 2.50                     | 0.52              |
| 3:b:279:VAL:HG11 | 3:b:303:LEU:HB3   | 1.91                     | 0.52              |
| 5:e:94:LEU:HD13  | 5:e:523:MET:HG3   | 1.92                     | 0.52              |
| 6:g:434:GLN:OE1  | 6:g:438:ARG:NH2   | 2.43                     | 0.52              |
| 3:B:232:ILE:HD13 | 3:B:288:ASN:HB3   | 1.92                     | 0.51              |
| 9:Z:244:VAL:HG12 | 9:Z:244:VAL:O     | 2.10                     | 0.51              |
| 2:a:214:TYR:OH   | 2:a:315:ASP:OD1   | 2.23                     | 0.51              |
| 6:g:77:ALA:O     | 6:g:81:ILE:HG12   | 2.10                     | 0.51              |
| 8:Q:284:ALA:HB2  | 8:Q:310:ILE:HD11  | 1.92                     | 0.51              |
| 9:Z:229:TYR:HE1  | 9:Z:287:LYS:HD3   | 1.76                     | 0.51              |
| 9:z:337:ASP:OD1  | 9:z:337:ASP:N     | 2.41                     | 0.51              |
| 10:P:185:VAL:HB  | 10:P:237:LEU:HB2  | 1.92                     | 0.51              |
| 8:Q:364:LYS:NZ   | 8:Q:366:GLU:OE2   | 2.44                     | 0.51              |
| 6:g:411:GLY:HA3  | 6:g:490:MET:HE3   | 1.91                     | 0.51              |
| 1:N:176:LEU:HG   | 1:N:177:THR:HG23  | 1.92                     | 0.51              |
| 2:A:47:ASP:OD1   | 6:G:526:HIS:NE2   | 2.43                     | 0.51              |
| 8:q:400:LYS:O    | 8:q:403:THR:OG1   | 2.23                     | 0.51              |
| 10:P:232:ALA:HA  | 10:P:250:ARG:HH22 | 1.75                     | 0.51              |
| 2:A:529:ASP:OD2  | 2:A:530:LEU:N     | 2.43                     | 0.51              |
| 11:B:601:ADP:PB  | 13:B:603:AF3:F1   | 2.57                     | 0.51              |
| 5:E:198:ASP:OD2  | 5:E:202:ARG:NH1   | 2.43                     | 0.51              |
| 7:H:516:VAL:HG11 | 8:Q:55:MET:HG3    | 1.93                     | 0.51              |
| 8:Q:116:GLU:OE2  | 8:Q:120:ARG:NE    | 2.43                     | 0.51              |
| 4:d:291:LYS:HG2  | 4:d:320:MET:HE2   | 1.92                     | 0.51              |
| 4:d:325:ILE:HD13 | 4:d:374:LEU:HD21  | 1.91                     | 0.51              |
| 9:z:148:LEU:HD11 | 9:z:402:ILE:HD11  | 1.93                     | 0.51              |
| 2:A:532:LYS:NZ   | 4:D:62:GLN:OE1    | 2.43                     | 0.51              |
| 4:D:48:ILE:HD12  | 4:D:107:THR:HG23  | 1.93                     | 0.51              |
| 5:E:305:GLY:HA2  | 5:E:323:ARG:HB2   | 1.92                     | 0.51              |
| 2:a:91:THR:OG1   | 11:a:601:ADP:O3B  | 2.29                     | 0.51              |
| 8:q:47:TYR:O     | 8:q:455:ASN:ND2   | 2.42                     | 0.51              |
| 3:B:65:ASN:HD22  | 3:B:170:LYS:HD3   | 1.76                     | 0.51              |
| 5:E:239:MET:SD   | 5:E:320:PRO:HA    | 2.51                     | 0.51              |
| 1:N:236:HIS:O    | 1:N:238:ALA:N     | 2.44                     | 0.51              |
| 5:E:81:MET:HG2   | 5:E:83:VAL:HG13   | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:103:ASN:ND2   | 2:A:444:SER:OG    | 2.29                     | 0.50              |
| 4:D:195:ILE:HG21  | 4:D:203:VAL:HG22  | 1.93                     | 0.50              |
| 9:Z:227:ASP:OD1   | 9:Z:346:HIS:NE2   | 2.44                     | 0.50              |
| 6:G:265:THR:HG21  | 9:Z:265:LYS:HB3   | 1.92                     | 0.50              |
| 8:Q:248:GLY:N     | 8:Q:276:MET:HE1   | 2.27                     | 0.50              |
| 2:a:238:ASP:HB3   | 2:a:329:SER:HA    | 1.93                     | 0.50              |
| 4:d:227:LEU:HD21  | 4:d:376:ILE:HD12  | 1.93                     | 0.50              |
| 9:z:61:ASN:HB2    | 9:z:92:THR:HG21   | 1.93                     | 0.50              |
| 9:z:63:LEU:O      | 9:z:67:MET:HG3    | 2.11                     | 0.50              |
| 6:G:77:ALA:O      | 6:G:81:ILE:HG12   | 2.11                     | 0.50              |
| 10:P:183:ILE:HG12 | 10:P:213:LYS:HB3  | 1.94                     | 0.50              |
| 3:B:516:ARG:NE    | 5:E:58:ASP:OD2    | 2.32                     | 0.50              |
| 5:E:149:ASP:OD1   | 5:E:417:ARG:NH1   | 2.44                     | 0.50              |
| 6:G:41:LEU:O      | 6:G:454:ASN:ND2   | 2.36                     | 0.50              |
| 2:a:384:MET:HG2   | 2:a:388:MET:HE2   | 1.93                     | 0.50              |
| 4:d:170:SER:HB2   | 4:d:411:VAL:HG21  | 1.94                     | 0.50              |
| 5:e:38:ILE:HD13   | 5:e:121:GLU:HB2   | 1.94                     | 0.50              |
| 2:A:431:GLY:O     | 2:A:435:GLN:NE2   | 2.33                     | 0.50              |
| 3:b:45:PRO:HG2    | 3:b:480:MET:HG3   | 1.92                     | 0.50              |
| 6:g:27:ILE:HG21   | 6:g:110:GLU:HB2   | 1.93                     | 0.50              |
| 6:g:452:ILE:HG13  | 6:g:480:VAL:HG11  | 1.93                     | 0.50              |
| 7:h:121:ILE:HA    | 7:h:434:LEU:HD13  | 1.94                     | 0.50              |
| 1:N:231:GLN:HG3   | 1:N:233:PHE:HE1   | 1.76                     | 0.50              |
| 2:A:281:THR:HG23  | 2:A:345:LEU:HD11  | 1.92                     | 0.50              |
| 2:a:127:GLU:HG3   | 2:a:426:TYR:CZ    | 2.47                     | 0.50              |
| 2:a:382:ASP:HB3   | 10:P:286:ARG:HH22 | 1.77                     | 0.50              |
| 8:Q:57:ILE:HG12   | 8:Q:63:LEU:HD23   | 1.94                     | 0.50              |
| 2:A:205:GLN:OE1   | 6:G:127:ARG:NH2   | 2.38                     | 0.50              |
| 2:A:400:LYS:NZ    | 2:A:404:GLU:OE2   | 2.42                     | 0.50              |
| 5:E:73:ASP:OD1    | 13:E:603:AF3:F2   | 2.20                     | 0.50              |
| 7:H:178:MET:HE3   | 7:H:372:PHE:HE2   | 1.75                     | 0.50              |
| 4:d:352:THR:OG1   | 4:d:354:ASP:OD1   | 2.23                     | 0.50              |
| 7:h:403:ASP:OD1   | 7:h:403:ASP:N     | 2.42                     | 0.50              |
| 7:h:421:ARG:O     | 7:h:425:ARG:HG2   | 2.12                     | 0.50              |
| 2:A:397:CYS:O     | 2:A:401:ARG:HG2   | 2.12                     | 0.49              |
| 6:G:184:GLN:HG3   | 6:G:193:ILE:HG12  | 1.93                     | 0.49              |
| 8:q:348:ASP:OD2   | 8:q:366:GLU:N     | 2.39                     | 0.49              |
| 8:q:483:GLU:OE2   | 8:q:490:LYS:NZ    | 2.45                     | 0.49              |
| 2:A:326:THR:HB    | 2:A:344:MET:HG3   | 1.94                     | 0.49              |
| 4:D:454:PHE:O     | 4:D:458:MET:HG2   | 2.12                     | 0.49              |
| 5:E:255:PHE:HB2   | 5:E:306:PHE:HB2   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:d:33:ILE:HD11  | 10:P:56:ASN:HD21 | 1.76                     | 0.49              |
| 9:z:24:ILE:HD13  | 9:z:107:ASP:HB2  | 1.94                     | 0.49              |
| 9:z:31:GLN:O     | 9:z:35:ARG:HG3   | 2.12                     | 0.49              |
| 5:E:342:VAL:HG21 | 5:E:348:LEU:HD13 | 1.93                     | 0.49              |
| 9:Z:8:ASN:ND2    | 9:Z:526:MET:SD   | 2.85                     | 0.49              |
| 2:a:385:CYS:HA   | 2:a:388:MET:HE3  | 1.94                     | 0.49              |
| 5:e:225:ILE:HD13 | 5:e:229:ILE:HD11 | 1.94                     | 0.49              |
| 8:q:116:GLU:OE2  | 8:q:120:ARG:NE   | 2.46                     | 0.49              |
| 9:z:44:MET:HE2   | 9:z:58:LYS:HD3   | 1.94                     | 0.49              |
| 9:z:429:VAL:HG21 | 9:z:437:VAL:HG21 | 1.94                     | 0.49              |
| 3:B:197:GLU:OE2  | 5:E:368:LYS:HB2  | 2.13                     | 0.49              |
| 3:B:326:VAL:HB   | 3:B:370:ALA:HB3  | 1.93                     | 0.49              |
| 2:a:34:SER:OG    | 2:a:43:LYS:NZ    | 2.46                     | 0.49              |
| 2:a:39:VAL:HG21  | 2:a:456:ALA:HB2  | 1.93                     | 0.49              |
| 2:a:78:LEU:HD11  | 2:a:516:PHE:HB3  | 1.95                     | 0.49              |
| 4:d:124:LEU:HD21 | 4:d:130:PRO:HB3  | 1.93                     | 0.49              |
| 7:h:200:VAL:HG11 | 7:h:353:ILE:HG22 | 1.94                     | 0.49              |
| 8:q:206:LYS:NZ   | 8:q:389:GLU:OE1  | 2.37                     | 0.49              |
| 3:B:160:MET:HE3  | 3:B:180:THR:HG22 | 1.94                     | 0.49              |
| 9:Z:178:ALA:O    | 9:Z:370:ARG:NH1  | 2.45                     | 0.49              |
| 2:a:122:ARG:HG3  | 4:d:178:GLN:HG3  | 1.95                     | 0.49              |
| 3:b:47:GLY:O     | 4:d:531:LYS:NZ   | 2.45                     | 0.49              |
| 9:z:97:LEU:HD13  | 9:z:450:VAL:HG21 | 1.94                     | 0.49              |
| 5:E:248:ILE:HG23 | 5:E:301:ILE:HD13 | 1.93                     | 0.49              |
| 6:G:520:ASP:OD1  | 6:G:521:ASP:N    | 2.43                     | 0.49              |
| 8:Q:191:PHE:HB2  | 8:Q:197:PHE:HD1  | 1.77                     | 0.49              |
| 3:b:79:PRO:HB2   | 5:e:60:MET:SD    | 2.53                     | 0.49              |
| 7:h:73:HIS:HB3   | 7:h:76:ALA:HB3   | 1.95                     | 0.49              |
| 7:h:152:ARG:NH1  | 7:h:184:MET:SD   | 2.85                     | 0.49              |
| 7:H:97:VAL:HG12  | 7:H:502:ALA:HA   | 1.95                     | 0.49              |
| 11:Q:601:ADP:O2B | 13:Q:603:AF3:F2  | 2.20                     | 0.49              |
| 2:a:47:ASP:HB2   | 2:a:51:ASP:HB2   | 1.94                     | 0.49              |
| 3:B:113:ALA:HB2  | 3:B:130:TRP:CH2  | 2.46                     | 0.49              |
| 3:B:326:VAL:HG13 | 3:B:327:THR:HG23 | 1.94                     | 0.49              |
| 4:D:144:GLY:HA2  | 4:D:432:LEU:HD11 | 1.95                     | 0.49              |
| 2:a:321:LYS:NZ   | 10:P:297:ASP:O   | 2.41                     | 0.49              |
| 3:b:255:ARG:HD3  | 5:e:265:LYS:HD2  | 1.94                     | 0.49              |
| 4:d:48:ILE:HG13  | 4:d:48:ILE:O     | 2.12                     | 0.49              |
| 1:N:244:ASP:OD2  | 1:N:289:TYR:N    | 2.40                     | 0.49              |
| 9:Z:166:ASP:O    | 9:Z:169:THR:OG1  | 2.30                     | 0.49              |
| 9:Z:179:ILE:HD13 | 9:Z:191:ILE:HG13 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:a:164:ASN:HB3  | 2:a:168:PHE:CD2   | 2.48                     | 0.49              |
| 2:a:397:CYS:O    | 2:a:401:ARG:HG2   | 2.12                     | 0.49              |
| 3:b:271:GLU:HG2  | 5:e:274:TYR:CZ    | 2.48                     | 0.49              |
| 4:d:62:GLN:HG3   | 4:d:68:VAL:HG22   | 1.94                     | 0.49              |
| 8:q:277:ASP:HB2  | 8:q:304:TYR:CZ    | 2.48                     | 0.49              |
| 9:z:200:SER:OG   | 9:z:203:ASP:OD2   | 2.28                     | 0.49              |
| 2:A:289:THR:HG23 | 2:A:316:LEU:HD22  | 1.95                     | 0.48              |
| 7:H:73:HIS:HB3   | 7:H:76:ALA:HB3    | 1.95                     | 0.48              |
| 2:a:220:VAL:HB   | 2:a:225:MET:HE3   | 1.94                     | 0.48              |
| 3:b:326:VAL:HG13 | 3:b:327:THR:HG23  | 1.95                     | 0.48              |
| 3:b:517:VAL:HG11 | 5:e:60:MET:HE3    | 1.94                     | 0.48              |
| 4:d:194:VAL:HG23 | 4:d:195:ILE:HG23  | 1.95                     | 0.48              |
| 3:B:414:GLU:HG2  | 3:B:446:LEU:HD23  | 1.96                     | 0.48              |
| 6:G:182:MET:HE1  | 6:G:216:ARG:HD2   | 1.96                     | 0.48              |
| 4:d:367:LEU:HD11 | 4:d:373:LEU:HG    | 1.93                     | 0.48              |
| 6:g:43:PRO:HA    | 6:g:162:THR:HA    | 1.94                     | 0.48              |
| 10:P:56:ASN:O    | 10:P:59:PRO:HD2   | 2.14                     | 0.48              |
| 4:D:490:THR:OG1  | 4:D:502:ASN:OD1   | 2.30                     | 0.48              |
| 7:H:413:GLU:OE1  | 7:H:445:ILE:HB    | 2.14                     | 0.48              |
| 2:a:164:ASN:HB3  | 2:a:168:PHE:HD2   | 1.78                     | 0.48              |
| 5:e:77:ILE:O     | 5:e:81:MET:HG3    | 2.13                     | 0.48              |
| 5:e:386:PHE:CE2  | 5:e:388:ARG:HD3   | 2.48                     | 0.48              |
| 8:q:169:MET:SD   | 11:q:601:ADP:N6   | 2.77                     | 0.48              |
| 2:A:331:LEU:O    | 2:A:338:GLU:HG3   | 2.14                     | 0.48              |
| 6:g:243:SER:OG   | 6:g:333:SER:O     | 2.29                     | 0.48              |
| 11:H:601:ADP:O1B | 13:H:603:AF3:F1   | 2.22                     | 0.48              |
| 3:b:151:ASP:HB3  | 3:b:154:LYS:HB2   | 1.94                     | 0.48              |
| 5:e:248:ILE:HD12 | 5:e:299:LEU:HD23  | 1.96                     | 0.48              |
| 7:h:427:ILE:HD11 | 7:h:432:GLN:HA    | 1.96                     | 0.48              |
| 1:N:289:TYR:CE2  | 1:N:293:GLY:HA2   | 2.48                     | 0.48              |
| 2:A:192:VAL:HG21 | 2:A:400:LYS:HB2   | 1.96                     | 0.48              |
| 7:H:136:ILE:HD11 | 7:H:416:LEU:HD11  | 1.96                     | 0.48              |
| 9:Z:175:SER:HB3  | 9:Z:206:LEU:HD13  | 1.95                     | 0.48              |
| 3:b:20:ARG:HD2   | 3:b:20:ARG:HA     | 1.68                     | 0.48              |
| 5:e:53:GLY:H     | 11:e:601:ADP:H5'1 | 1.79                     | 0.48              |
| 9:Z:103:LEU:HD21 | 9:Z:515:ILE:HG21  | 1.96                     | 0.48              |
| 2:a:266:ARG:NH1  | 4:d:273:ASP:OD2   | 2.47                     | 0.48              |
| 3:b:52:LEU:HB2   | 3:b:62:MET:HB3    | 1.94                     | 0.48              |
| 7:H:197:ILE:HD13 | 7:H:372:PHE:HB2   | 1.96                     | 0.48              |
| 9:Z:44:MET:HE1   | 9:Z:58:LYS:HD2    | 1.94                     | 0.48              |
| 9:Z:97:LEU:HD13  | 9:Z:450:VAL:HG21  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:g:319:ASP:OD1  | 6:g:322:ARG:NH1  | 2.47                     | 0.48              |
| 9:z:179:ILE:HD13 | 9:z:191:ILE:HG13 | 1.96                     | 0.48              |
| 11:D:601:ADP:O2B | 13:D:603:AF3:F1  | 2.21                     | 0.48              |
| 8:Q:410:PRO:O    | 8:Q:415:THR:OG1  | 2.23                     | 0.48              |
| 9:Z:134:LEU:HA   | 9:Z:137:VAL:HG12 | 1.96                     | 0.48              |
| 9:Z:480:ASP:HB2  | 9:Z:487:MET:HG2  | 1.95                     | 0.48              |
| 6:g:20:ARG:HG2   | 6:g:20:ARG:HH11  | 1.79                     | 0.48              |
| 8:q:86:ILE:HG22  | 8:q:105:LEU:HD12 | 1.96                     | 0.48              |
| 2:A:219:VAL:HA   | 2:A:353:GLN:HE22 | 1.78                     | 0.47              |
| 4:D:248:LEU:HD21 | 4:D:333:ILE:HG23 | 1.96                     | 0.47              |
| 2:a:192:VAL:HG12 | 2:a:193:ASN:H    | 1.79                     | 0.47              |
| 6:g:79:SER:O     | 6:g:83:ILE:HG12  | 2.14                     | 0.47              |
| 6:g:258:ILE:HG23 | 6:g:263:ASP:HB2  | 1.95                     | 0.47              |
| 7:h:145:LYS:NZ   | 7:h:150:GLU:HB2  | 2.29                     | 0.47              |
| 5:e:210:LYS:HB3  | 5:e:384:THR:HG23 | 1.96                     | 0.47              |
| 5:E:157:VAL:HG12 | 5:E:157:VAL:O    | 2.13                     | 0.47              |
| 7:h:66:LEU:HD11  | 7:h:98:THR:HG21  | 1.96                     | 0.47              |
| 11:h:601:ADP:O3B | 13:h:603:AF3:F3  | 2.22                     | 0.47              |
| 8:Q:400:LYS:O    | 8:Q:403:THR:OG1  | 2.24                     | 0.47              |
| 6:g:67:LEU:HB3   | 6:g:81:ILE:HD12  | 1.95                     | 0.47              |
| 10:P:186:HIS:CE1 | 10:P:188:TYR:HB3 | 2.49                     | 0.47              |
| 5:E:145:ILE:HG23 | 5:E:514:LYS:HD2  | 1.95                     | 0.47              |
| 5:E:242:LYS:NZ   | 5:E:244:GLU:OE2  | 2.43                     | 0.47              |
| 7:H:448:GLN:NE2  | 7:H:452:ASN:OD1  | 2.47                     | 0.47              |
| 8:q:324:LEU:HA   | 8:q:327:THR:HG22 | 1.97                     | 0.47              |
| 9:z:166:ASP:O    | 9:z:169:THR:OG1  | 2.32                     | 0.47              |
| 6:g:521:ASP:OD2  | 6:g:522:ILE:N    | 2.48                     | 0.47              |
| 10:P:60:LYS:HA   | 10:P:63:ILE:HG12 | 1.96                     | 0.47              |
| 1:N:314:ARG:NH2  | 7:H:221:SER:O    | 2.47                     | 0.47              |
| 6:G:157:ASN:O    | 6:G:161:THR:HG23 | 2.15                     | 0.47              |
| 7:H:303:PHE:HD2  | 7:H:310:CYS:HB3  | 1.79                     | 0.47              |
| 7:H:516:VAL:HG11 | 8:Q:55:MET:HE2   | 1.96                     | 0.47              |
| 8:Q:220:GLY:O    | 8:Q:374:THR:OG1  | 2.25                     | 0.47              |
| 2:a:353:GLN:NE2  | 2:a:360:GLU:OE1  | 2.33                     | 0.47              |
| 3:b:323:LEU:O    | 3:b:327:THR:OG1  | 2.25                     | 0.47              |
| 9:z:278:LYS:HA   | 9:z:289:PHE:CE2  | 2.50                     | 0.47              |
| 2:A:294:ASP:O    | 2:A:298:LYS:HG2  | 2.15                     | 0.47              |
| 11:A:601:ADP:O2B | 13:A:603:AF3:F3  | 2.23                     | 0.47              |
| 5:E:10:ASP:OD2   | 7:H:24:SER:OG    | 2.33                     | 0.47              |
| 4:d:513:LEU:HD23 | 4:d:513:LEU:O    | 2.14                     | 0.47              |
| 6:g:447:ILE:HB   | 6:g:448:PRO:HD3  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:h:92:ASP:HB3   | 7:h:395:ILE:HD11 | 1.96                     | 0.47              |
| 1:N:219:CYS:HB2  | 1:N:233:PHE:HB2  | 1.97                     | 0.47              |
| 2:A:254:ILE:HD11 | 2:A:263:ILE:HD12 | 1.96                     | 0.47              |
| 3:B:20:ARG:HD2   | 3:B:20:ARG:HA    | 1.69                     | 0.47              |
| 4:D:227:LEU:HB2  | 4:D:339:THR:HG21 | 1.96                     | 0.47              |
| 5:E:35:LYS:NZ    | 5:E:125:ASP:OD1  | 2.46                     | 0.47              |
| 8:Q:11:PHE:CE1   | 9:Z:69:ILE:HD11  | 2.50                     | 0.47              |
| 2:a:51:ASP:OD2   | 6:g:528:LYS:NZ   | 2.46                     | 0.47              |
| 2:a:263:ILE:HG23 | 4:d:272:MET:HE1  | 1.97                     | 0.47              |
| 2:A:359:ASP:OD2  | 2:A:360:GLU:N    | 2.48                     | 0.47              |
| 9:Z:159:LYS:HA   | 9:Z:159:LYS:HD3  | 1.58                     | 0.47              |
| 9:z:196:MET:HE2  | 9:z:375:LEU:HD21 | 1.97                     | 0.47              |
| 9:z:449:LYS:HB3  | 9:z:459:LEU:HD11 | 1.97                     | 0.47              |
| 9:z:487:MET:HE2  | 9:z:492:VAL:HG21 | 1.97                     | 0.47              |
| 3:B:214:LEU:HD11 | 3:B:371:CYS:HB3  | 1.98                     | 0.46              |
| 4:D:249:ILE:HD12 | 4:D:251:PHE:CE1  | 2.50                     | 0.46              |
| 5:E:119:GLU:HB3  | 5:E:450:ALA:HB1  | 1.97                     | 0.46              |
| 7:H:145:LYS:HZ2  | 7:H:150:GLU:HB2  | 1.79                     | 0.46              |
| 3:b:113:ALA:HB2  | 3:b:130:TRP:CH2  | 2.49                     | 0.46              |
| 6:G:232:TYR:HD2  | 6:G:351:GLU:HG3  | 1.79                     | 0.46              |
| 2:a:197:ILE:HD12 | 2:a:392:LEU:HD23 | 1.96                     | 0.46              |
| 1:N:233:PHE:HD2  | 1:N:266:TRP:CE3  | 2.33                     | 0.46              |
| 3:B:187:VAL:HG21 | 3:B:397:LEU:HB2  | 1.98                     | 0.46              |
| 3:B:521:ILE:HB   | 5:E:61:MET:SD    | 2.55                     | 0.46              |
| 5:E:251:LEU:HD23 | 5:E:342:VAL:HB   | 1.97                     | 0.46              |
| 5:e:229:ILE:HD12 | 5:e:373:VAL:HG22 | 1.96                     | 0.46              |
| 8:q:101:THR:N    | 13:q:603:AF3:F1  | 2.31                     | 0.46              |
| 6:G:79:SER:O     | 6:G:83:ILE:HG23  | 2.15                     | 0.46              |
| 6:G:502:LYS:HA   | 6:G:502:LYS:HD2  | 1.76                     | 0.46              |
| 7:H:34:GLU:HA    | 7:H:37:ARG:HG3   | 1.97                     | 0.46              |
| 4:d:439:TYR:O    | 4:d:442:THR:OG1  | 2.24                     | 0.46              |
| 7:H:23:VAL:HG13  | 7:H:109:LYS:HE2  | 1.98                     | 0.46              |
| 9:Z:399:LYS:NZ   | 9:Z:403:ASP:OD2  | 2.49                     | 0.46              |
| 7:h:34:GLU:HA    | 7:h:37:ARG:HG3   | 1.98                     | 0.46              |
| 8:q:131:GLY:HA3  | 8:q:437:ALA:HB3  | 1.97                     | 0.46              |
| 2:A:238:ASP:HB3  | 2:A:329:SER:HA   | 1.97                     | 0.46              |
| 7:H:273:ILE:HD11 | 8:Q:266:MET:HA   | 1.97                     | 0.46              |
| 2:a:27:SER:O     | 2:a:31:ILE:HG12  | 2.16                     | 0.46              |
| 2:A:227:LYS:HB3  | 2:A:353:GLN:HB3  | 1.97                     | 0.46              |
| 4:D:69:THR:HG21  | 4:D:80:GLN:HG3   | 1.98                     | 0.46              |
| 4:D:73:ASP:OD1   | 13:D:603:AF3:F3  | 2.23                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:52:LEU:O     | 5:E:465:ASN:ND2  | 2.41                     | 0.46              |
| 5:e:63:ASP:OD1   | 5:e:67:ASP:N     | 2.49                     | 0.46              |
| 8:q:26:GLU:HA    | 8:q:30:TYR:CD2   | 2.51                     | 0.46              |
| 2:A:216:LEU:HB2  | 2:A:362:ILE:HB   | 1.97                     | 0.46              |
| 2:a:28:ILE:HG13  | 2:a:72:ALA:HB1   | 1.98                     | 0.46              |
| 6:g:133:MET:HE2  | 6:g:506:TYR:CD1  | 2.50                     | 0.46              |
| 7:h:97:VAL:HG12  | 7:h:502:ALA:HA   | 1.98                     | 0.46              |
| 8:q:73:LEU:HD13  | 8:q:87:VAL:HG22  | 1.98                     | 0.46              |
| 1:N:251:GLY:HA2  | 1:N:268:MET:HE3  | 1.98                     | 0.46              |
| 3:B:6:LEU:HD23   | 4:d:32:GLN:HB3   | 1.98                     | 0.46              |
| 3:B:204:LYS:NZ   | 3:B:357:ASP:OD2  | 2.37                     | 0.46              |
| 5:E:255:PHE:HB2  | 5:E:306:PHE:CB   | 2.46                     | 0.46              |
| 6:G:129:ALA:O    | 6:G:133:MET:HG3  | 2.14                     | 0.46              |
| 7:H:221:SER:HB2  | 7:H:225:PHE:CG   | 2.51                     | 0.46              |
| 8:Q:247:ASP:OD1  | 8:Q:248:GLY:N    | 2.48                     | 0.46              |
| 9:Z:487:MET:HE1  | 9:Z:492:VAL:HG21 | 1.97                     | 0.46              |
| 5:e:97:SER:HB3   | 7:h:202:GLY:HA2  | 1.96                     | 0.46              |
| 5:e:289:ILE:HG13 | 5:e:313:LEU:HB3  | 1.97                     | 0.46              |
| 8:q:259:ILE:HG21 | 8:q:265:LEU:HB2  | 1.98                     | 0.46              |
| 3:B:407:VAL:HG13 | 3:B:497:PHE:HB2  | 1.98                     | 0.46              |
| 1:N:311:ARG:HG2  | 5:E:304:TRP:CZ2  | 2.43                     | 0.45              |
| 4:D:86:PRO:O     | 4:D:90:MET:HG3   | 2.16                     | 0.45              |
| 2:a:138:VAL:HG21 | 2:a:499:LYS:HD2  | 1.97                     | 0.45              |
| 2:a:228:ARG:HG3  | 2:a:352:VAL:HG22 | 1.97                     | 0.45              |
| 2:a:349:GLU:HB2  | 2:a:366:ASN:HB2  | 1.97                     | 0.45              |
| 2:a:411:GLY:O    | 2:a:498:ASN:ND2  | 2.41                     | 0.45              |
| 4:d:415:LEU:HD13 | 4:d:511:PRO:HB3  | 1.98                     | 0.45              |
| 6:g:226:HIS:ND1  | 6:g:305:MET:SD   | 2.89                     | 0.45              |
| 6:g:411:GLY:N    | 11:g:601:ADP:O2' | 2.44                     | 0.45              |
| 7:h:202:GLY:O    | 7:h:375:ARG:NH2  | 2.49                     | 0.45              |
| 9:z:175:SER:HB3  | 9:z:206:LEU:HD13 | 1.98                     | 0.45              |
| 7:H:193:LYS:HG3  | 7:H:194:MET:HE2  | 1.98                     | 0.45              |
| 8:Q:93:GLN:NE2   | 8:Q:99:ASP:O     | 2.46                     | 0.45              |
| 5:e:464:GLU:HB2  | 5:e:470:PRO:HG3  | 1.98                     | 0.45              |
| 6:g:157:ASN:O    | 6:g:161:THR:HG23 | 2.16                     | 0.45              |
| 9:z:190:MET:O    | 9:z:371:SER:OG   | 2.34                     | 0.45              |
| 3:B:245:ASP:HB2  | 3:B:297:TYR:CZ   | 2.51                     | 0.45              |
| 8:Q:82:ALA:O     | 8:Q:86:ILE:HG12  | 2.17                     | 0.45              |
| 8:q:156:ASP:OD1  | 8:q:157:ILE:N    | 2.49                     | 0.45              |
| 10:P:56:ASN:HD22 | 10:P:57:THR:HG22 | 1.82                     | 0.45              |
| 4:D:48:ILE:HD11  | 4:D:110:VAL:HB   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:e:10:ASP:OD2   | 7:h:24:SER:OG     | 2.29                     | 0.45              |
| 7:h:516:VAL:HG21 | 8:q:55:MET:HE3    | 1.99                     | 0.45              |
| 8:q:412:GLY:HA3  | 8:q:492:MET:HE3   | 1.98                     | 0.45              |
| 7:H:384:GLU:OE1  | 7:H:387:ARG:NH1   | 2.43                     | 0.45              |
| 2:a:82:GLN:NE2   | 2:a:88:ASP:O      | 2.49                     | 0.45              |
| 3:b:50:LYS:HD3   | 4:d:534:ASP:HB3   | 1.97                     | 0.45              |
| 5:e:306:PHE:CE1  | 5:e:323:ARG:HB3   | 2.51                     | 0.45              |
| 1:N:217:GLY:O    | 1:N:234:HIS:ND1   | 2.48                     | 0.45              |
| 8:Q:238:LYS:HB2  | 8:Q:288:ALA:HA    | 1.98                     | 0.45              |
| 8:Q:440:LYS:HA   | 8:Q:440:LYS:HD3   | 1.74                     | 0.45              |
| 3:b:79:PRO:O     | 3:b:83:VAL:HG23   | 2.16                     | 0.45              |
| 4:d:48:ILE:HD11  | 4:d:110:VAL:HG11  | 1.98                     | 0.45              |
| 6:g:293:GLU:HG3  | 6:g:320:ASN:HD22  | 1.82                     | 0.45              |
| 7:h:187:ASP:OD1  | 7:h:187:ASP:N     | 2.44                     | 0.45              |
| 2:A:204:SER:OG   | 2:A:205:GLN:N     | 2.49                     | 0.45              |
| 3:B:293:ARG:HA   | 3:B:315:ALA:O     | 2.16                     | 0.45              |
| 5:E:123:LEU:HD22 | 5:E:128:ILE:HD12  | 1.97                     | 0.45              |
| 8:Q:38:GLU:O     | 8:Q:42:THR:HG23   | 2.16                     | 0.45              |
| 8:Q:154:LEU:HD13 | 8:Q:403:THR:HG22  | 1.99                     | 0.45              |
| 2:a:120:GLY:HA3  | 2:a:437:ALA:HB3   | 1.98                     | 0.45              |
| 3:b:187:VAL:HG21 | 3:b:397:LEU:HB2   | 1.99                     | 0.45              |
| 4:d:534:ASP:OD1  | 4:d:535:VAL:N     | 2.50                     | 0.45              |
| 6:g:278:LEU:HD22 | 6:g:335:PRO:HG2   | 1.97                     | 0.45              |
| 8:q:505:TYR:OH   | 8:q:509:LYS:NZ    | 2.39                     | 0.45              |
| 4:D:42:LYS:NZ    | 5:e:125:ASP:OD2   | 2.40                     | 0.45              |
| 4:D:266:VAL:HG13 | 4:D:271:GLN:HB2   | 1.98                     | 0.45              |
| 4:D:503:ILE:HG13 | 4:D:508:VAL:HB    | 1.98                     | 0.45              |
| 5:E:94:LEU:HD13  | 5:E:523:MET:HG3   | 1.99                     | 0.45              |
| 3:b:45:PRO:HG3   | 11:b:601:ADP:C5   | 2.52                     | 0.45              |
| 2:A:508:ILE:HD11 | 2:A:512:LYS:HE3   | 1.98                     | 0.45              |
| 8:Q:402:LEU:HD21 | 8:Q:408:LEU:HD21  | 1.98                     | 0.45              |
| 5:E:196:VAL:HG13 | 5:E:196:VAL:O     | 2.17                     | 0.45              |
| 9:z:376:ILE:HG22 | 9:z:384:LEU:HD22  | 1.99                     | 0.45              |
| 2:A:86:VAL:HG12  | 2:A:88:ASP:H      | 1.82                     | 0.44              |
| 2:A:127:GLU:HG3  | 2:A:426:TYR:CE2   | 2.52                     | 0.44              |
| 4:D:218:ILE:HD11 | 4:D:397:VAL:HG22  | 1.99                     | 0.44              |
| 6:G:249:LYS:NZ   | 9:Z:243:GLU:O     | 2.41                     | 0.44              |
| 8:q:524:ILE:HG23 | 9:z:46:MET:HE3    | 1.99                     | 0.44              |
| 9:z:195:GLU:HB3  | 9:z:384:LEU:HD13  | 1.99                     | 0.44              |
| 10:P:170:PHE:HE1 | 10:P:185:VAL:HG11 | 1.81                     | 0.44              |
| 9:Z:130:ALA:HB1  | 9:Z:418:MET:SD    | 2.57                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:220:VAL:HB   | 2:A:225:MET:HE3   | 1.98                     | 0.44              |
| 2:a:529:ASP:OD1  | 2:a:530:LEU:N     | 2.50                     | 0.44              |
| 4:d:38:ILE:HG12  | 4:d:117:LEU:HB3   | 1.99                     | 0.44              |
| 4:d:91:LEU:HD23  | 4:d:110:VAL:HG13  | 1.99                     | 0.44              |
| 4:d:421:LEU:HD21 | 4:d:509:VAL:HG21  | 1.98                     | 0.44              |
| 9:z:33:VAL:HG12  | 9:z:34:LEU:HD12   | 1.98                     | 0.44              |
| 2:A:36:LEU:O     | 2:A:455:ASN:ND2   | 2.45                     | 0.44              |
| 4:D:399:GLU:O    | 4:D:402:GLU:HG3   | 2.18                     | 0.44              |
| 6:G:225:THR:HG22 | 6:G:313:ARG:HB2   | 1.99                     | 0.44              |
| 6:G:418:VAL:O    | 6:G:422:LEU:HD23  | 2.17                     | 0.44              |
| 8:Q:218:LEU:HD21 | 8:Q:362:VAL:HG13  | 1.98                     | 0.44              |
| 4:d:467:GLU:HG3  | 4:d:468:ASN:N     | 2.32                     | 0.44              |
| 6:g:182:MET:SD   | 6:g:372:CYS:HB3   | 2.58                     | 0.44              |
| 6:G:462:LEU:HD23 | 6:G:462:LEU:HA    | 1.87                     | 0.44              |
| 8:Q:470:VAL:HG11 | 8:Q:478:VAL:HG11  | 1.99                     | 0.44              |
| 9:Z:172:VAL:HG13 | 9:Z:395:LEU:HD23  | 1.98                     | 0.44              |
| 3:B:11:ILE:O     | 3:B:12:PHE:CD1    | 2.71                     | 0.44              |
| 7:H:200:VAL:HG11 | 7:H:353:ILE:HG22  | 1.98                     | 0.44              |
| 9:Z:455:SER:OG   | 9:Z:481:LEU:O     | 2.32                     | 0.44              |
| 3:b:214:LEU:HD11 | 3:b:371:CYS:HB3   | 2.00                     | 0.44              |
| 3:b:249:ILE:HG21 | 5:e:277:LEU:HG    | 1.98                     | 0.44              |
| 5:e:62:VAL:HG22  | 5:e:68:VAL:HG22   | 2.00                     | 0.44              |
| 10:P:154:LYS:HE3 | 10:P:282:LEU:HD21 | 1.98                     | 0.44              |
| 3:B:231:ARG:NH1  | 3:B:233:GLU:OE2   | 2.44                     | 0.44              |
| 5:e:530:ILE:HD11 | 7:h:58:ILE:HD13   | 2.00                     | 0.44              |
| 9:z:80:VAL:HG12  | 9:z:95:ASN:HD21   | 1.82                     | 0.44              |
| 3:B:167:LEU:HD22 | 3:B:172:LEU:HD12  | 2.00                     | 0.44              |
| 8:Q:155:ARG:HH21 | 8:Q:193:ASP:HA    | 1.83                     | 0.44              |
| 3:b:509:GLU:O    | 3:b:513:VAL:HG13  | 2.18                     | 0.44              |
| 6:g:246:GLU:HB3  | 6:g:297:SER:HB2   | 2.00                     | 0.44              |
| 8:q:393:ASP:O    | 8:q:397:ASN:ND2   | 2.51                     | 0.44              |
| 1:N:238:ALA:N    | 1:N:260:ASP:OD1   | 2.51                     | 0.44              |
| 2:A:313:LYS:HE2  | 2:A:317:LYS:HE3   | 1.99                     | 0.44              |
| 6:G:67:LEU:HB3   | 6:G:81:ILE:HD12   | 2.00                     | 0.44              |
| 2:a:302:GLU:OE1  | 6:g:339:ARG:NH2   | 2.42                     | 0.44              |
| 5:e:78:LEU:HD23  | 5:e:81:MET:SD     | 2.58                     | 0.44              |
| 5:e:248:ILE:N    | 5:e:354:GLY:O     | 2.47                     | 0.44              |
| 10:P:285:VAL:O   | 10:P:286:ARG:HD3  | 2.18                     | 0.44              |
| 5:E:533:ILE:HD13 | 7:H:48:LEU:HB3    | 2.00                     | 0.43              |
| 10:P:146:GLU:HA  | 10:P:149:ARG:HG2  | 1.99                     | 0.43              |
| 2:A:11:ARG:O     | 5:e:2:ALA:N       | 2.51                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:G:43:PRO:HA    | 6:G:162:THR:HA    | 1.99                     | 0.43              |
| 7:H:287:LYS:HA   | 7:H:287:LYS:HD2   | 1.85                     | 0.43              |
| 8:Q:136:CYS:HB2  | 8:Q:512:THR:HG21  | 2.00                     | 0.43              |
| 2:a:179:ILE:HD13 | 2:a:195:VAL:HG23  | 2.01                     | 0.43              |
| 5:e:242:LYS:NZ   | 5:e:244:GLU:OE2   | 2.38                     | 0.43              |
| 7:h:232:TYR:HD2  | 7:h:348:PHE:HD2   | 1.66                     | 0.43              |
| 10:P:232:ALA:HA  | 10:P:250:ARG:HH12 | 1.83                     | 0.43              |
| 2:A:44:MET:HB2   | 6:G:522:ILE:HG12  | 1.99                     | 0.43              |
| 6:G:137:LEU:HD23 | 6:G:137:LEU:HA    | 1.85                     | 0.43              |
| 7:H:60:ASN:ND2   | 7:H:165:SER:O     | 2.51                     | 0.43              |
| 7:H:67:LYS:HG2   | 7:H:84:LYS:HE3    | 2.00                     | 0.43              |
| 8:Q:81:PRO:HB2   | 9:Z:46:MET:CE     | 2.49                     | 0.43              |
| 7:h:326:CYS:HB3  | 7:h:344:ARG:H     | 1.84                     | 0.43              |
| 7:h:499:ARG:HA   | 7:h:499:ARG:HD3   | 1.74                     | 0.43              |
| 6:G:391:LEU:HD23 | 6:G:391:LEU:HA    | 1.89                     | 0.43              |
| 9:Z:210:LEU:HD21 | 9:Z:323:ARG:HB3   | 2.01                     | 0.43              |
| 4:d:429:GLU:HG2  | 4:d:461:ILE:HB    | 2.00                     | 0.43              |
| 5:e:284:LYS:HD2  | 5:e:284:LYS:HA    | 1.75                     | 0.43              |
| 6:g:266:ARG:HA   | 6:g:266:ARG:HD2   | 1.71                     | 0.43              |
| 7:h:280:LYS:NZ   | 7:h:335:ASN:OD1   | 2.46                     | 0.43              |
| 7:h:427:ILE:HD12 | 7:h:431:GLN:HB2   | 2.01                     | 0.43              |
| 3:B:90:VAL:HG21  | 5:E:391:ASN:HA    | 2.01                     | 0.43              |
| 3:B:242:THR:HG21 | 3:B:335:PHE:CE2   | 2.53                     | 0.43              |
| 4:D:345:VAL:HG22 | 4:D:355:MET:SD    | 2.58                     | 0.43              |
| 6:G:266:ARG:HE   | 6:G:270:MET:HG3   | 1.83                     | 0.43              |
| 6:G:319:ASP:OD1  | 6:G:322:ARG:NH1   | 2.52                     | 0.43              |
| 8:Q:101:THR:N    | 13:Q:603:AF3:F1   | 2.31                     | 0.43              |
| 3:b:131:ARG:NH2  | 3:b:512:GLU:OE2   | 2.45                     | 0.43              |
| 7:h:467:ARG:NH1  | 7:h:471:GLY:O     | 2.51                     | 0.43              |
| 8:q:191:PHE:HB2  | 8:q:197:PHE:HD1   | 1.83                     | 0.43              |
| 8:Q:117:GLU:O    | 8:Q:121:ILE:HG23  | 2.19                     | 0.43              |
| 9:Z:155:SER:O    | 9:Z:158:THR:OG1   | 2.30                     | 0.43              |
| 2:a:44:MET:SD    | 6:g:75:PRO:HB2    | 2.58                     | 0.43              |
| 2:a:57:ASP:OD1   | 13:a:603:AF3:F2   | 2.25                     | 0.43              |
| 4:d:116:LEU:O    | 4:d:119:SER:OG    | 2.36                     | 0.43              |
| 7:h:292:LYS:HG3  | 7:h:319:LEU:CD1   | 2.47                     | 0.43              |
| 8:q:207:ILE:O    | 8:q:378:ARG:HA    | 2.18                     | 0.43              |
| 8:q:218:LEU:HD21 | 8:q:362:VAL:HG13  | 2.00                     | 0.43              |
| 8:q:283:ILE:O    | 8:q:286:THR:OG1   | 2.36                     | 0.43              |
| 8:q:533:PRO:HB2  | 8:q:534:LYS:HD2   | 1.99                     | 0.43              |
| 9:z:370:ARG:HA   | 9:z:370:ARG:HD3   | 1.81                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:P:192:ILE:HD12 | 10:P:233:LEU:HD13 | 2.01                     | 0.43              |
| 2:A:184:ILE:O     | 2:A:185:ARG:HG2   | 2.19                     | 0.43              |
| 6:G:91:VAL:O      | 6:G:400:ASN:ND2   | 2.47                     | 0.43              |
| 6:g:144:VAL:HG21  | 6:g:407:LEU:HG    | 2.01                     | 0.43              |
| 9:z:244:VAL:HG12  | 9:z:244:VAL:O     | 2.18                     | 0.43              |
| 10:P:56:ASN:ND2   | 10:P:57:THR:HG22  | 2.34                     | 0.43              |
| 1:N:176:LEU:HD23  | 1:N:176:LEU:H     | 1.83                     | 0.43              |
| 2:A:127:GLU:HG3   | 2:A:426:TYR:CZ    | 2.54                     | 0.43              |
| 3:b:417:MET:HE2   | 3:b:504:LEU:HD22  | 2.01                     | 0.43              |
| 4:d:85:HIS:CD2    | 10:P:60:LYS:HE3   | 2.54                     | 0.43              |
| 5:e:109:VAL:HG13  | 5:e:516:GLN:HG2   | 2.01                     | 0.43              |
| 5:e:196:VAL:HG12  | 5:e:381:ARG:O     | 2.18                     | 0.43              |
| 5:e:385:ILE:HG21  | 5:e:402:LEU:HD13  | 2.00                     | 0.43              |
| 3:B:323:LEU:O     | 3:B:327:THR:OG1   | 2.32                     | 0.43              |
| 2:a:103:ASN:OD1   | 2:a:443:ARG:NH2   | 2.52                     | 0.43              |
| 4:d:511:PRO:HG2   | 4:d:514:VAL:HG23  | 2.01                     | 0.43              |
| 9:z:134:LEU:HA    | 9:z:137:VAL:HG12  | 2.00                     | 0.43              |
| 10:P:251:VAL:HB   | 10:P:255:LEU:HD12 | 2.00                     | 0.43              |
| 2:A:82:GLN:NE2    | 2:A:88:ASP:O      | 2.50                     | 0.43              |
| 4:D:249:ILE:HD13  | 4:D:249:ILE:HA    | 1.90                     | 0.43              |
| 8:Q:76:LEU:HD23   | 8:Q:76:LEU:HA     | 1.90                     | 0.43              |
| 9:Z:213:ASP:OD1   | 9:Z:213:ASP:N     | 2.51                     | 0.43              |
| 4:d:53:GLY:H      | 11:d:601:ADP:H5'1 | 1.83                     | 0.43              |
| 11:d:601:ADP:O2B  | 13:d:603:AF3:F3   | 2.27                     | 0.43              |
| 7:h:521:LYS:HG2   | 8:q:57:ILE:HD12   | 2.01                     | 0.43              |
| 1:N:218:THR:HG22  | 1:N:234:HIS:HB2   | 2.01                     | 0.42              |
| 6:G:108:VAL:HG11  | 6:G:443:ALA:HB2   | 2.01                     | 0.42              |
| 8:Q:151:ALA:O     | 8:Q:152:LYS:HG2   | 2.19                     | 0.42              |
| 3:b:68:ALA:HB2    | 3:b:99:THR:HG21   | 2.01                     | 0.42              |
| 5:e:223:LYS:HE3   | 5:e:225:ILE:HD11  | 2.01                     | 0.42              |
| 5:e:498:THR:O     | 5:e:504:GLN:NE2   | 2.52                     | 0.42              |
| 7:h:145:LYS:HE2   | 7:h:150:GLU:HB2   | 2.00                     | 0.42              |
| 9:z:165:ALA:O     | 9:z:169:THR:HG23  | 2.19                     | 0.42              |
| 1:N:177:THR:C     | 1:N:179:ASP:H     | 2.27                     | 0.42              |
| 2:a:514:LEU:HD23  | 2:a:514:LEU:HA    | 1.87                     | 0.42              |
| 2:a:519:GLU:OE1   | 4:d:393:SER:OG    | 2.31                     | 0.42              |
| 6:g:278:LEU:HD23  | 6:g:278:LEU:HA    | 1.90                     | 0.42              |
| 10:P:299:GLU:N    | 10:P:299:GLU:OE1  | 2.52                     | 0.42              |
| 3:B:45:PRO:HG3    | 11:B:601:ADP:C5   | 2.54                     | 0.42              |
| 5:E:193:VAL:HG21  | 5:E:409:ILE:HB    | 2.01                     | 0.42              |
| 6:G:223:ASP:OD1   | 6:G:231:ARG:NH1   | 2.53                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:H:187:ASP:N    | 7:H:187:ASP:OD1   | 2.43                     | 0.42              |
| 9:Z:211:VAL:HG23 | 9:Z:373:THR:HG21  | 2.01                     | 0.42              |
| 4:d:482:ASN:O    | 4:d:486:GLN:HG2   | 2.19                     | 0.42              |
| 6:g:98:VAL:HG21  | 6:g:508:THR:HB    | 2.00                     | 0.42              |
| 8:q:33:ILE:HD13  | 8:q:116:GLU:HB2   | 2.00                     | 0.42              |
| 4:D:415:LEU:HD23 | 4:D:415:LEU:HA    | 1.90                     | 0.42              |
| 7:H:121:ILE:HA   | 7:H:434:LEU:HD13  | 2.00                     | 0.42              |
| 8:Q:131:GLY:HA3  | 8:Q:437:ALA:HB3   | 2.00                     | 0.42              |
| 2:a:156:MET:HE1  | 2:a:169:ALA:N     | 2.34                     | 0.42              |
| 2:a:331:LEU:O    | 2:a:338:GLU:HG3   | 2.20                     | 0.42              |
| 3:b:257:ARG:HE   | 4:d:263:GLN:HE21  | 1.67                     | 0.42              |
| 5:e:403:HIS:HA   | 5:e:406:LEU:HD12  | 2.02                     | 0.42              |
| 2:A:233:LYS:HB2  | 2:A:283:ALA:HA    | 2.01                     | 0.42              |
| 3:B:495:GLU:OE1  | 3:B:500:LYS:HD3   | 2.20                     | 0.42              |
| 3:B:500:LYS:HD2  | 3:B:500:LYS:HA    | 1.81                     | 0.42              |
| 5:E:231:ASP:OD1  | 5:E:231:ASP:O     | 2.38                     | 0.42              |
| 11:G:601:ADP:O2B | 13:G:603:AF3:F2   | 2.28                     | 0.42              |
| 6:g:83:ILE:HG23  | 6:g:508:THR:HG22  | 2.01                     | 0.42              |
| 7:h:442:LEU:HD23 | 7:h:442:LEU:HA    | 1.84                     | 0.42              |
| 2:A:216:LEU:HD21 | 2:A:319:ILE:HD11  | 2.01                     | 0.42              |
| 5:E:295:THR:HG21 | 5:E:348:LEU:HG    | 2.01                     | 0.42              |
| 6:G:226:HIS:CD2  | 6:G:228:ARG:H     | 2.35                     | 0.42              |
| 2:a:37:GLY:H     | 11:a:601:ADP:H5'1 | 1.83                     | 0.42              |
| 2:a:86:VAL:HG12  | 2:a:88:ASP:H      | 1.83                     | 0.42              |
| 4:d:257:LYS:HB2  | 4:d:306:ARG:NH1   | 2.34                     | 0.42              |
| 6:g:407:LEU:HD23 | 6:g:407:LEU:HA    | 1.92                     | 0.42              |
| 2:A:160:ILE:HD13 | 2:A:384:MET:HG3   | 2.01                     | 0.42              |
| 4:D:291:LYS:HD3  | 4:D:322:ILE:HD11  | 2.02                     | 0.42              |
| 5:E:306:PHE:CE1  | 5:E:323:ARG:HB3   | 2.54                     | 0.42              |
| 6:G:51:LEU:HD21  | 9:Z:72:PRO:HG3    | 2.02                     | 0.42              |
| 6:G:483:GLU:HG3  | 6:G:484:THR:HG23  | 2.01                     | 0.42              |
| 8:Q:71:THR:HA    | 8:Q:74:ARG:HG2    | 2.01                     | 0.42              |
| 4:d:152:SER:HA   | 4:d:422:ILE:HG22  | 2.02                     | 0.42              |
| 2:A:171:MET:HE3  | 2:A:375:ILE:HD13  | 2.00                     | 0.42              |
| 2:A:506:PRO:HB2  | 2:A:509:VAL:HG23  | 2.02                     | 0.42              |
| 2:a:419:LEU:HD23 | 2:a:419:LEU:HA    | 1.89                     | 0.42              |
| 3:b:33:ILE:HD11  | 3:b:111:ARG:HB2   | 2.02                     | 0.42              |
| 3:b:50:LYS:CD    | 4:d:534:ASP:HB3   | 2.50                     | 0.42              |
| 7:h:18:GLY:O     | 7:h:21:GLN:HG3    | 2.20                     | 0.42              |
| 2:A:181:TYR:OH   | 2:A:189:ARG:NE    | 2.49                     | 0.42              |
| 4:D:301:GLN:NE2  | 4:D:330:ARG:HG2   | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:Z:237:LEU:HB2  | 9:Z:297:ILE:HG12 | 2.02                     | 0.42              |
| 6:g:45:SER:O     | 9:z:117:ARG:NH2  | 2.52                     | 0.42              |
| 1:N:187:LYS:NZ   | 4:D:303:SER:O    | 2.52                     | 0.42              |
| 1:N:248:SER:C    | 1:N:250:THR:H    | 2.28                     | 0.42              |
| 4:D:169:THR:HA   | 4:D:172:ASN:OD1  | 2.20                     | 0.42              |
| 4:D:435:ARG:HA   | 4:D:435:ARG:HD3  | 1.79                     | 0.42              |
| 7:H:94:THR:OG1   | 13:H:603:AF3:F3  | 2.24                     | 0.42              |
| 6:g:64:ASN:HB2   | 6:g:95:THR:HG21  | 2.02                     | 0.42              |
| 9:z:277:LEU:HD21 | 9:z:344:LEU:HD11 | 2.02                     | 0.42              |
| 2:A:499:LYS:HA   | 2:A:504:PHE:HE1  | 1.84                     | 0.41              |
| 6:G:384:LEU:HD23 | 6:G:384:LEU:HA   | 1.87                     | 0.41              |
| 7:H:246:LEU:HG   | 7:H:274:LEU:HD22 | 2.01                     | 0.41              |
| 7:H:446:PRO:HA   | 7:H:449:LEU:HD12 | 2.02                     | 0.41              |
| 8:Q:15:LEU:HG    | 8:Q:19:ALA:HB3   | 2.01                     | 0.41              |
| 8:q:470:VAL:HG11 | 8:q:478:VAL:HG11 | 2.02                     | 0.41              |
| 9:z:234:ASN:N    | 9:z:333:LEU:O    | 2.47                     | 0.41              |
| 6:G:165:ILE:HD12 | 6:G:387:VAL:HG13 | 2.01                     | 0.41              |
| 5:e:170:LYS:O    | 5:e:182:HIS:NE2  | 2.43                     | 0.41              |
| 5:e:179:ASN:O    | 5:e:182:HIS:HB2  | 2.20                     | 0.41              |
| 7:h:297:ASP:N    | 7:h:297:ASP:OD1  | 2.53                     | 0.41              |
| 2:A:22:VAL:HG22  | 2:A:101:LEU:HG   | 2.02                     | 0.41              |
| 2:A:402:VAL:HG23 | 2:A:506:PRO:HG3  | 2.02                     | 0.41              |
| 3:B:86:ASP:OD1   | 5:E:392:LYS:HE3  | 2.20                     | 0.41              |
| 3:B:263:LYS:O    | 3:B:267:ILE:HG12 | 2.21                     | 0.41              |
| 3:B:480:MET:HE2  | 3:B:480:MET:HA   | 2.02                     | 0.41              |
| 4:D:42:LYS:HZ3   | 4:D:46:ASP:CG    | 2.27                     | 0.41              |
| 5:E:284:LYS:HA   | 5:E:284:LYS:HD2  | 1.68                     | 0.41              |
| 5:E:441:PRO:O    | 5:E:445:GLN:HG3  | 2.20                     | 0.41              |
| 7:H:107:GLN:HG3  | 7:H:441:ALA:HB2  | 2.03                     | 0.41              |
| 4:d:459:GLU:OE2  | 4:d:481:ARG:NH2  | 2.51                     | 0.41              |
| 5:e:35:LYS:NZ    | 5:e:125:ASP:OD1  | 2.42                     | 0.41              |
| 6:g:201:VAL:HG11 | 6:g:388:GLU:HG3  | 2.02                     | 0.41              |
| 6:g:435:TRP:HB2  | 6:g:436:PRO:HD3  | 2.01                     | 0.41              |
| 2:A:31:ILE:O     | 2:A:43:LYS:HE3   | 2.21                     | 0.41              |
| 3:b:242:THR:HG21 | 3:b:335:PHE:CE2  | 2.55                     | 0.41              |
| 4:d:191:VAL:HG21 | 4:d:412:ILE:HB   | 2.03                     | 0.41              |
| 4:d:435:ARG:HD3  | 4:d:435:ARG:HA   | 1.83                     | 0.41              |
| 5:e:129:HIS:HB3  | 5:e:132:ARG:HG2  | 2.02                     | 0.41              |
| 5:e:375:GLU:HG3  | 5:e:376:GLN:HG3  | 2.02                     | 0.41              |
| 7:h:145:LYS:HZ1  | 7:h:150:GLU:HB2  | 1.86                     | 0.41              |
| 7:h:152:ARG:NH2  | 7:h:181:ASP:OD1  | 2.48                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:q:292:VAL:HG22 | 8:q:313:VAL:HB   | 2.02                     | 0.41              |
| 2:A:45:LEU:HD23  | 6:G:523:VAL:HB   | 2.02                     | 0.41              |
| 4:D:103:GLY:HA3  | 4:D:410:CYS:HB3  | 2.03                     | 0.41              |
| 5:E:123:LEU:HD23 | 5:E:123:LEU:HA   | 1.82                     | 0.41              |
| 6:G:256:ILE:HB   | 9:Z:246:SER:HA   | 2.02                     | 0.41              |
| 8:Q:73:LEU:HD11  | 8:Q:105:LEU:HD22 | 2.02                     | 0.41              |
| 9:Z:201:GLU:HA   | 9:Z:377:LYS:O    | 2.21                     | 0.41              |
| 4:d:246:ILE:HD13 | 4:d:376:ILE:HD13 | 2.02                     | 0.41              |
| 7:h:197:ILE:HG21 | 7:h:386:GLU:HG3  | 2.02                     | 0.41              |
| 7:h:259:THR:HG22 | 7:h:261:GLU:H    | 1.85                     | 0.41              |
| 7:H:442:LEU:HD23 | 7:H:442:LEU:HA   | 1.93                     | 0.41              |
| 9:Z:64:LEU:HA    | 9:Z:67:MET:HE3   | 2.02                     | 0.41              |
| 3:b:333:SER:H    | 5:e:312:HIS:CG   | 2.37                     | 0.41              |
| 6:g:415:GLU:OE2  | 6:g:502:LYS:NZ   | 2.49                     | 0.41              |
| 2:A:246:MET:SD   | 4:D:272:MET:HE2  | 2.60                     | 0.41              |
| 3:B:168:SER:OG   | 11:B:601:ADP:N7  | 2.50                     | 0.41              |
| 4:D:244:ALA:HA   | 4:D:296:ASN:HD21 | 1.85                     | 0.41              |
| 8:Q:191:PHE:HB2  | 8:Q:197:PHE:CD1  | 2.55                     | 0.41              |
| 9:Z:375:LEU:HD12 | 9:Z:375:LEU:HA   | 1.89                     | 0.41              |
| 4:d:94:LEU:HD13  | 4:d:525:THR:OG1  | 2.20                     | 0.41              |
| 7:h:107:GLN:HG3  | 7:h:441:ALA:HB2  | 2.01                     | 0.41              |
| 7:h:122:ILE:HD11 | 7:h:515:SER:HB3  | 2.03                     | 0.41              |
| 10:P:248:PHE:HZ  | 10:P:271:PHE:HD2 | 1.69                     | 0.41              |
| 2:A:44:MET:HE2   | 6:G:519:ILE:HD13 | 2.03                     | 0.41              |
| 2:A:45:LEU:HD13  | 2:A:64:LEU:HD12  | 2.02                     | 0.41              |
| 4:D:405:ILE:O    | 4:D:409:LEU:HG   | 2.21                     | 0.41              |
| 8:Q:114:LEU:HD22 | 8:Q:440:LYS:HD2  | 2.03                     | 0.41              |
| 5:e:162:THR:O    | 5:e:166:ILE:HG12 | 2.21                     | 0.41              |
| 5:e:184:GLN:NE2  | 5:e:222:THR:O    | 2.54                     | 0.41              |
| 5:e:257:PRO:HA   | 5:e:258:PRO:HD3  | 1.94                     | 0.41              |
| 7:h:456:ASP:OD2  | 7:h:459:ASN:ND2  | 2.54                     | 0.41              |
| 8:q:97:VAL:HG13  | 8:q:401:VAL:HG21 | 2.01                     | 0.41              |
| 10:P:87:LEU:C    | 10:P:89:LYS:H    | 2.29                     | 0.41              |
| 3:B:271:GLU:HG2  | 5:E:274:TYR:CZ   | 2.56                     | 0.41              |
| 6:G:20:ARG:HG2   | 6:G:20:ARG:HH11  | 1.86                     | 0.41              |
| 7:H:149:VAL:O    | 7:H:153:LYS:HG2  | 2.21                     | 0.41              |
| 7:H:197:ILE:HG21 | 7:H:386:GLU:HG3  | 2.03                     | 0.41              |
| 7:H:337:LEU:HD23 | 7:H:337:LEU:HA   | 1.86                     | 0.41              |
| 3:b:65:ASN:HD22  | 3:b:170:LYS:HD3  | 1.86                     | 0.41              |
| 4:d:373:LEU:HD23 | 4:d:373:LEU:HA   | 1.87                     | 0.41              |
| 4:d:407:ASP:O    | 4:d:411:VAL:HG23 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:e:456:GLU:OE2  | 5:e:478:ARG:NH1  | 2.46                     | 0.41              |
| 6:g:183:VAL:HG11 | 6:g:195:ILE:HD13 | 2.02                     | 0.41              |
| 7:h:104:PHE:O    | 7:h:108:VAL:HG22 | 2.20                     | 0.41              |
| 9:z:140:SER:HA   | 9:z:406:CYS:HA   | 2.03                     | 0.41              |
| 9:z:159:LYS:HD2  | 9:z:393:ASP:OD2  | 2.21                     | 0.41              |
| 9:z:338:ASP:N    | 9:z:338:ASP:OD1  | 2.53                     | 0.41              |
| 10:P:198:MET:HB3 | 10:P:259:PHE:HZ  | 1.85                     | 0.41              |
| 2:A:384:MET:HE1  | 6:G:511:GLU:OE1  | 2.22                     | 0.41              |
| 5:E:119:GLU:O    | 5:E:122:GLN:HG3  | 2.21                     | 0.41              |
| 6:G:134:ILE:HD12 | 6:G:503:LEU:HD22 | 2.03                     | 0.41              |
| 8:Q:47:TYR:O     | 8:Q:455:ASN:ND2  | 2.47                     | 0.41              |
| 9:Z:520:GLU:HG2  | 9:Z:522:MET:HG3  | 2.02                     | 0.41              |
| 2:a:294:ASP:O    | 2:a:298:LYS:HG2  | 2.20                     | 0.41              |
| 3:b:40:LYS:C     | 3:b:42:THR:H     | 2.28                     | 0.41              |
| 5:e:377:CYS:HB2  | 5:e:380:SER:HB2  | 2.02                     | 0.41              |
| 7:h:145:LYS:HD2  | 7:h:147:ASP:N    | 2.35                     | 0.41              |
| 7:h:266:ILE:HD13 | 7:h:266:ILE:HA   | 1.94                     | 0.41              |
| 5:E:332:LEU:HD23 | 5:E:332:LEU:HA   | 1.95                     | 0.40              |
| 6:G:130:LEU:O    | 6:G:134:ILE:HG12 | 2.21                     | 0.40              |
| 6:G:219:MET:HE2  | 6:G:375:LEU:HD13 | 2.02                     | 0.40              |
| 8:Q:111:LEU:HD23 | 8:Q:111:LEU:HA   | 1.94                     | 0.40              |
| 8:Q:520:ARG:HB3  | 9:Z:44:MET:HG3   | 2.03                     | 0.40              |
| 4:d:224:VAL:HG23 | 4:d:377:THR:HG22 | 2.03                     | 0.40              |
| 5:e:405:ALA:O    | 5:e:409:ILE:HG12 | 2.22                     | 0.40              |
| 2:A:445:LEU:HD23 | 2:A:445:LEU:HA   | 1.89                     | 0.40              |
| 3:B:99:THR:OG1   | 13:B:603:AF3:F2  | 2.24                     | 0.40              |
| 6:G:329:ALA:HB2  | 6:G:344:GLY:HA3  | 2.03                     | 0.40              |
| 7:H:30:GLN:OE1   | 7:H:106:LYS:HB2  | 2.21                     | 0.40              |
| 2:a:197:ILE:HG21 | 2:a:389:GLU:HG3  | 2.02                     | 0.40              |
| 9:z:178:ALA:O    | 9:z:370:ARG:NH1  | 2.53                     | 0.40              |
| 3:B:244:MET:HE3  | 3:B:244:MET:HB3  | 1.90                     | 0.40              |
| 4:D:408:ALA:O    | 4:D:412:ILE:HG12 | 2.21                     | 0.40              |
| 5:E:129:HIS:HB3  | 5:E:132:ARG:HG2  | 2.02                     | 0.40              |
| 9:Z:61:ASN:HB2   | 9:Z:92:THR:HG21  | 2.04                     | 0.40              |
| 9:Z:210:LEU:HD22 | 9:Z:324:LEU:HG   | 2.03                     | 0.40              |
| 2:a:70:PRO:HB3   | 4:d:68:VAL:HG21  | 2.04                     | 0.40              |
| 2:a:204:SER:OG   | 2:a:207:GLU:OE1  | 2.33                     | 0.40              |
| 2:a:229:ILE:HD12 | 2:a:306:MET:HG2  | 2.03                     | 0.40              |
| 3:b:495:GLU:OE2  | 11:b:601:ADP:O2' | 2.34                     | 0.40              |
| 5:e:203:ASP:OD2  | 7:h:357:ARG:NH1  | 2.51                     | 0.40              |
| 5:e:255:PHE:HB2  | 5:e:306:PHE:CB   | 2.51                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:g:236:PRO:HG3   | 6:g:350:LEU:HB2  | 2.03                     | 0.40              |
| 3:B:59:ALA:O      | 4:D:89:ARG:NH2   | 2.44                     | 0.40              |
| 6:G:67:LEU:HD23   | 6:G:67:LEU:HA    | 1.84                     | 0.40              |
| 7:H:109:LYS:O     | 7:H:113:GLU:HG3  | 2.21                     | 0.40              |
| 8:Q:81:PRO:HA     | 8:Q:84:LYS:HB2   | 2.03                     | 0.40              |
| 2:a:505:GLU:OE2   | 11:a:601:ADP:O2' | 2.27                     | 0.40              |
| 3:b:35:ILE:HD13   | 3:b:35:ILE:HA    | 1.98                     | 0.40              |
| 3:b:42:THR:HB     | 3:b:65:ASN:OD1   | 2.22                     | 0.40              |
| 4:d:129:HIS:CD2   | 4:d:130:PRO:HD2  | 2.56                     | 0.40              |
| 5:e:185:MET:HA    | 5:e:188:ILE:HG12 | 2.02                     | 0.40              |
| 9:z:271:VAL:O     | 9:z:275:ILE:HG12 | 2.22                     | 0.40              |
| 9:z:333:LEU:HD11  | 9:z:343:CYS:SG   | 2.61                     | 0.40              |
| 10:P:285:VAL:HG23 | 10:P:286:ARG:H   | 1.86                     | 0.40              |
| 10:P:285:VAL:C    | 10:P:286:ARG:HD3 | 2.46                     | 0.40              |
| 4:D:256:PRO:HD3   | 4:D:282:TYR:CD2  | 2.57                     | 0.40              |
| 6:G:407:LEU:HD23  | 6:G:407:LEU:HA   | 1.95                     | 0.40              |
| 7:H:40:LEU:HD13   | 7:H:99:LEU:HD12  | 2.04                     | 0.40              |
| 7:H:90:VAL:HG12   | 7:H:92:ASP:H     | 1.87                     | 0.40              |
| 2:a:66:GLU:HG2    | 6:g:526:HIS:HB2  | 2.04                     | 0.40              |
| 5:e:532:ASP:HB3   | 7:h:47:LYS:HD2   | 2.03                     | 0.40              |
| 6:g:62:ASP:OD1    | 13:g:603:AF3:F3  | 2.29                     | 0.40              |
| 7:h:26:ILE:HG23   | 7:h:105:LEU:HB3  | 2.01                     | 0.40              |
| 8:q:233:SER:HA    | 8:q:351:TYR:HA   | 2.04                     | 0.40              |
| 9:z:237:LEU:HD23  | 9:z:237:LEU:HA   | 1.90                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles           |
|-----|-------|---------------|-----------|----------|----------|-----------------------|
| 1   | N     | 118/395 (30%) | 100 (85%) | 18 (15%) | 0        | <b>100</b> <b>100</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | A     | 534/536 (100%)  | 513 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 2   | a     | 530/536 (99%)   | 507 (96%)  | 23 (4%)  | 0        | 100         | 100 |
| 3   | B     | 524/526 (100%)  | 509 (97%)  | 15 (3%)  | 0        | 100         | 100 |
| 3   | b     | 523/526 (99%)   | 508 (97%)  | 15 (3%)  | 0        | 100         | 100 |
| 4   | D     | 518/520 (100%)  | 507 (98%)  | 11 (2%)  | 0        | 100         | 100 |
| 4   | d     | 518/520 (100%)  | 497 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 5   | E     | 533/540 (99%)   | 520 (98%)  | 13 (2%)  | 0        | 100         | 100 |
| 5   | e     | 539/540 (100%)  | 525 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 6   | G     | 524/528 (99%)   | 510 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 6   | g     | 524/528 (99%)   | 515 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 7   | H     | 526/528 (100%)  | 509 (97%)  | 17 (3%)  | 0        | 100         | 100 |
| 7   | h     | 523/528 (99%)   | 505 (97%)  | 18 (3%)  | 0        | 100         | 100 |
| 8   | Q     | 536/538 (100%)  | 522 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 8   | q     | 531/538 (99%)   | 516 (97%)  | 15 (3%)  | 0        | 100         | 100 |
| 9   | Z     | 523/527 (99%)   | 510 (98%)  | 13 (2%)  | 0        | 100         | 100 |
| 9   | z     | 525/527 (100%)  | 513 (98%)  | 12 (2%)  | 0        | 100         | 100 |
| 10  | P     | 183/301 (61%)   | 161 (88%)  | 20 (11%) | 2 (1%)   | 12          | 37  |
| All | All   | 8732/9182 (95%) | 8447 (97%) | 283 (3%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | P     | 55  | VAL  |
| 10  | P     | 300 | 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   | N     | 107/334 (32%) | 107 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 2   | A     | 447/447 (100%)  | 447 (100%)  | 0        | 100         | 100 |
| 2   | a     | 444/447 (99%)   | 444 (100%)  | 0        | 100         | 100 |
| 3   | B     | 418/418 (100%)  | 418 (100%)  | 0        | 100         | 100 |
| 3   | b     | 417/418 (100%)  | 417 (100%)  | 0        | 100         | 100 |
| 4   | D     | 442/442 (100%)  | 442 (100%)  | 0        | 100         | 100 |
| 4   | d     | 441/442 (100%)  | 441 (100%)  | 0        | 100         | 100 |
| 5   | E     | 451/455 (99%)   | 451 (100%)  | 0        | 100         | 100 |
| 5   | e     | 456/455 (100%)  | 456 (100%)  | 0        | 100         | 100 |
| 6   | G     | 456/457 (100%)  | 456 (100%)  | 0        | 100         | 100 |
| 6   | g     | 456/457 (100%)  | 456 (100%)  | 0        | 100         | 100 |
| 7   | H     | 435/435 (100%)  | 435 (100%)  | 0        | 100         | 100 |
| 7   | h     | 432/435 (99%)   | 432 (100%)  | 0        | 100         | 100 |
| 8   | Q     | 442/442 (100%)  | 442 (100%)  | 0        | 100         | 100 |
| 8   | q     | 438/442 (99%)   | 438 (100%)  | 0        | 100         | 100 |
| 9   | Z     | 437/439 (100%)  | 437 (100%)  | 0        | 100         | 100 |
| 9   | z     | 438/439 (100%)  | 438 (100%)  | 0        | 100         | 100 |
| 10  | P     | 171/266 (64%)   | 171 (100%)  | 0        | 100         | 100 |
| All | All   | 7328/7670 (96%) | 7328 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 194 | HIS  |
| 1   | N     | 252 | ASN  |
| 1   | N     | 285 | ASN  |
| 2   | A     | 284 | ASN  |
| 2   | A     | 347 | GLN  |
| 2   | A     | 353 | GLN  |
| 3   | B     | 65  | ASN  |
| 3   | B     | 78  | ASN  |
| 3   | B     | 227 | ASN  |
| 3   | B     | 269 | HIS  |
| 3   | B     | 381 | GLN  |
| 3   | B     | 391 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 464 | GLN  |
| 4   | D     | 25  | GLN  |
| 4   | D     | 82  | GLN  |
| 5   | E     | 85  | HIS  |
| 5   | E     | 298 | ASN  |
| 5   | E     | 411 | ASN  |
| 5   | E     | 472 | GLN  |
| 6   | G     | 28  | ASN  |
| 6   | G     | 111 | HIS  |
| 6   | G     | 390 | ASN  |
| 6   | G     | 420 | HIS  |
| 7   | H     | 170 | GLN  |
| 7   | H     | 264 | GLN  |
| 7   | H     | 431 | GLN  |
| 7   | H     | 481 | ASN  |
| 8   | Q     | 53  | ASN  |
| 9   | Z     | 334 | ASN  |
| 2   | a     | 20  | GLN  |
| 2   | a     | 187 | GLN  |
| 2   | a     | 217 | ASN  |
| 2   | a     | 347 | GLN  |
| 3   | b     | 157 | GLN  |
| 3   | b     | 464 | GLN  |
| 4   | d     | 80  | GLN  |
| 4   | d     | 172 | ASN  |
| 4   | d     | 263 | GLN  |
| 4   | d     | 482 | ASN  |
| 4   | d     | 537 | ASN  |
| 5   | e     | 55  | ASN  |
| 5   | e     | 184 | GLN  |
| 5   | e     | 278 | GLN  |
| 5   | e     | 469 | ASN  |
| 6   | g     | 74  | HIS  |
| 6   | g     | 111 | HIS  |
| 7   | h     | 331 | GLN  |
| 7   | h     | 448 | GLN  |
| 8   | q     | 34  | GLN  |
| 8   | q     | 93  | GLN  |
| 8   | q     | 172 | GLN  |
| 8   | q     | 175 | ASN  |
| 8   | q     | 397 | ASN  |
| 9   | z     | 61  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | z     | 70  | GLN  |
| 9   | z     | 467 | GLN  |
| 9   | z     | 514 | ASN  |
| 10  | P     | 56  | ASN  |
| 10  | P     | 153 | HIS  |
| 10  | P     | 186 | 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 ⓘ

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 11  | ADP  | e     | 601 | 12   | 24,29,29     | 0.90 | 0           | 29,45,45    | 1.22 | 2 (6%)      |
| 11  | ADP  | Z     | 601 | 12   | 24,29,29     | 0.84 | 0           | 29,45,45    | 1.25 | 2 (6%)      |
| 13  | AF3  | a     | 603 | -    | 0,3,3        | -    | -           | -           |      |             |
| 13  | AF3  | g     | 603 | -    | 0,3,3        | -    | -           | -           |      |             |
| 13  | AF3  | h     | 603 | -    | 0,3,3        | -    | -           | -           |      |             |
| 13  | AF3  | D     | 603 | -    | 0,3,3        | -    | -           | -           |      |             |
| 11  | ADP  | E     | 601 | 12   | 24,29,29     | 0.90 | 0           | 29,45,45    | 1.22 | 3 (10%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | AF3  | A     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 13  | AF3  | B     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 13  | AF3  | d     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | D     | 601 | 12   | 24,29,29     | 0.90 | 0        | 29,45,45    | 1.21 | 2 (6%)   |
| 13  | AF3  | e     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 13  | AF3  | q     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | G     | 601 | 12   | 24,29,29     | 0.85 | 0        | 29,45,45    | 1.23 | 2 (6%)   |
| 11  | ADP  | d     | 601 | 12   | 24,29,29     | 0.88 | 0        | 29,45,45    | 1.26 | 2 (6%)   |
| 13  | AF3  | Z     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | Q     | 601 | 12   | 24,29,29     | 0.85 | 0        | 29,45,45    | 1.23 | 2 (6%)   |
| 11  | ADP  | h     | 601 | 12   | 24,29,29     | 0.89 | 0        | 29,45,45    | 1.27 | 3 (10%)  |
| 13  | AF3  | H     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | H     | 601 | 12   | 24,29,29     | 0.92 | 1 (4%)   | 29,45,45    | 1.27 | 3 (10%)  |
| 13  | AF3  | E     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | A     | 601 | 12   | 24,29,29     | 0.86 | 0        | 29,45,45    | 1.23 | 2 (6%)   |
| 13  | AF3  | z     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 13  | AF3  | b     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | a     | 601 | 12   | 24,29,29     | 0.85 | 0        | 29,45,45    | 1.22 | 2 (6%)   |
| 11  | ADP  | g     | 601 | 12   | 24,29,29     | 0.85 | 0        | 29,45,45    | 1.24 | 2 (6%)   |
| 11  | ADP  | q     | 601 | 12   | 24,29,29     | 0.85 | 0        | 29,45,45    | 1.26 | 2 (6%)   |
| 11  | ADP  | z     | 601 | 12   | 24,29,29     | 0.84 | 0        | 29,45,45    | 1.23 | 2 (6%)   |
| 11  | ADP  | b     | 601 | 12   | 24,29,29     | 0.90 | 0        | 29,45,45    | 1.24 | 2 (6%)   |
| 11  | ADP  | B     | 601 | 12   | 24,29,29     | 0.88 | 0        | 29,45,45    | 1.21 | 2 (6%)   |
| 13  | AF3  | G     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |
| 13  | AF3  | Q     | 603 | -    | 0,3,3        | -    | -        | -           |      |          |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 11  | ADP  | e     | 601 | 12   | -       | 1/12/32/32 | 0/3/3/3 |
| 11  | ADP  | a     | 601 | 12   | -       | 6/12/32/32 | 0/3/3/3 |
| 11  | ADP  | g     | 601 | 12   | -       | 3/12/32/32 | 0/3/3/3 |
| 11  | ADP  | h     | 601 | 12   | -       | 1/12/32/32 | 0/3/3/3 |
| 11  | ADP  | q     | 601 | 12   | -       | 6/12/32/32 | 0/3/3/3 |
| 11  | ADP  | D     | 601 | 12   | -       | 1/12/32/32 | 0/3/3/3 |
| 11  | ADP  | Z     | 601 | 12   | -       | 4/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 11  | ADP  | z     | 601 | 12   | -       | 3/12/32/32 | 0/3/3/3 |
| 11  | ADP  | b     | 601 | 12   | -       | 1/12/32/32 | 0/3/3/3 |
| 11  | ADP  | G     | 601 | 12   | -       | 2/12/32/32 | 0/3/3/3 |
| 11  | ADP  | d     | 601 | 12   | -       | 1/12/32/32 | 0/3/3/3 |
| 11  | ADP  | B     | 601 | 12   | -       | 0/12/32/32 | 0/3/3/3 |
| 11  | ADP  | H     | 601 | 12   | -       | 3/12/32/32 | 0/3/3/3 |
| 11  | ADP  | E     | 601 | 12   | -       | 0/12/32/32 | 0/3/3/3 |
| 11  | ADP  | Q     | 601 | 12   | -       | 6/12/32/32 | 0/3/3/3 |
| 11  | ADP  | A     | 601 | 12   | -       | 6/12/32/32 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 11  | H     | 601 | ADP  | PA-O3A | 2.07 | 1.61        | 1.59     |

All (35) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | a     | 601 | ADP  | N3-C2-N1 | -3.74 | 123.59      | 128.67   |
| 11  | H     | 601 | ADP  | N3-C2-N1 | -3.71 | 123.64      | 128.67   |
| 11  | A     | 601 | ADP  | N3-C2-N1 | -3.70 | 123.64      | 128.67   |
| 11  | Q     | 601 | ADP  | N3-C2-N1 | -3.70 | 123.65      | 128.67   |
| 11  | q     | 601 | ADP  | N3-C2-N1 | -3.70 | 123.65      | 128.67   |
| 11  | Z     | 601 | ADP  | N3-C2-N1 | -3.70 | 123.65      | 128.67   |
| 11  | D     | 601 | ADP  | N3-C2-N1 | -3.69 | 123.66      | 128.67   |
| 11  | d     | 601 | ADP  | N3-C2-N1 | -3.69 | 123.67      | 128.67   |
| 11  | h     | 601 | ADP  | N3-C2-N1 | -3.69 | 123.67      | 128.67   |
| 11  | E     | 601 | ADP  | N3-C2-N1 | -3.68 | 123.68      | 128.67   |
| 11  | B     | 601 | ADP  | N3-C2-N1 | -3.67 | 123.69      | 128.67   |
| 11  | z     | 601 | ADP  | N3-C2-N1 | -3.64 | 123.73      | 128.67   |
| 11  | e     | 601 | ADP  | N3-C2-N1 | -3.64 | 123.73      | 128.67   |
| 11  | b     | 601 | ADP  | N3-C2-N1 | -3.61 | 123.78      | 128.67   |
| 11  | G     | 601 | ADP  | N3-C2-N1 | -3.53 | 123.89      | 128.67   |
| 11  | g     | 601 | ADP  | N3-C2-N1 | -3.46 | 123.98      | 128.67   |
| 11  | h     | 601 | ADP  | C4-C5-N7 | -2.76 | 106.42      | 109.34   |
| 11  | a     | 601 | ADP  | C4-C5-N7 | -2.71 | 106.47      | 109.34   |
| 11  | b     | 601 | ADP  | C4-C5-N7 | -2.68 | 106.50      | 109.34   |
| 11  | d     | 601 | ADP  | C4-C5-N7 | -2.68 | 106.50      | 109.34   |
| 11  | Q     | 601 | ADP  | C4-C5-N7 | -2.68 | 106.51      | 109.34   |
| 11  | q     | 601 | ADP  | C4-C5-N7 | -2.66 | 106.52      | 109.34   |
| 11  | H     | 601 | ADP  | C4-C5-N7 | -2.66 | 106.52      | 109.34   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 11  | A     | 601 | ADP  | C4-C5-N7   | -2.66 | 106.53      | 109.34   |
| 11  | D     | 601 | ADP  | C4-C5-N7   | -2.65 | 106.54      | 109.34   |
| 11  | e     | 601 | ADP  | C4-C5-N7   | -2.64 | 106.55      | 109.34   |
| 11  | B     | 601 | ADP  | C4-C5-N7   | -2.63 | 106.56      | 109.34   |
| 11  | E     | 601 | ADP  | C4-C5-N7   | -2.61 | 106.58      | 109.34   |
| 11  | g     | 601 | ADP  | C4-C5-N7   | -2.60 | 106.59      | 109.34   |
| 11  | G     | 601 | ADP  | C4-C5-N7   | -2.60 | 106.59      | 109.34   |
| 11  | z     | 601 | ADP  | C4-C5-N7   | -2.53 | 106.66      | 109.34   |
| 11  | Z     | 601 | ADP  | C4-C5-N7   | -2.49 | 106.71      | 109.34   |
| 11  | H     | 601 | ADP  | O4'-C1'-N9 | 2.22  | 111.69      | 108.75   |
| 11  | h     | 601 | ADP  | O4'-C1'-N9 | 2.09  | 111.51      | 108.75   |
| 11  | E     | 601 | ADP  | O4'-C1'-N9 | 2.03  | 111.43      | 108.75   |

There are no chirality outliers.

All (44) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | A     | 601 | ADP  | C5'-O5'-PA-O1A  |
| 11  | A     | 601 | ADP  | C5'-O5'-PA-O2A  |
| 11  | A     | 601 | ADP  | C5'-O5'-PA-O3A  |
| 11  | H     | 601 | ADP  | PA-O3A-PB-O3B   |
| 11  | H     | 601 | ADP  | C5'-O5'-PA-O3A  |
| 11  | Q     | 601 | ADP  | C5'-O5'-PA-O1A  |
| 11  | Q     | 601 | ADP  | C5'-O5'-PA-O2A  |
| 11  | Q     | 601 | ADP  | C5'-O5'-PA-O3A  |
| 11  | a     | 601 | ADP  | C5'-O5'-PA-O2A  |
| 11  | a     | 601 | ADP  | C5'-O5'-PA-O3A  |
| 11  | g     | 601 | ADP  | C5'-O5'-PA-O1A  |
| 11  | q     | 601 | ADP  | C5'-O5'-PA-O1A  |
| 11  | q     | 601 | ADP  | C5'-O5'-PA-O3A  |
| 11  | Q     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 11  | Z     | 601 | ADP  | O4'-C4'-C5'-O5' |
| 11  | Z     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 11  | q     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 11  | A     | 601 | ADP  | O4'-C4'-C5'-O5' |
| 11  | a     | 601 | ADP  | O4'-C4'-C5'-O5' |
| 11  | A     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 11  | D     | 601 | ADP  | PB-O3A-PA-O5'   |
| 11  | b     | 601 | ADP  | PB-O3A-PA-O5'   |
| 11  | d     | 601 | ADP  | PB-O3A-PA-O5'   |
| 11  | e     | 601 | ADP  | PB-O3A-PA-O5'   |
| 11  | h     | 601 | ADP  | PB-O3A-PA-O5'   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | Q     | 601 | ADP  | O4'-C4'-C5'-O5' |
| 11  | a     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 11  | q     | 601 | ADP  | O4'-C4'-C5'-O5' |
| 11  | Z     | 601 | ADP  | C5'-O5'-PA-O1A  |
| 11  | a     | 601 | ADP  | C5'-O5'-PA-O1A  |
| 11  | g     | 601 | ADP  | C5'-O5'-PA-O3A  |
| 11  | q     | 601 | ADP  | C5'-O5'-PA-O2A  |
| 11  | z     | 601 | ADP  | C5'-O5'-PA-O1A  |
| 11  | z     | 601 | ADP  | O4'-C4'-C5'-O5' |
| 11  | G     | 601 | ADP  | PB-O3A-PA-O2A   |
| 11  | Q     | 601 | ADP  | PB-O3A-PA-O2A   |
| 11  | Z     | 601 | ADP  | PB-O3A-PA-O2A   |
| 11  | g     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 11  | G     | 601 | ADP  | PB-O3A-PA-O1A   |
| 11  | a     | 601 | ADP  | PB-O3A-PA-O1A   |
| 11  | z     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 11  | A     | 601 | ADP  | PB-O3A-PA-O2A   |
| 11  | q     | 601 | ADP  | PB-O3A-PA-O2A   |
| 11  | H     | 601 | ADP  | C3'-C4'-C5'-O5' |

There are no ring outliers.

29 monomers are involved in 42 short contacts:

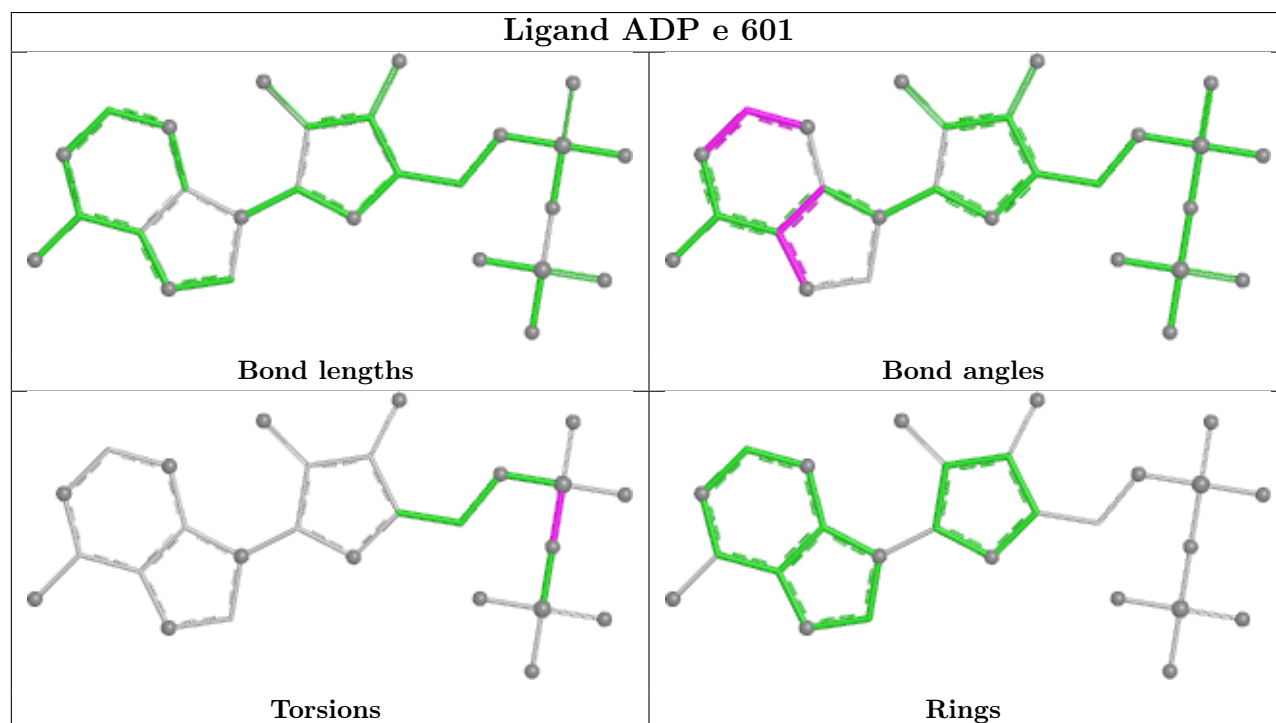
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | e     | 601 | ADP  | 1       | 0            |
| 11  | Z     | 601 | ADP  | 1       | 0            |
| 13  | a     | 603 | AF3  | 2       | 0            |
| 13  | g     | 603 | AF3  | 3       | 0            |
| 13  | h     | 603 | AF3  | 1       | 0            |
| 13  | D     | 603 | AF3  | 2       | 0            |
| 13  | A     | 603 | AF3  | 1       | 0            |
| 13  | B     | 603 | AF3  | 4       | 0            |
| 13  | d     | 603 | AF3  | 1       | 0            |
| 11  | D     | 601 | ADP  | 1       | 0            |
| 13  | q     | 603 | AF3  | 2       | 0            |
| 11  | G     | 601 | ADP  | 2       | 0            |
| 11  | d     | 601 | ADP  | 3       | 0            |
| 13  | Z     | 603 | AF3  | 1       | 0            |
| 11  | Q     | 601 | ADP  | 3       | 0            |
| 11  | h     | 601 | ADP  | 1       | 0            |
| 13  | H     | 603 | AF3  | 2       | 0            |
| 11  | H     | 601 | ADP  | 2       | 0            |

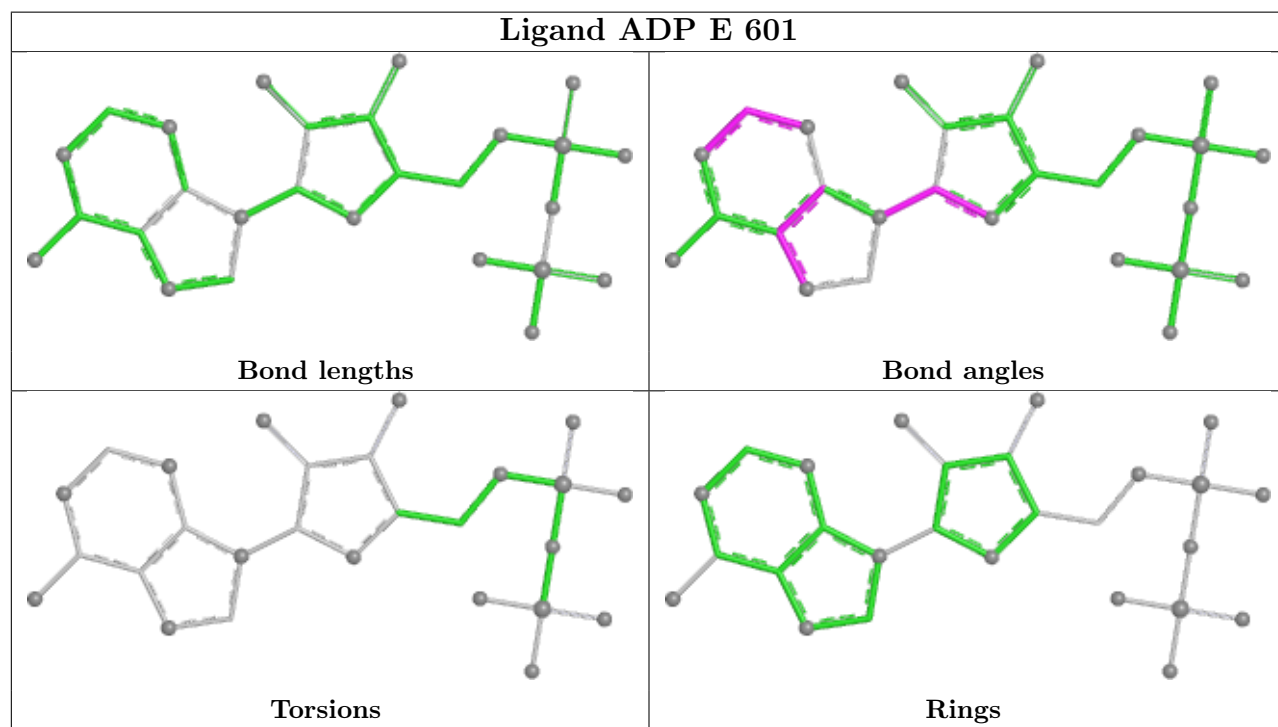
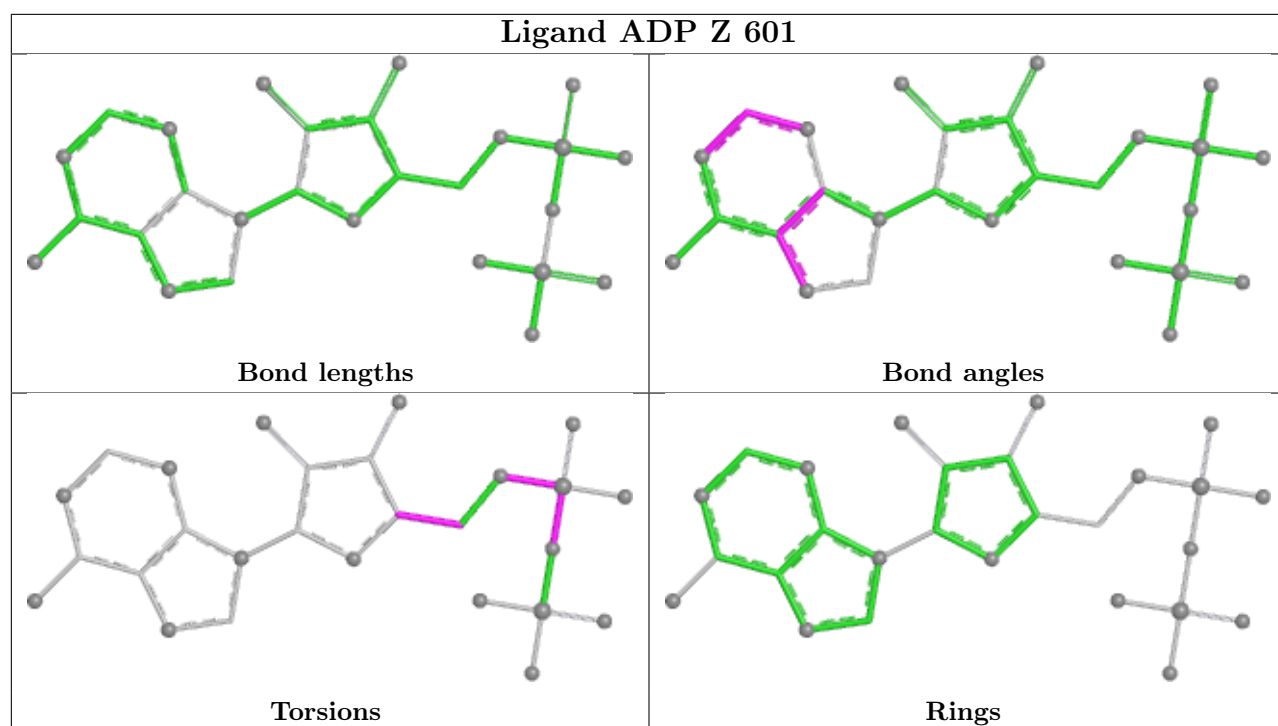
*Continued on next page...*

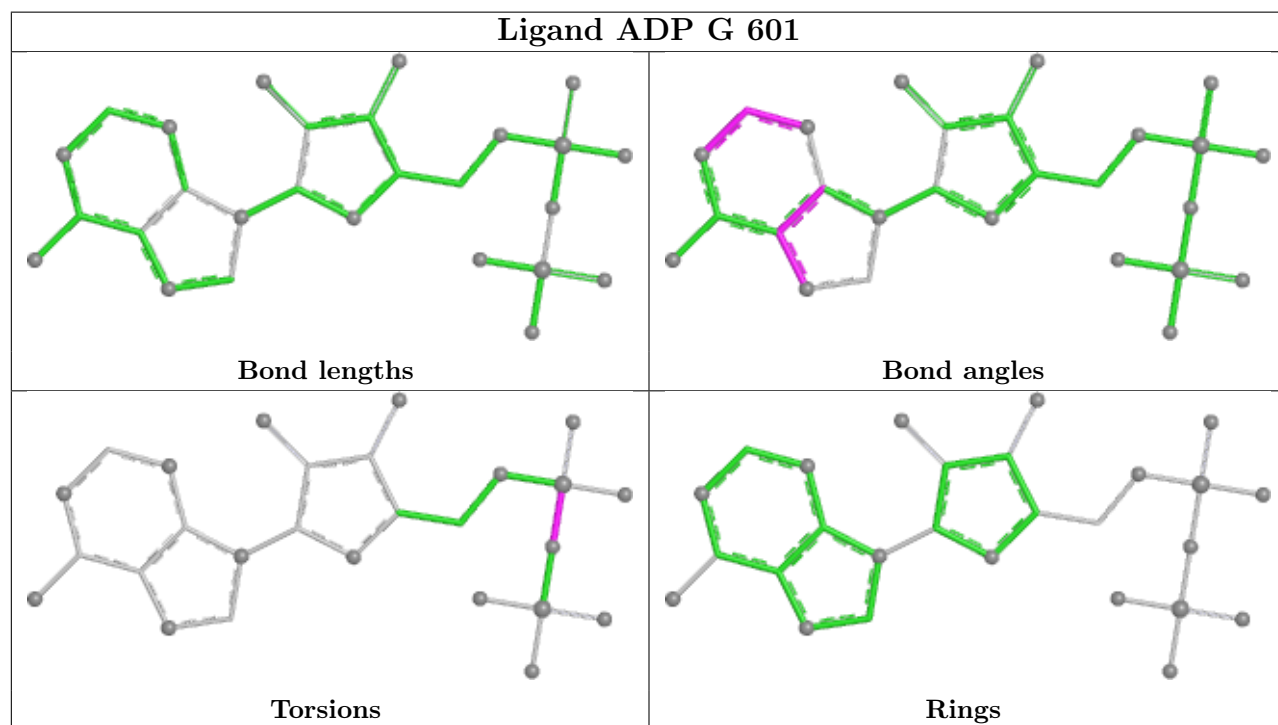
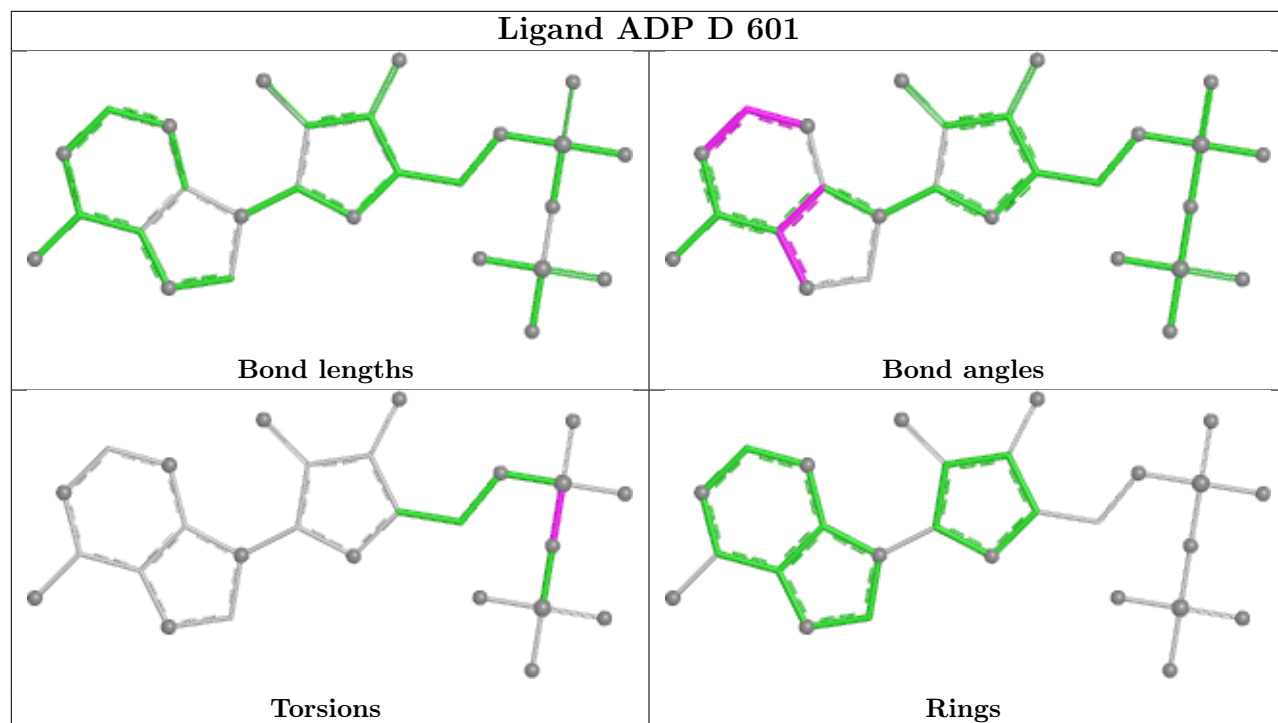
*Continued from previous page...*

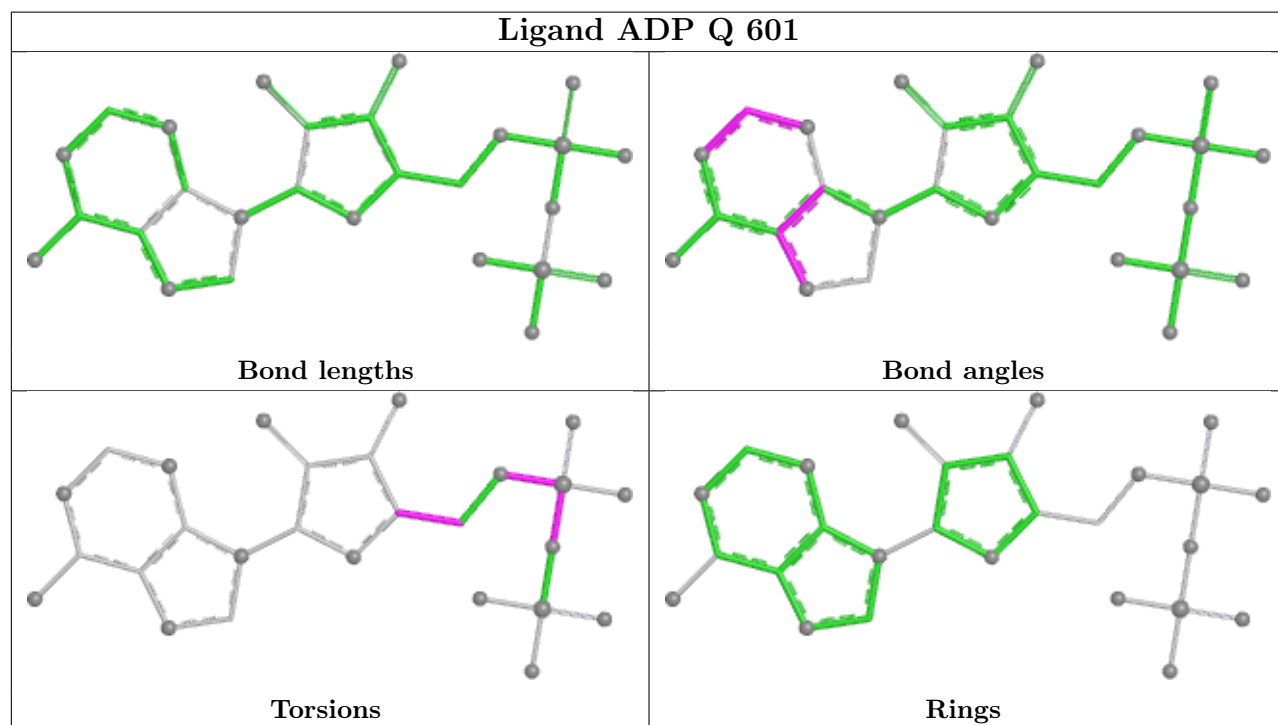
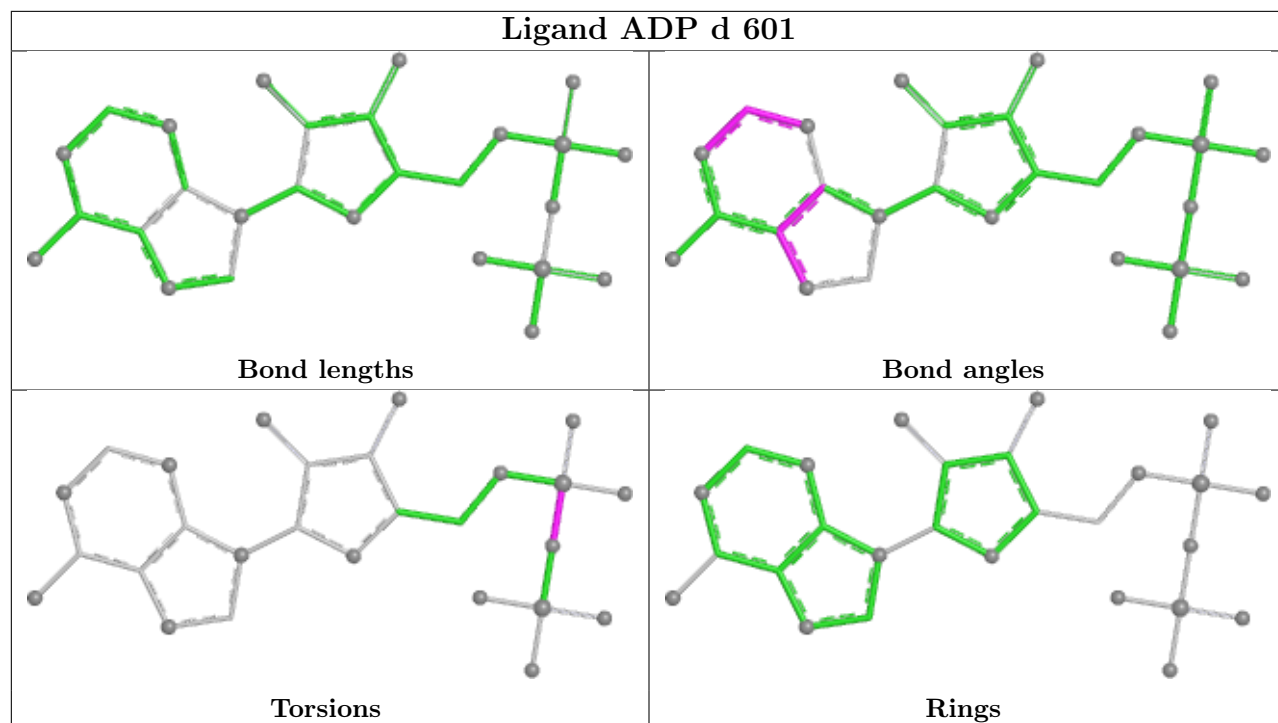
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | E     | 603 | AF3  | 1       | 0            |
| 11  | A     | 601 | ADP  | 1       | 0            |
| 13  | z     | 603 | AF3  | 1       | 0            |
| 11  | a     | 601 | ADP  | 4       | 0            |
| 11  | g     | 601 | ADP  | 3       | 0            |
| 11  | q     | 601 | ADP  | 2       | 0            |
| 11  | z     | 601 | ADP  | 1       | 0            |
| 11  | b     | 601 | ADP  | 3       | 0            |
| 11  | B     | 601 | ADP  | 4       | 0            |
| 13  | G     | 603 | AF3  | 3       | 0            |
| 13  | Q     | 603 | AF3  | 2       | 0            |

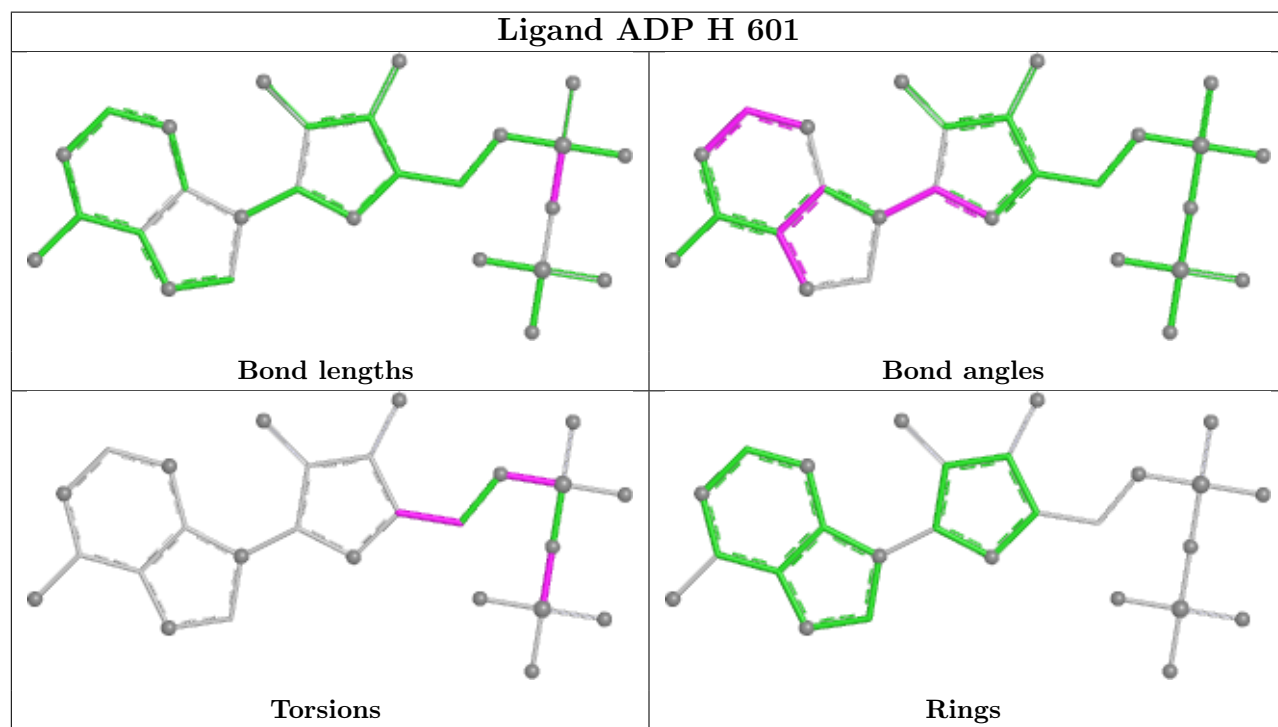
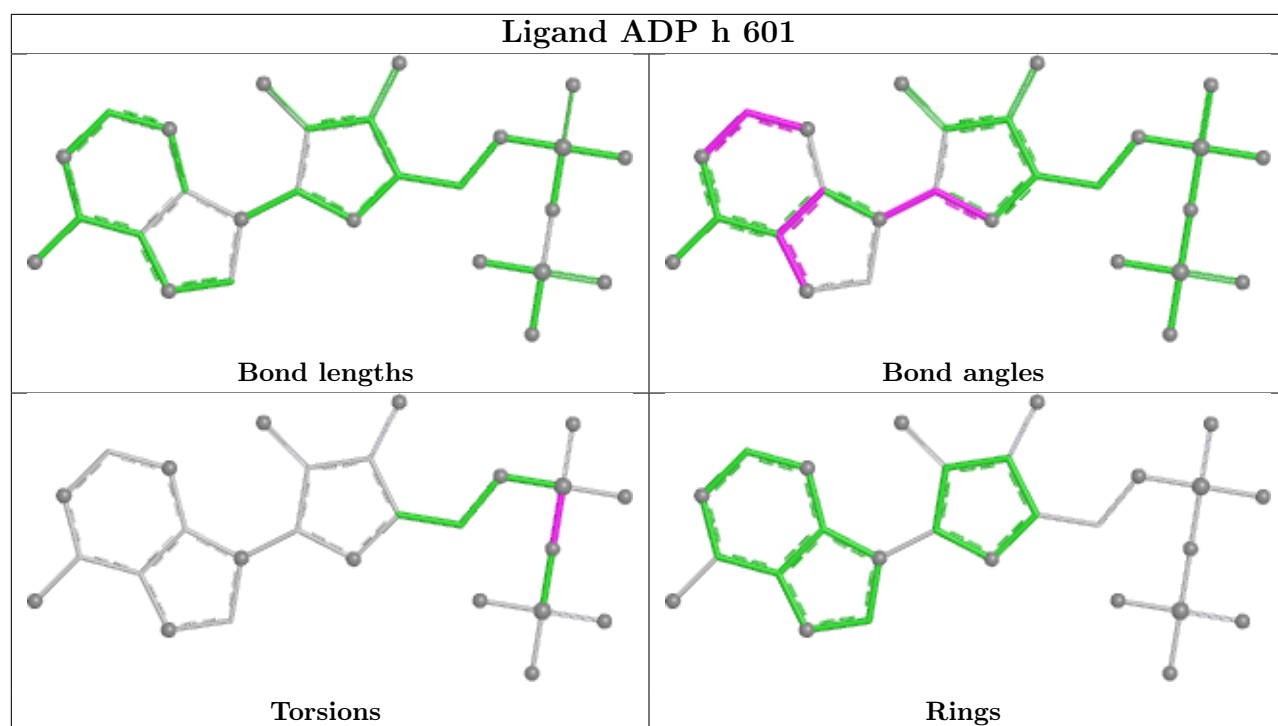
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



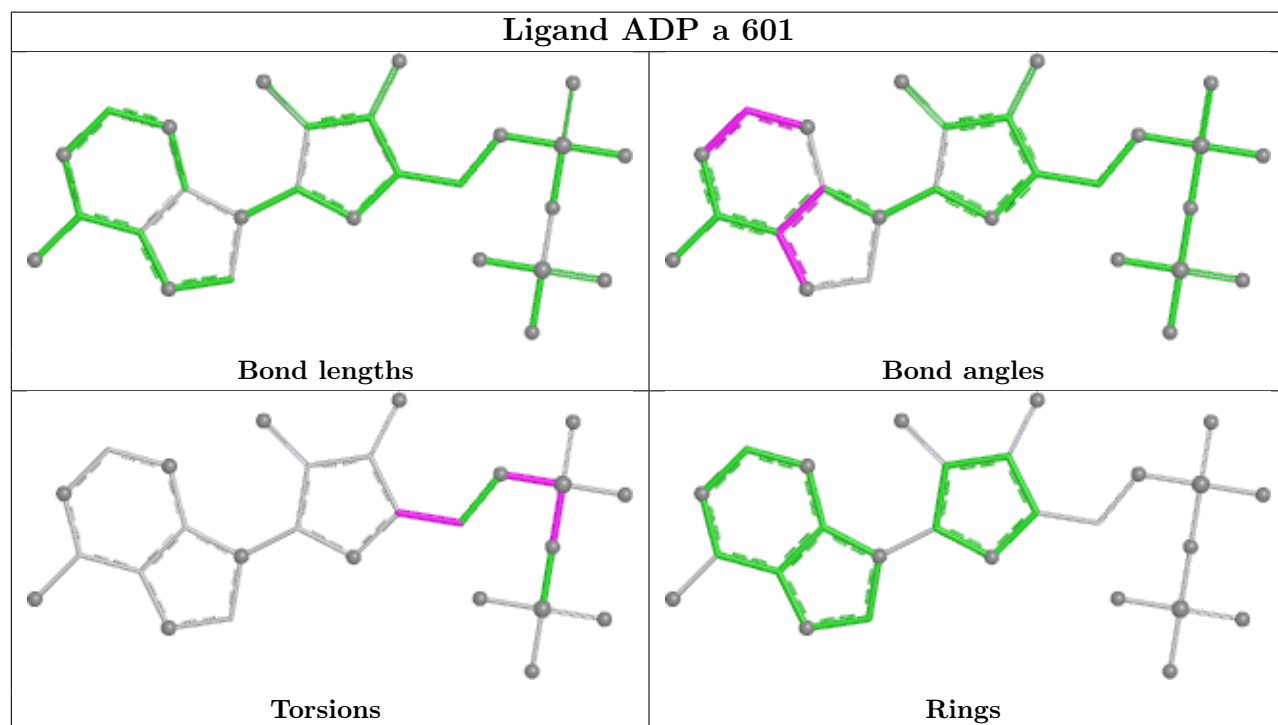
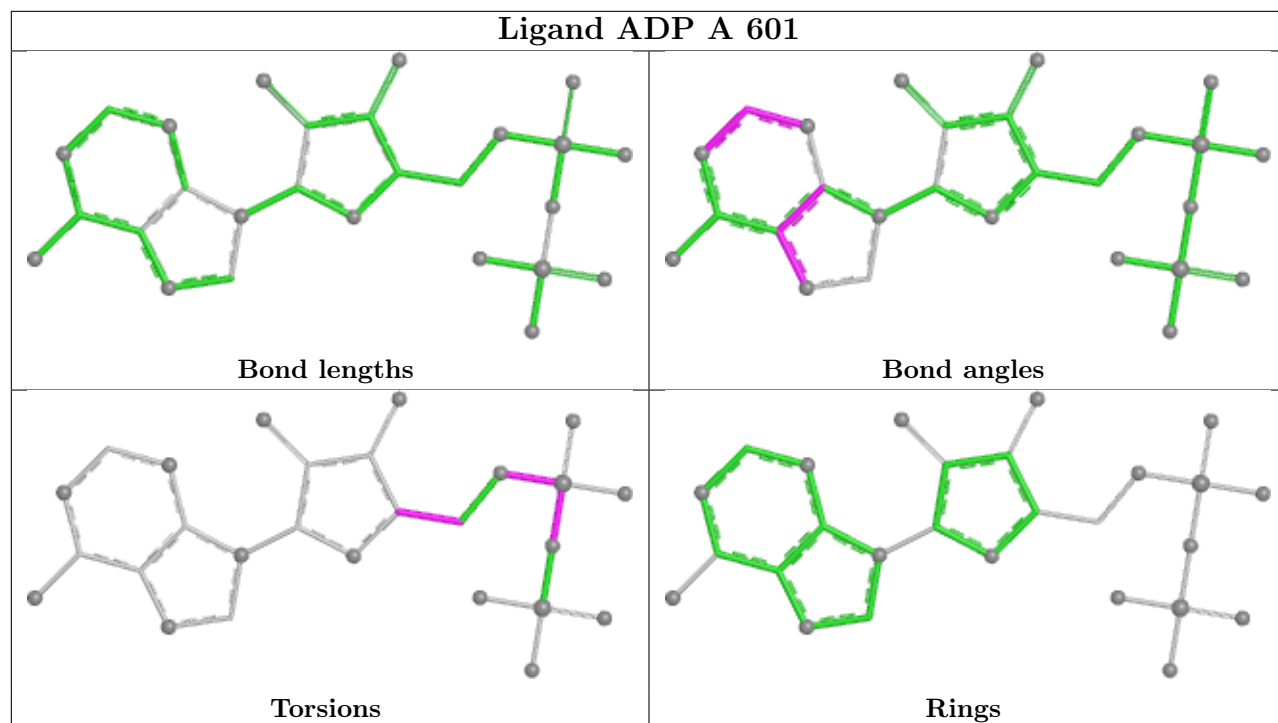


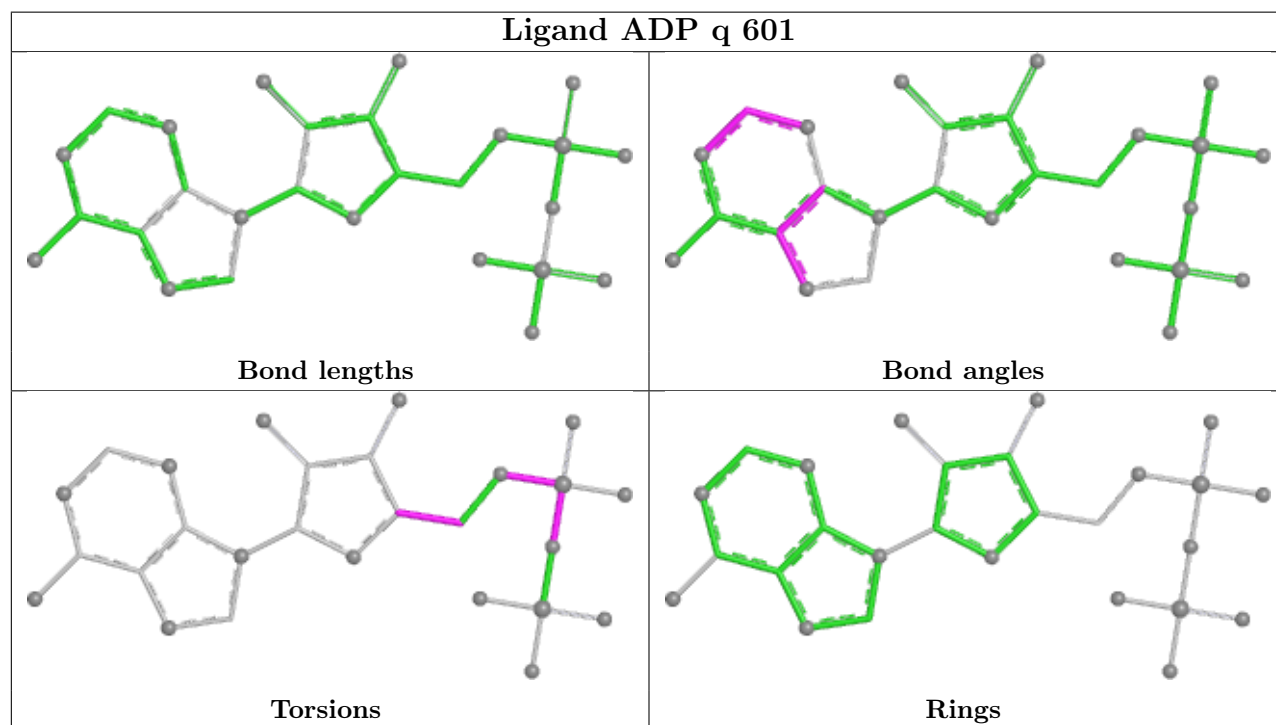
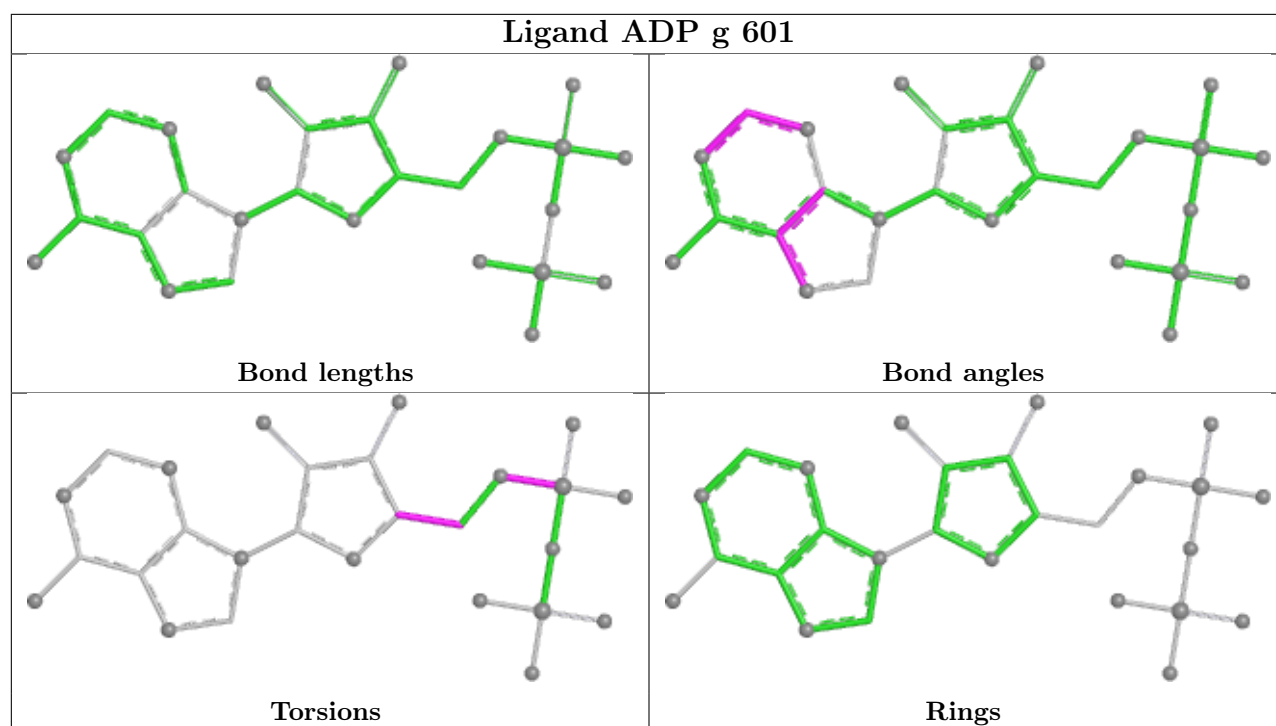


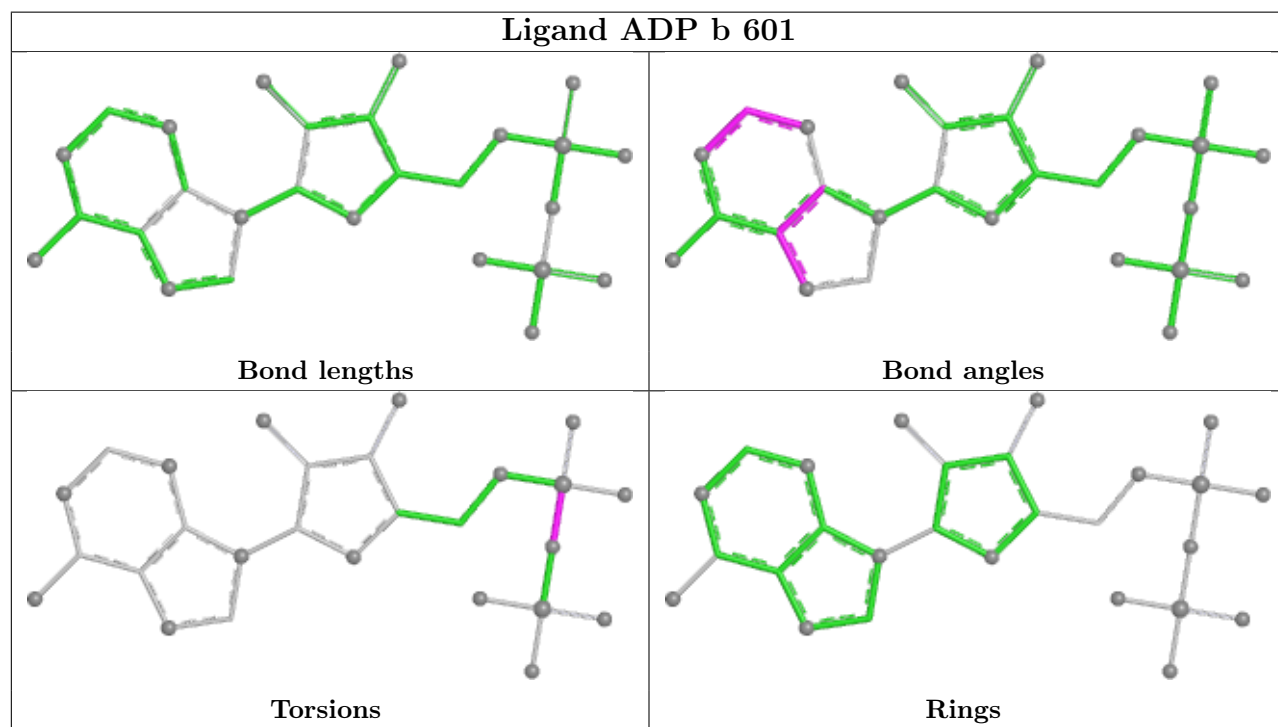
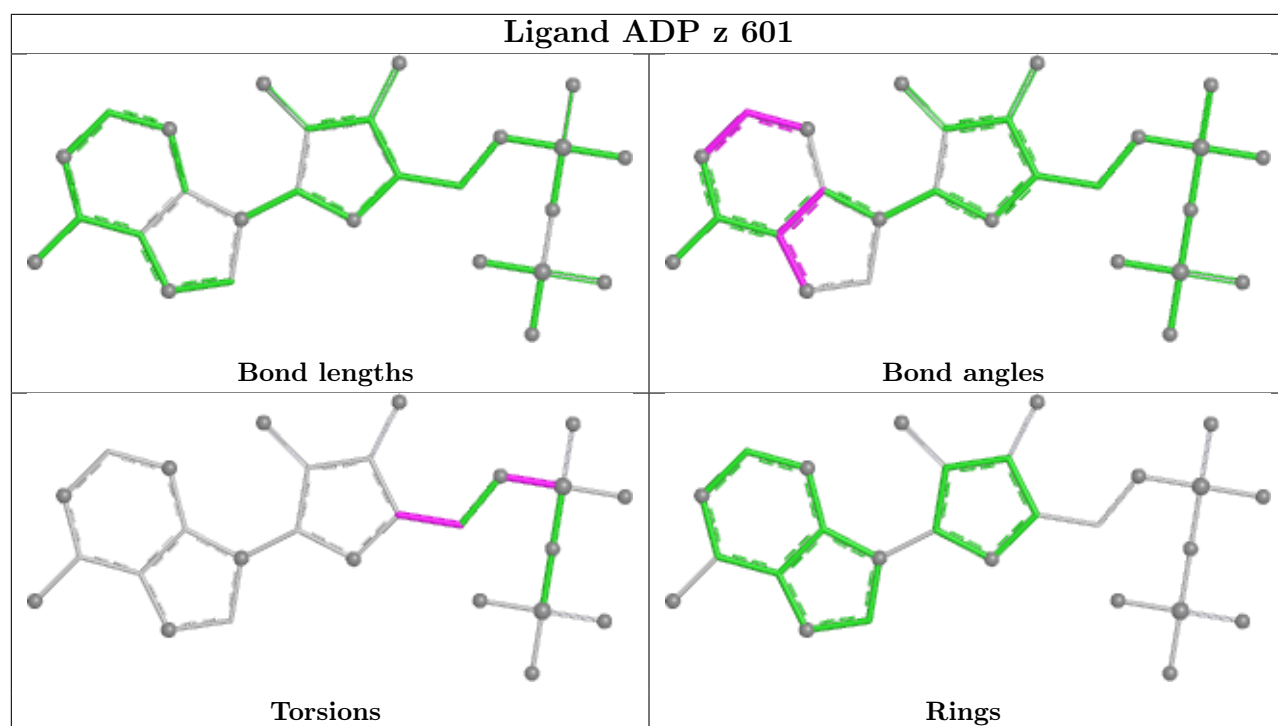


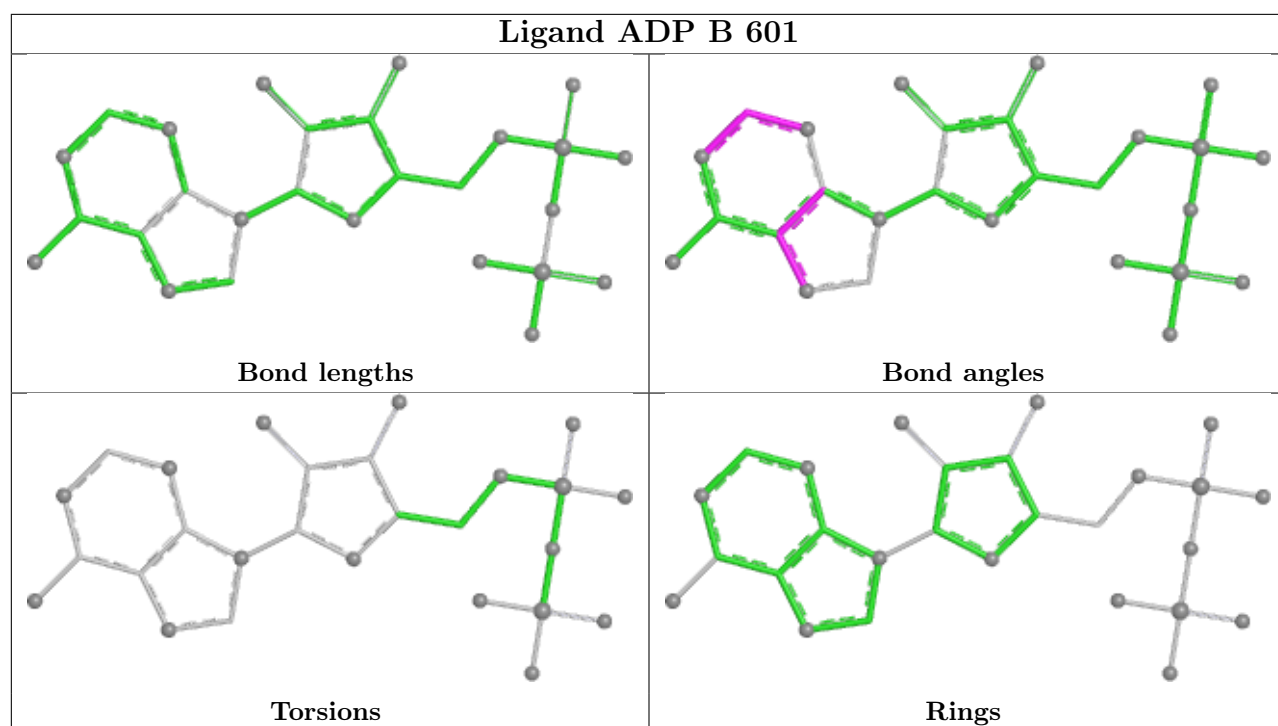












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

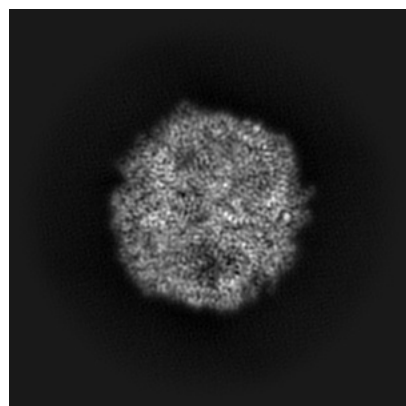
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40487. These allow visual inspection of the internal detail of the map and identification of artifacts.

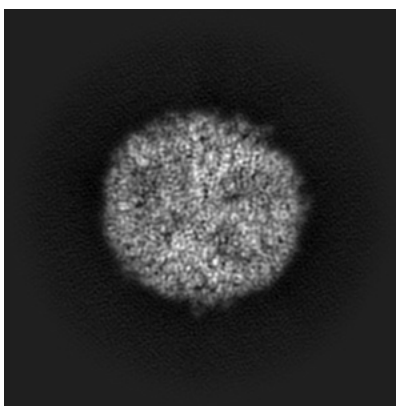
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

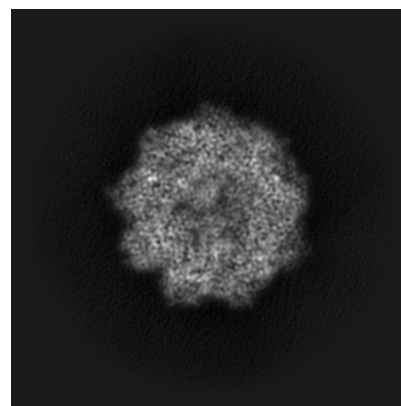
#### 6.1.1 Primary map



X

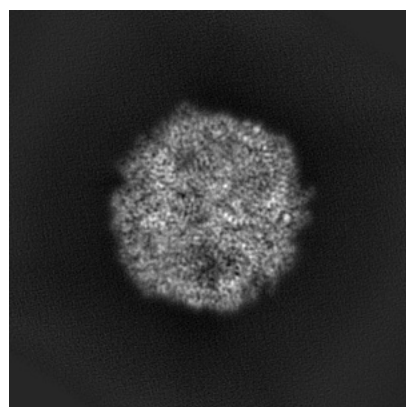


Y

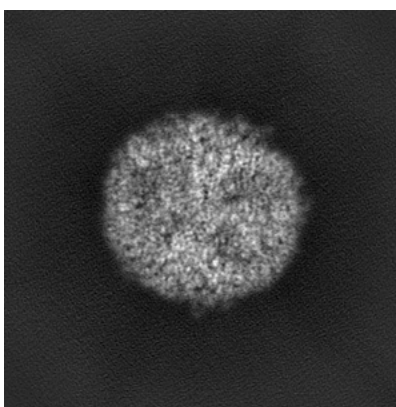


Z

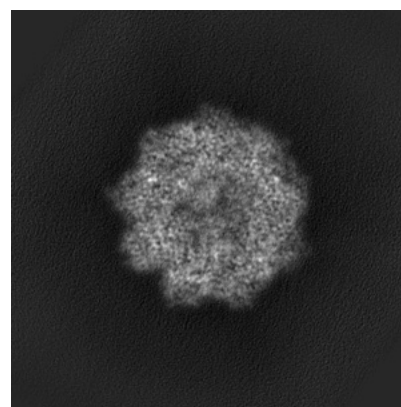
#### 6.1.2 Raw map



X



Y

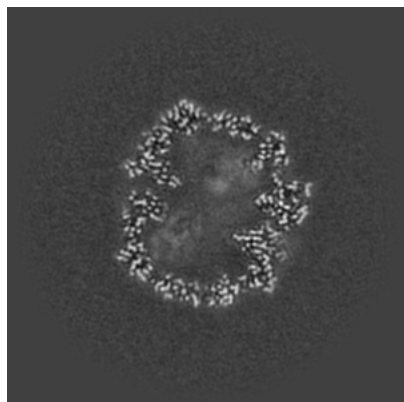


Z

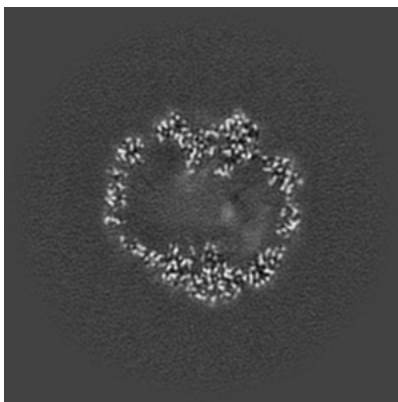
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

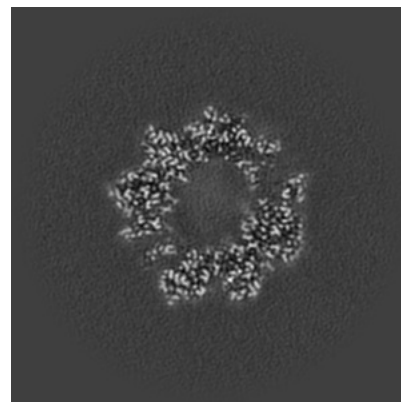
### 6.2.1 Primary map



X Index: 150

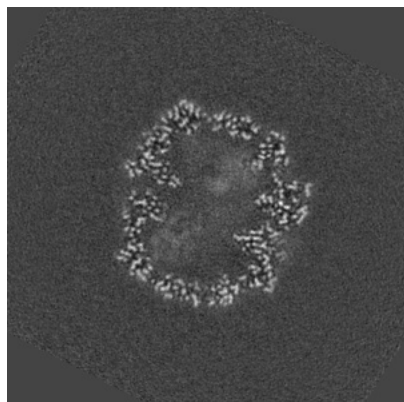


Y Index: 150

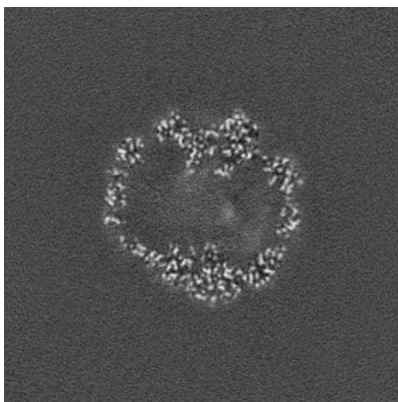


Z Index: 150

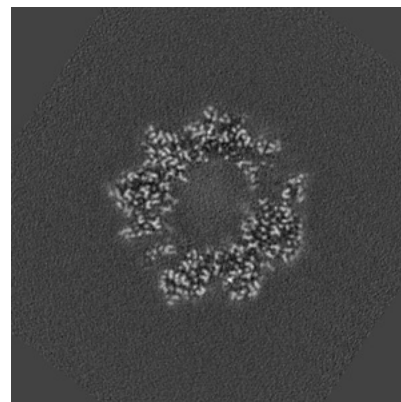
### 6.2.2 Raw map



X Index: 150



Y Index: 150



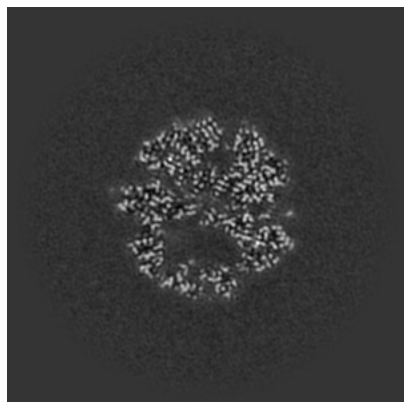
Z Index: 150

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

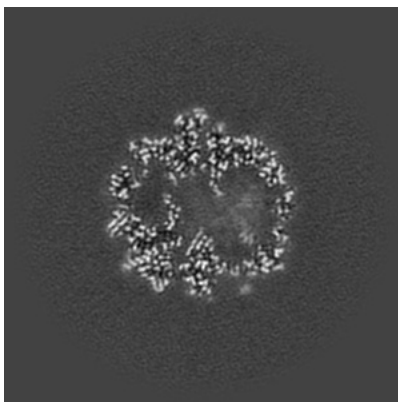


## 6.3 Largest variance slices [i](#)

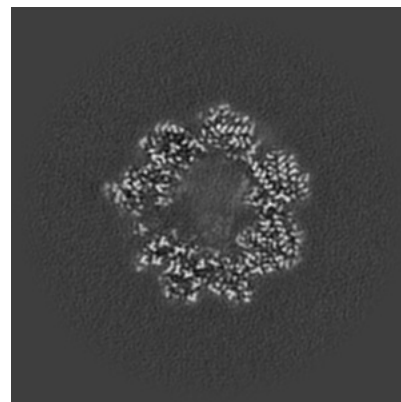
### 6.3.1 Primary map



X Index: 182

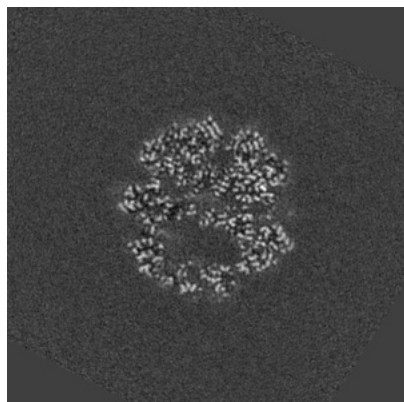


Y Index: 173

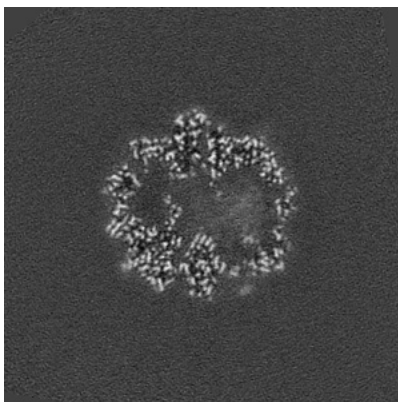


Z Index: 143

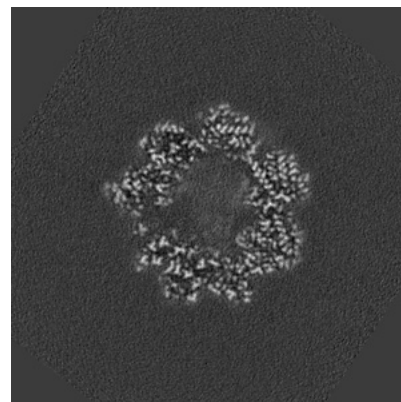
### 6.3.2 Raw map



X Index: 183



Y Index: 172

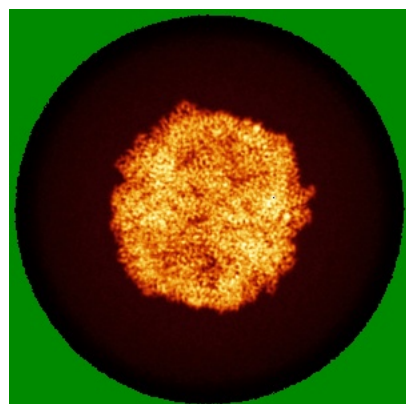


Z Index: 143

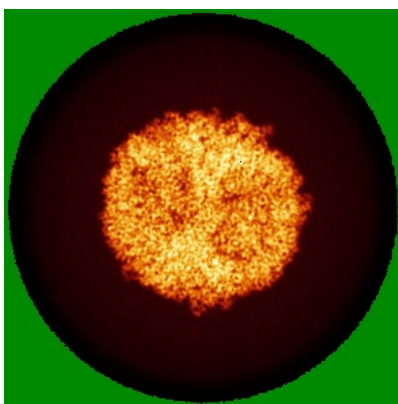
The images above show the largest variance slices of the map in three orthogonal directions.

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

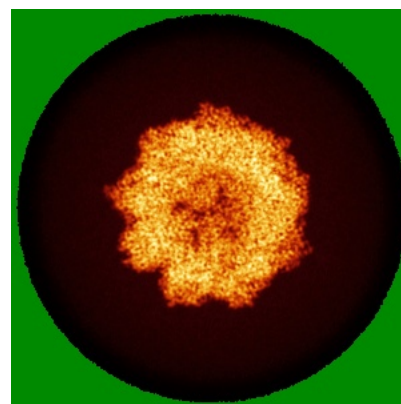
### 6.4.1 Primary map



X

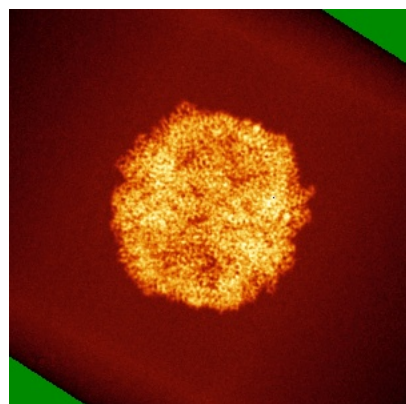


Y

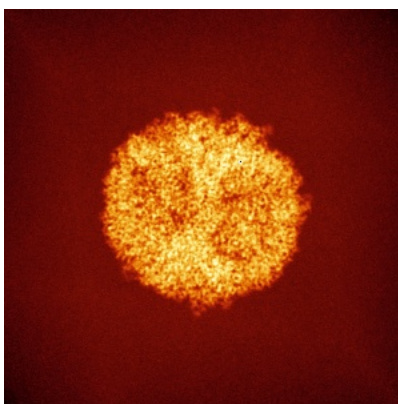


Z

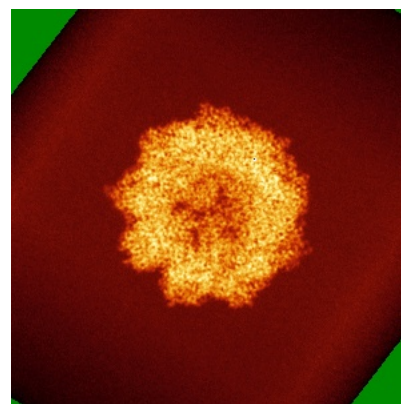
### 6.4.2 Raw map



X



Y



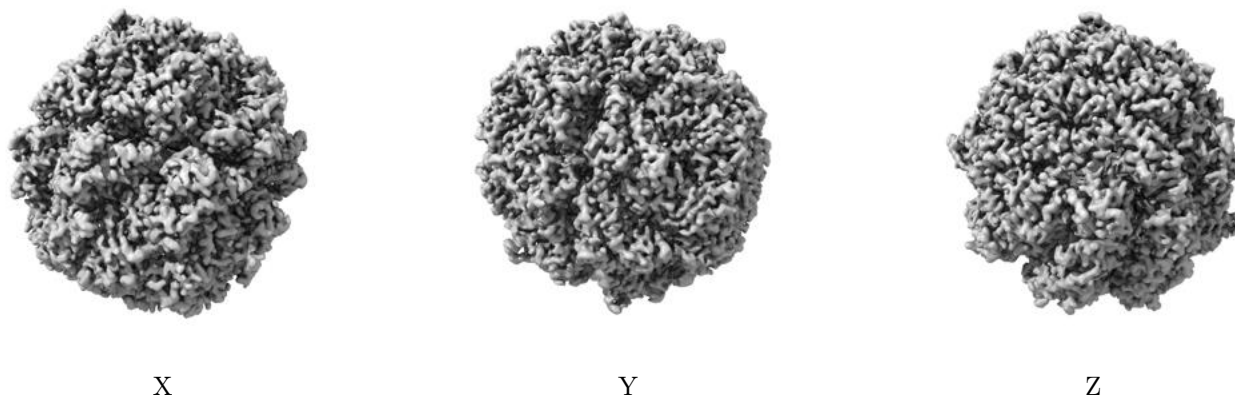
Z

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



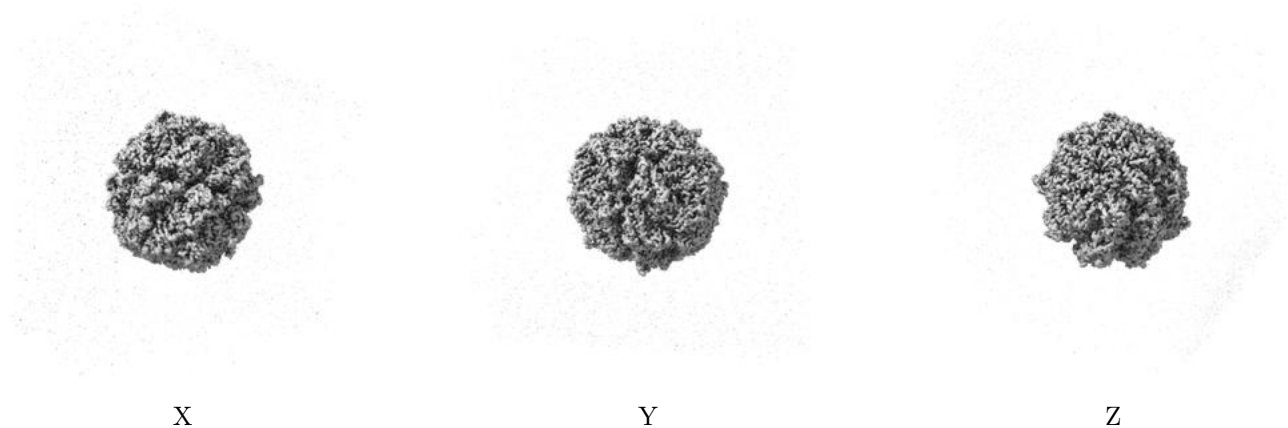
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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.

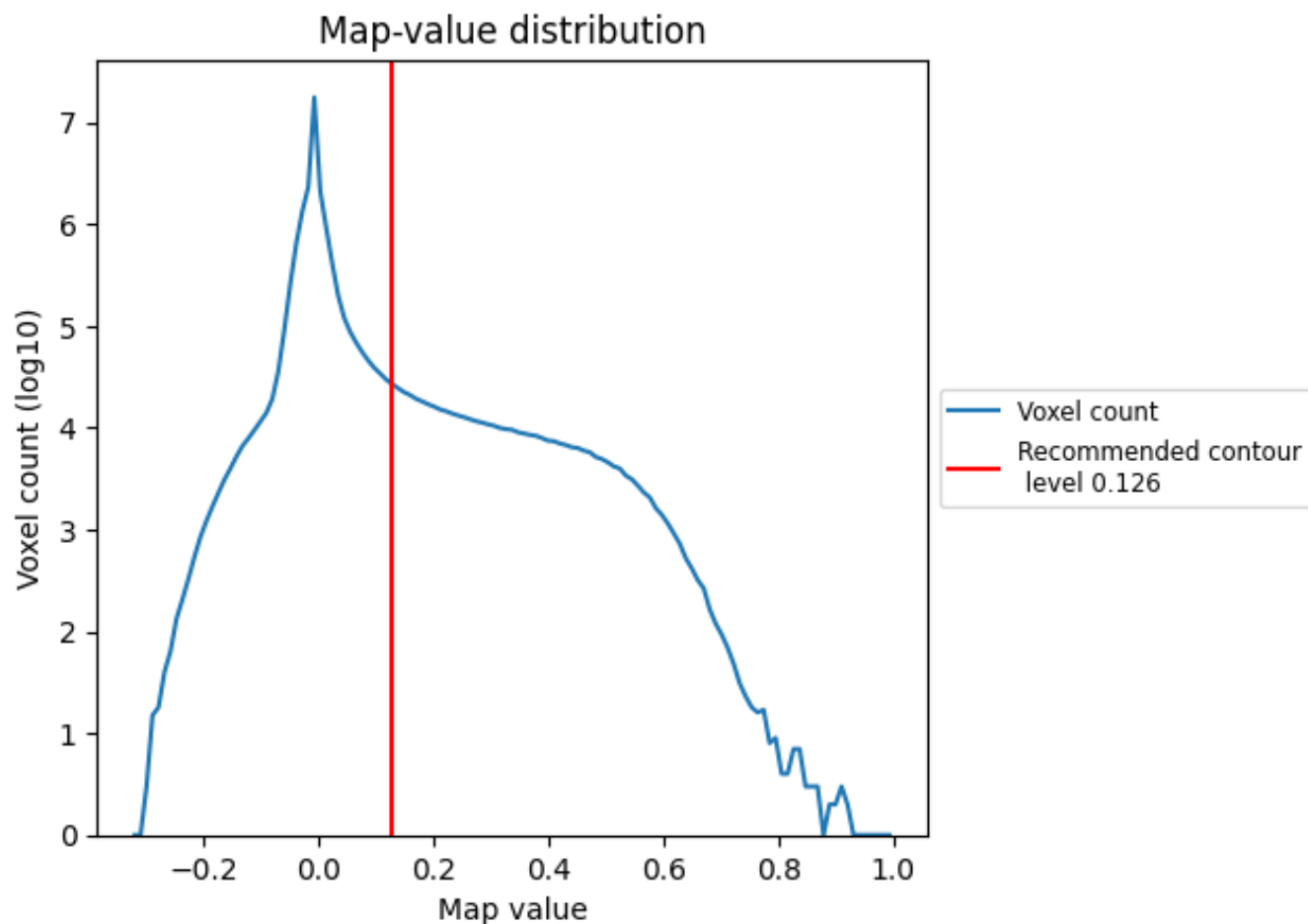
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

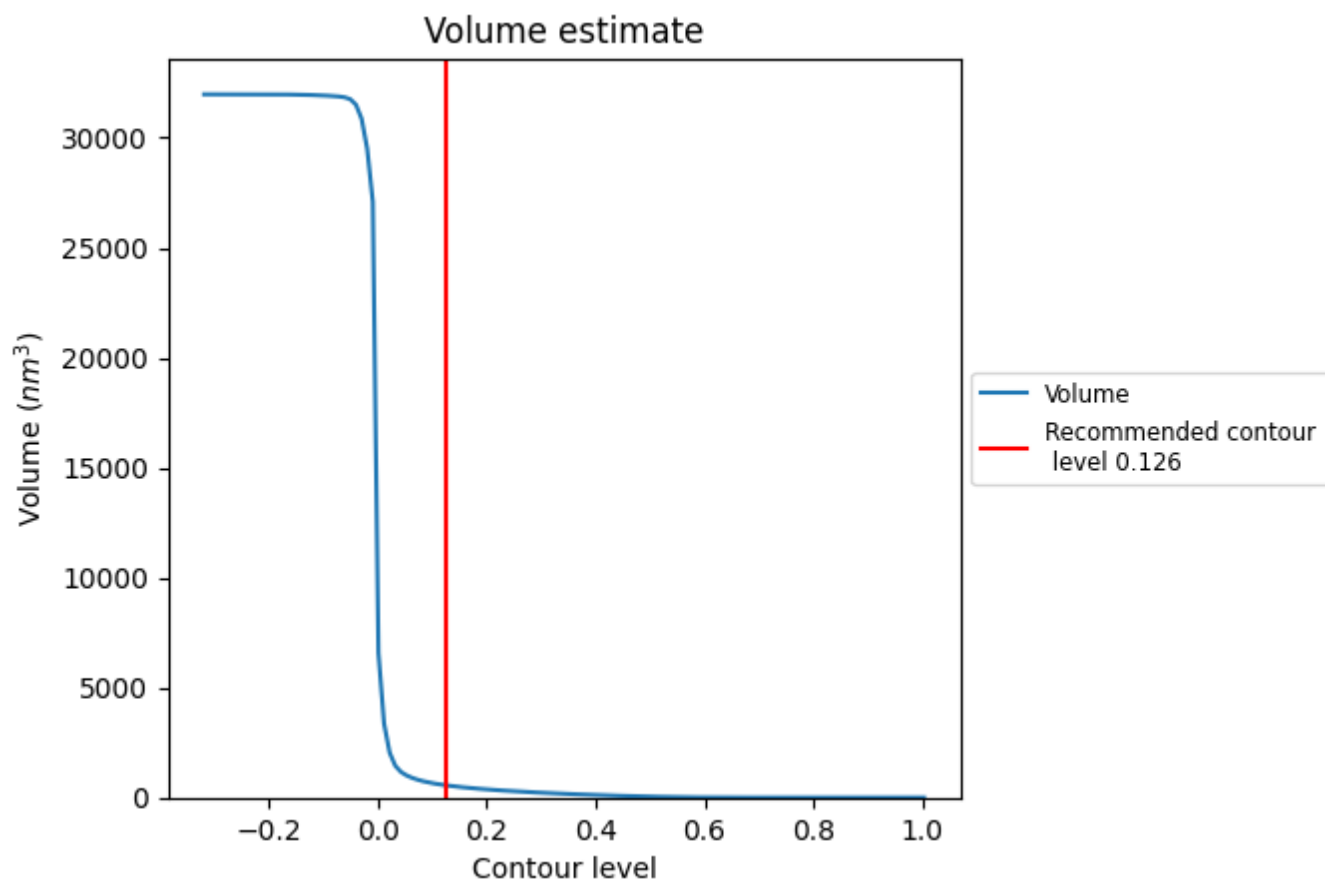
This section contains the results of statistical analysis of the map.

### 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.

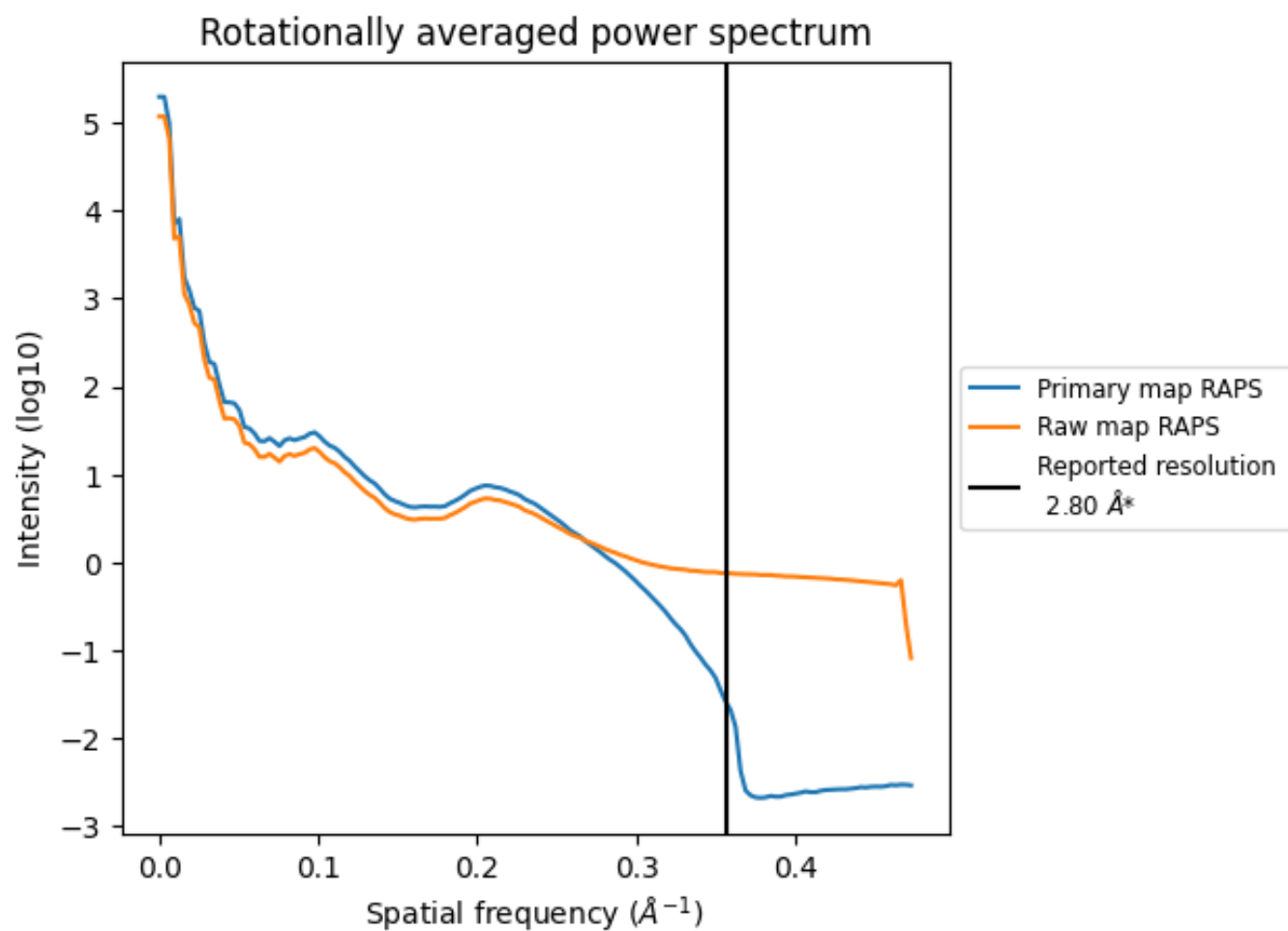
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 553 nm<sup>3</sup>; this corresponds to an approximate mass of 500 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 ⓘ

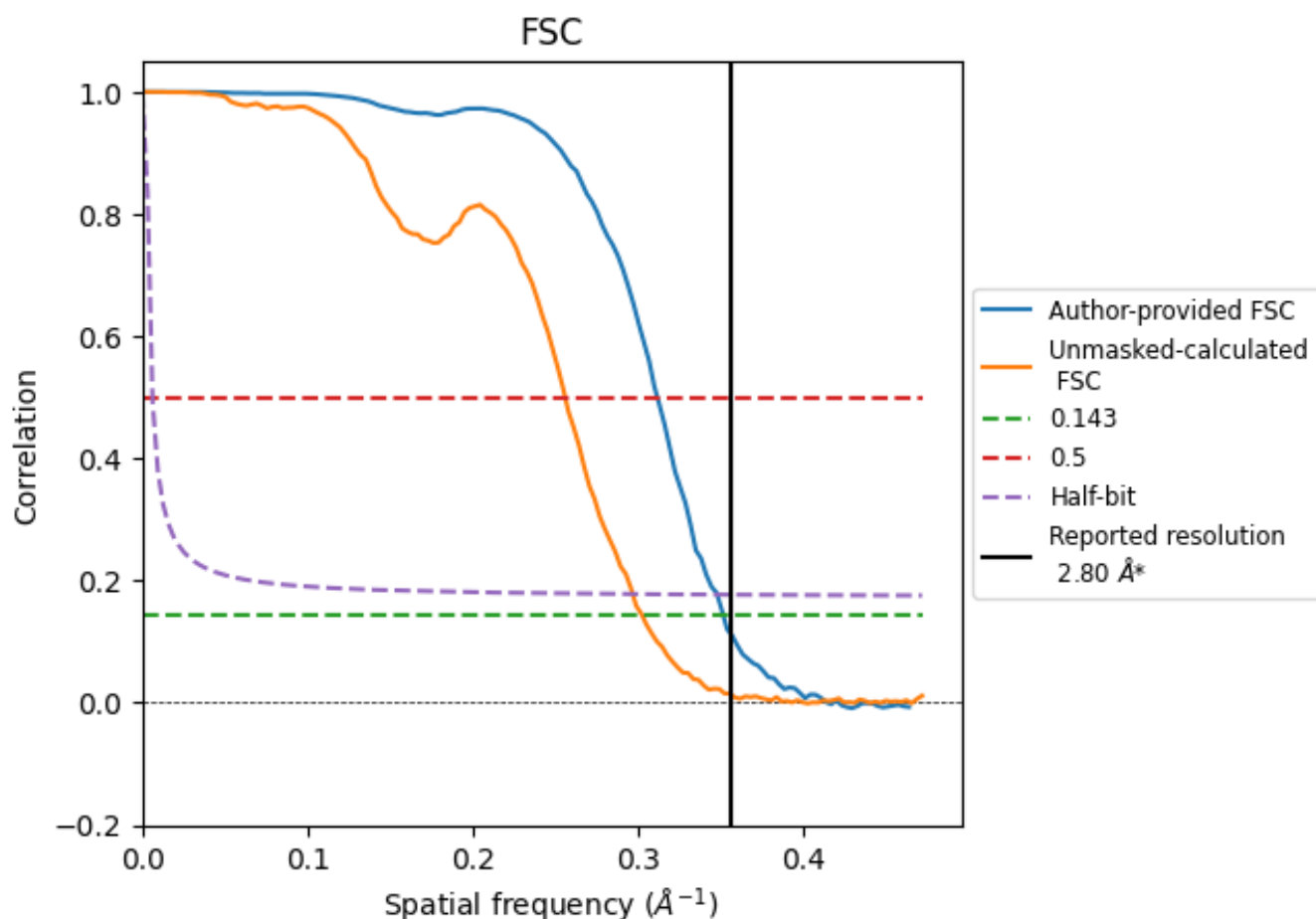


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

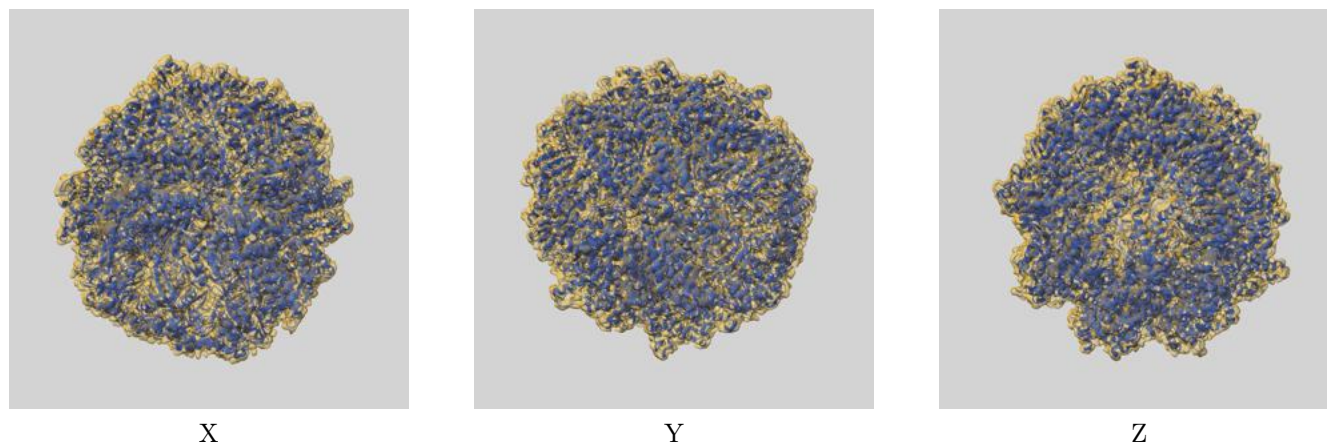
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.80                               | -    | -        |
| Author-provided FSC curve | 2.84                               | 3.20 | 2.87     |
| Unmasked-calculated*      | 3.30                               | 3.90 | 3.36     |

\*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 3.30 differs from the reported value 2.8 by more than 10 %

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

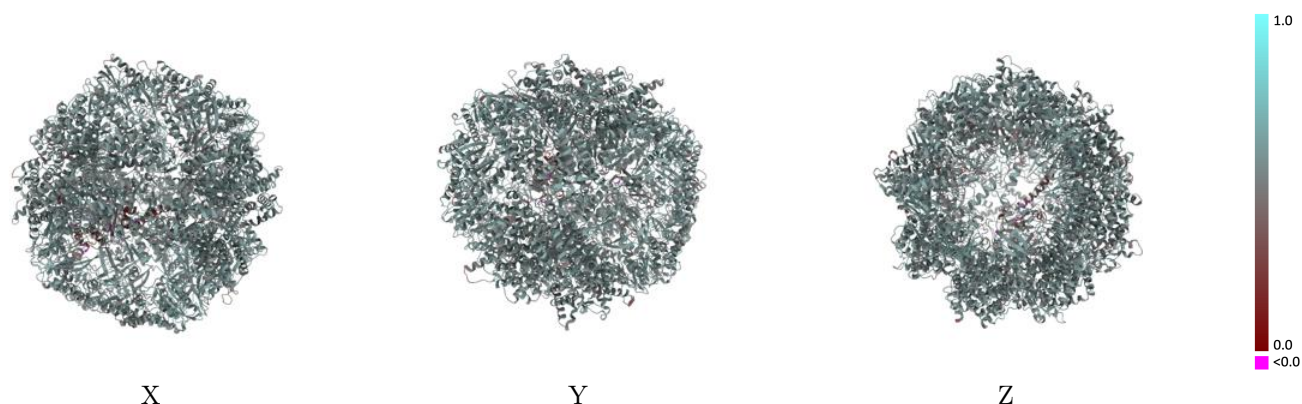
This section contains information regarding the fit between EMDB map EMD-40487 and PDB model 8SHG. Per-residue inclusion information can be found in section 3 on page 10.

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



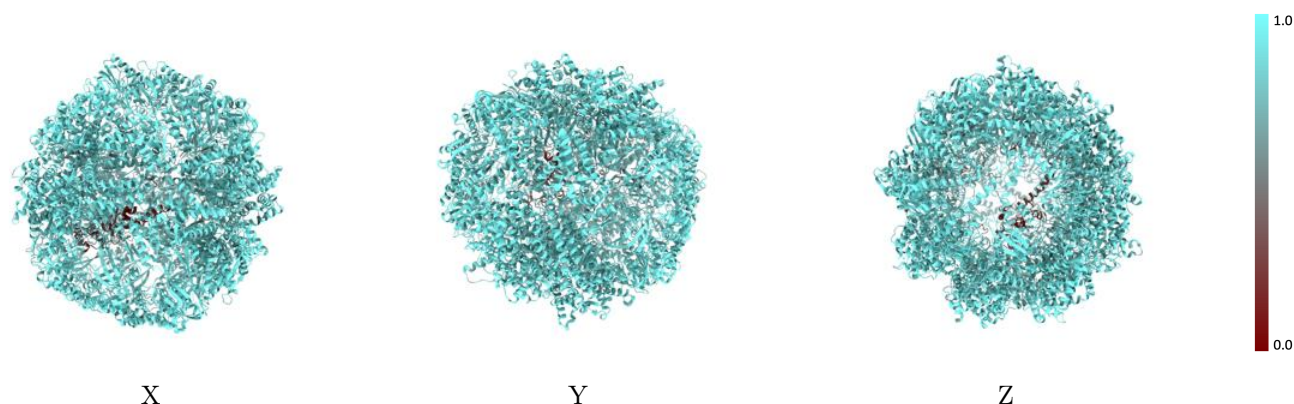
The images above show the 3D surface view of the map at the recommended contour level 0.126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

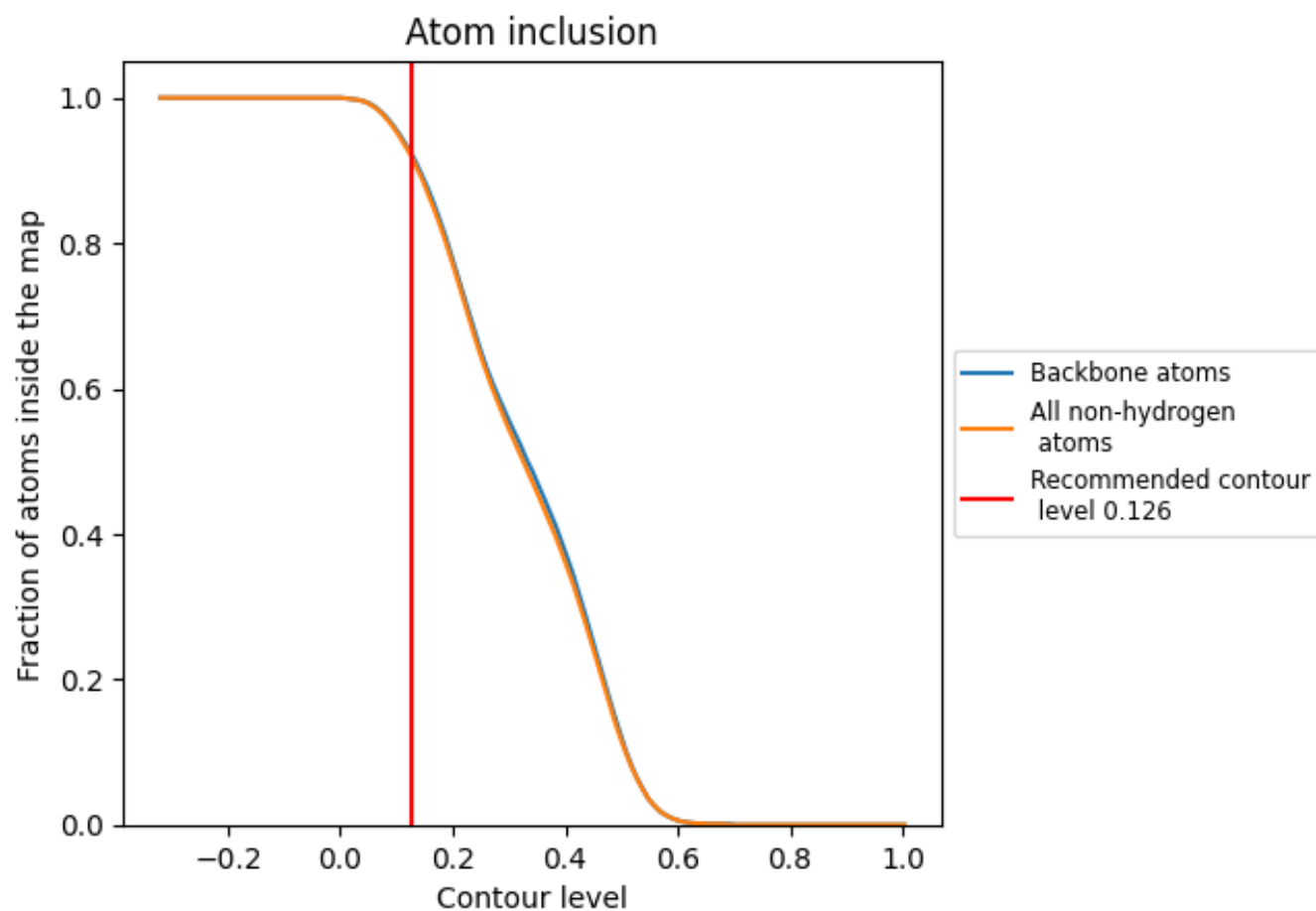
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 92% of all backbone atoms, 92% 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   |  0.9200   |  0.5450   |
| A     |  0.9330   |  0.5480   |
| B     |  0.9450   |  0.5570   |
| D     |  0.9410   |  0.5510   |
| E     |  0.9310   |  0.5530   |
| G     |  0.9360   |  0.5550   |
| H     |  0.9370   |  0.5530   |
| N     |  0.7430   |  0.4300   |
| P     |  0.3630   |  0.3280   |
| Q     |  0.9280   |  0.5460   |
| Z     |  0.9410   |  0.5520   |
| a     |  0.9340   |  0.5460   |
| b     |  0.9520   |  0.5590   |
| d     |  0.9400   |  0.5500   |
| e     |  0.9300  |  0.5500  |
| g     |  0.9390 |  0.5550 |
| h     |  0.9390 |  0.5530 |
| q     |  0.9380 |  0.5480 |
| z     |  0.9340 |  0.5490 |

