



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:16 AM UTC

PDB ID : 5OGC / pdb\_00005ogc  
EMDB ID : EMD-3803  
Title : Molecular basis of human kinesin-8 function and inhibition  
Authors : Locke, J.; Joseph, A.P.; Topf, M.; Moores, C.A.  
Deposited on : 2017-07-12  
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

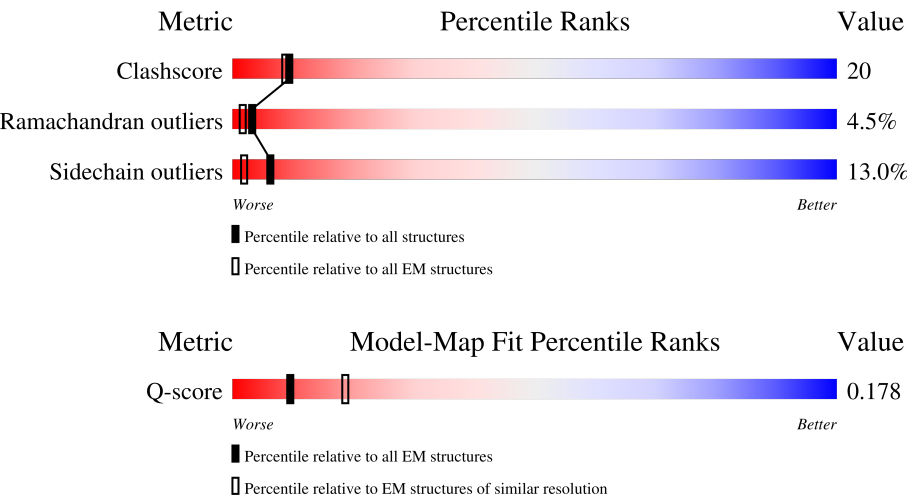
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 1575 ( 4.30 - 5.30 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1-K   | 377    |                  |
| 1   | 2-K   | 377    |                  |
| 2   | 1-A   | 451    |                  |
| 2   | 2-A   | 451    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3   | 1-B   | 445    |  |
| 3   | 2-B   | 445    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 7   | GTP  | 1-A   | 503 | -         | -        | X       | -                |
| 7   | GTP  | 2-A   | 503 | -         | -        | X       | -                |

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18580 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 Kinesin-like protein KIF18A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 1-K   | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2569  | 1605 | 463 | 489 | 12 |         |       |
| 1   | 2-K   | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2569  | 1605 | 463 | 489 | 12 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | -2      | GLY      | -      | expression tag | UNP Q8NI77 |
| K     | -1      | SER      | -      | expression tag | UNP Q8NI77 |
| K     | 0       | HIS      | -      | expression tag | UNP Q8NI77 |

- Molecule 2 is a protein called Tubulin alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 1-A   | 412      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3227  | 2043 | 551 | 613 | 20 |         |       |
| 2   | 2-A   | 412      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3227  | 2043 | 551 | 613 | 20 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 136     | SER      | LEU    | conflict | UNP F2Z4C1 |
| A     | 265     | GLY      | ILE    | conflict | UNP F2Z4C1 |
| A     | 358     | GLU      | GLN    | conflict | UNP F2Z4C1 |

- Molecule 3 is a protein called Tubulin beta chain.

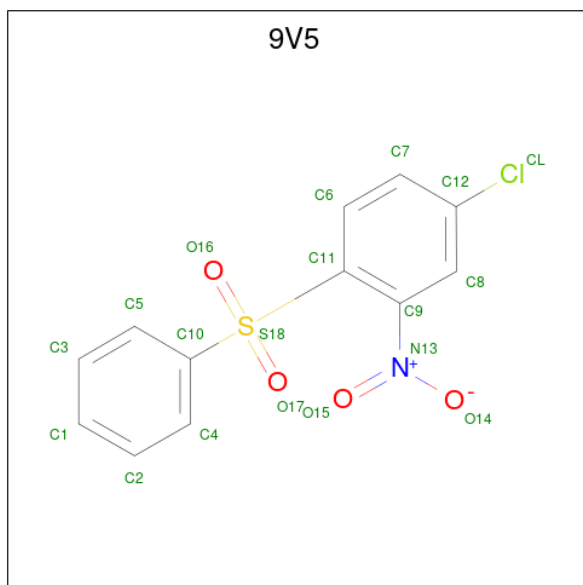
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 1-B   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3351  | 2105 | 575 | 646 | 25 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 2-B   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3351  | 2105 | 575 | 646 | 25 |         |       |

- Molecule 4 is 4-chloranyl-2-nitro-1-(phenylsulfonyl)benzene (CCD ID: 9V5) (formula:  $C_{12}H_8ClNO_4S$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |   |
|-----|-------|----------|-------|----|----|---|---|---------|---|
| 4   | 1-K   | 1        | Total | C  | Cl | N | O | S       | 0 |
|     |       |          | 19    | 12 | 1  | 1 | 4 | 1       |   |
| 4   | 2-K   | 1        | Total | C  | Cl | N | O | S       | 0 |
|     |       |          | 19    | 12 | 1  | 1 | 4 | 1       |   |

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 5   | 1-A   | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 5   | 2-A   | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula:  $Mg$ ).

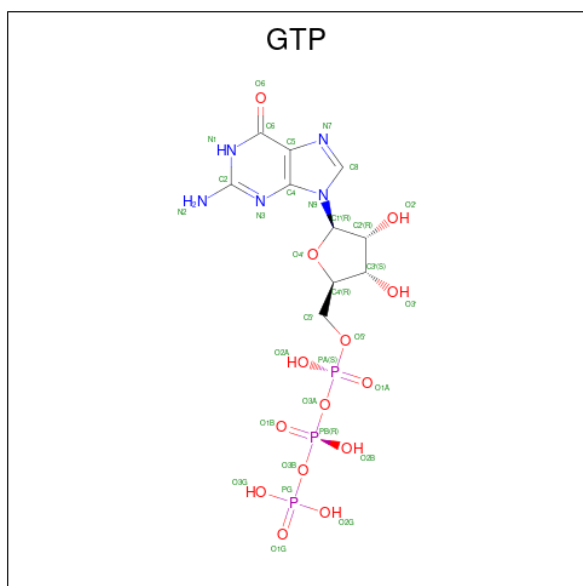
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 6   | 1-A   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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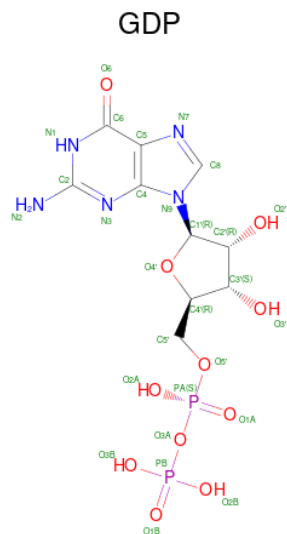
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 6   | 2-A   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



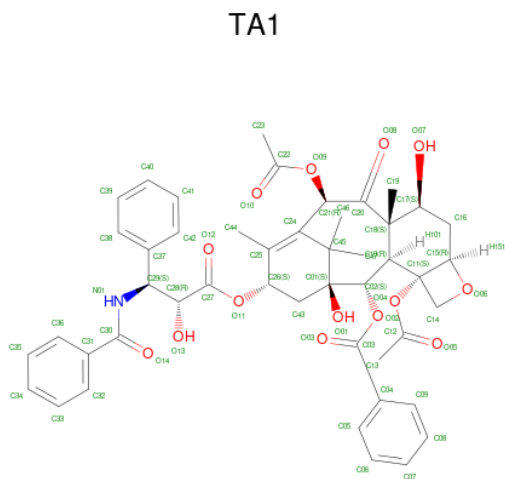
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 7   | 1-A   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 7   | 2-A   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 8   | 1-B   | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 8   | 2-B   | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

- Molecule 9 is TAXOL (CCD ID: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).

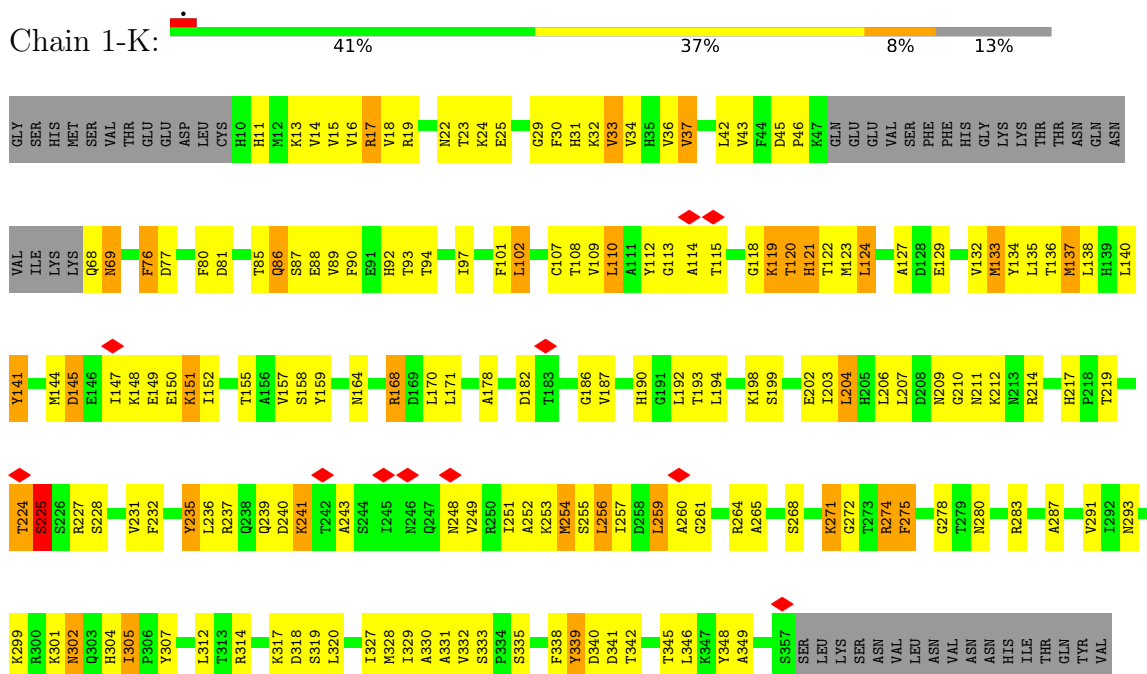


| Mol | Chain | Residues | Atoms       |         |        |         | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|
| 9   | 1-B   | 1        | Total<br>62 | C<br>47 | N<br>1 | O<br>14 | 0       |
| 9   | 2-B   | 1        | Total<br>62 | C<br>47 | N<br>1 | O<br>14 | 0       |

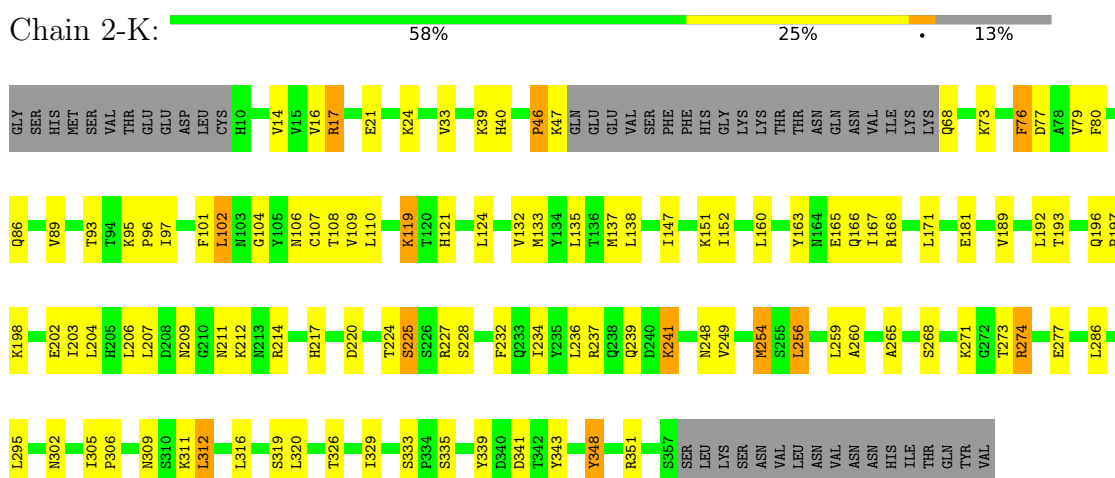
### 3 Residue-property plots

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.

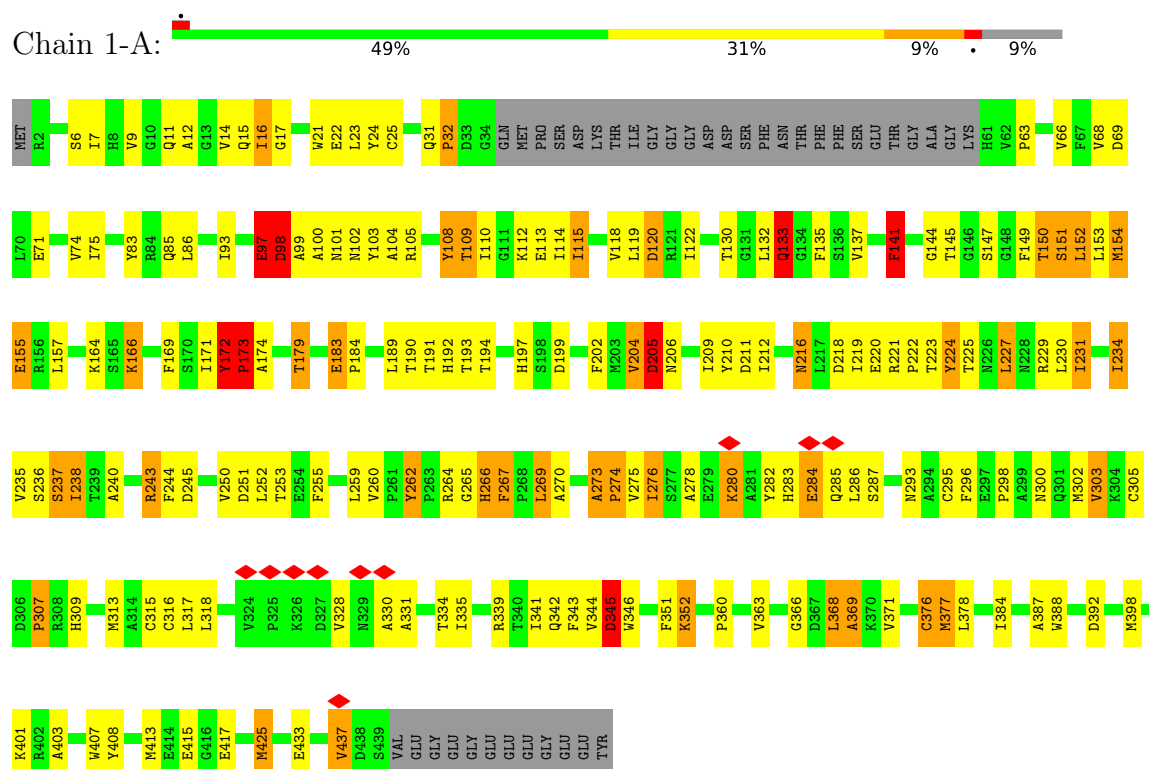
#### • Molecule 1: Kinesin-like protein KIF18A



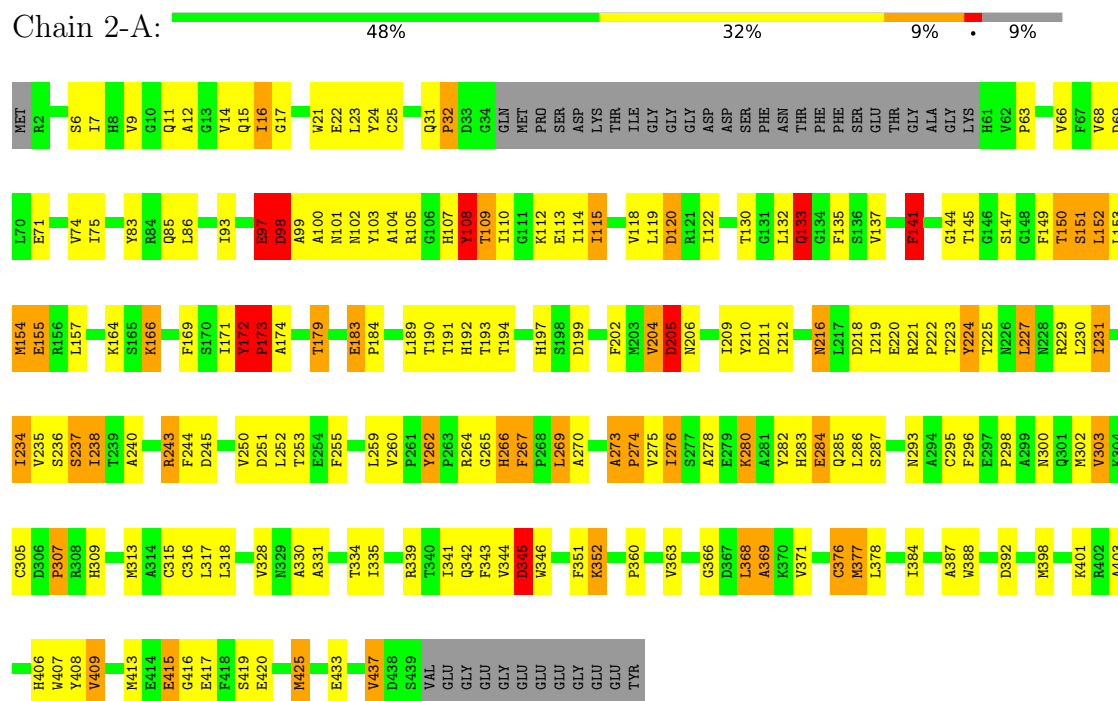
#### • Molecule 1: Kinesin-like protein KIF18A



- Molecule 2: Tubulin alpha chain

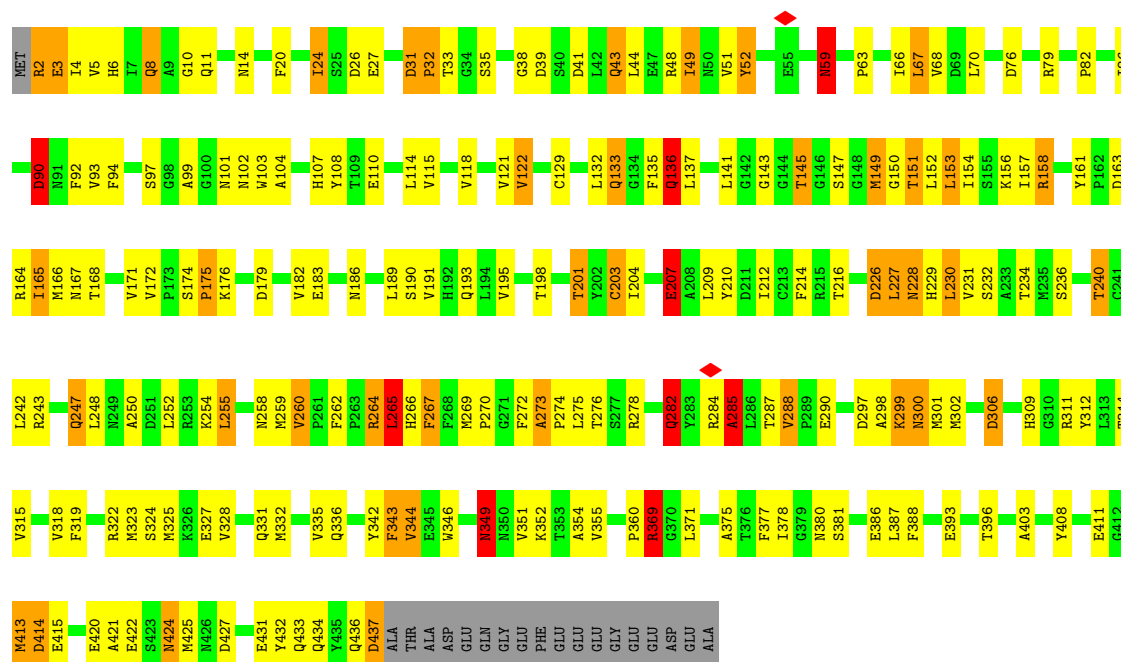


- Molecule 2: Tubulin alpha chain



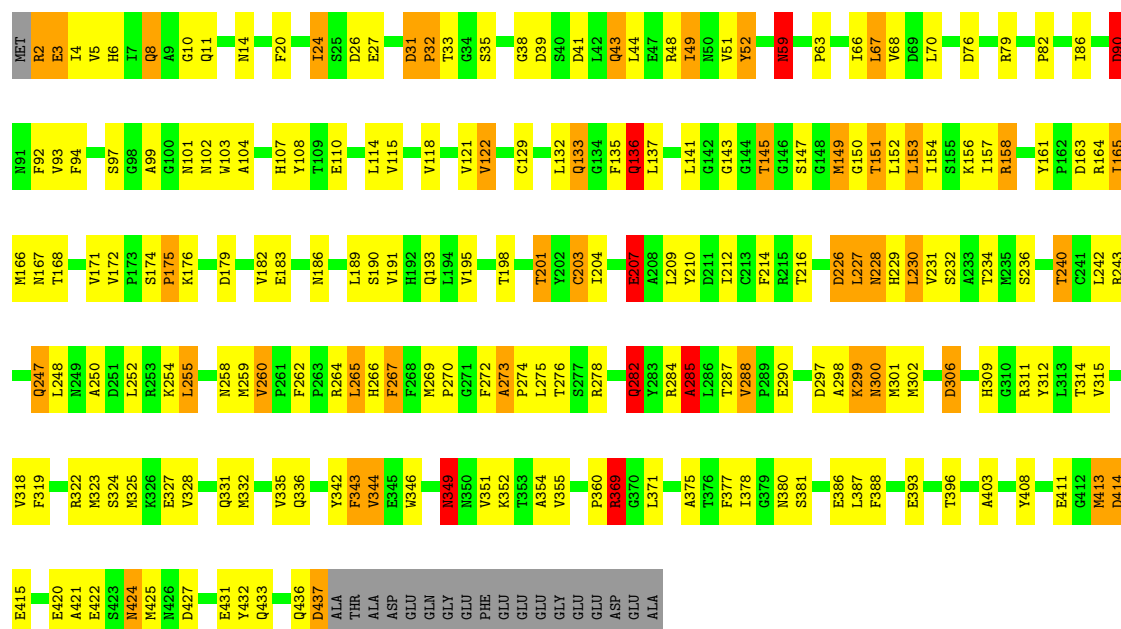
- Molecule 3: Tubulin beta chain





• Molecule 3: Tubulin beta chain

Chain 2-B: 49% 35% 9% . .



## 4 Experimental information

| Property                             | Value                                      | Source    |
|--------------------------------------|--------------------------------------------|-----------|
| EM reconstruction method             | HELICAL                                    | Depositor |
| Imposed symmetry                     | HELICAL, twist=0°, rise=81 Å, axial sym=C1 | Depositor |
| Number of segments used              | 135382                                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                          | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION    | Depositor |
| Microscope                           | FEI POLARA 300                             | Depositor |
| Voltage (kV)                         | 300                                        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 5                                          | Depositor |
| Minimum defocus (nm)                 | 500                                        | Depositor |
| Maximum defocus (nm)                 | 3500                                       | Depositor |
| Magnification                        | Not provided                               |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)                  | Depositor |
| Maximum map value                    | 0.204                                      | Depositor |
| Minimum map value                    | 0.000                                      | Depositor |
| Average map value                    | 0.020                                      | Depositor |
| Map value standard deviation         | 0.034                                      | Depositor |
| Recommended contour level            | 0.05                                       | Depositor |
| Map size (Å)                         | 112.59, 80.62, 104.25                      | wwPDB     |
| Map dimensions                       | 81, 58, 75                                 | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                           | wwPDB     |
| Pixel spacing (Å)                    | 1.39, 1.3900001, 1.39                      | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 9V5, GTP, GDP, ZN, TA1

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   | 1-K   | 0.32         | 0/2611         | 0.60        | 0/3524           |
| 1   | 2-K   | 0.32         | 0/2611         | 0.60        | 0/3524           |
| 2   | 1-A   | 0.81         | 0/3300         | 1.54        | 25/4482 (0.6%)   |
| 2   | 2-A   | 0.81         | 0/3300         | 1.54        | 25/4482 (0.6%)   |
| 3   | 1-B   | 0.82         | 2/3426 (0.1%)  | 1.53        | 29/4642 (0.6%)   |
| 3   | 2-B   | 0.82         | 2/3426 (0.1%)  | 1.53        | 29/4642 (0.6%)   |
| All | All   | 0.71         | 4/18674 (0.0%) | 1.34        | 108/25296 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 1-K   | 0                   | 27                  |
| 1   | 2-K   | 1                   | 3                   |
| 2   | 1-A   | 0                   | 27                  |
| 2   | 2-A   | 0                   | 32                  |
| 3   | 1-B   | 0                   | 28                  |
| 3   | 2-B   | 0                   | 28                  |
| All | All   | 1                   | 145                 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | 1-B   | 431 | GLU  | CD-OE2 | -5.61 | 1.14        | 1.25     |
| 3   | 2-B   | 431 | GLU  | CD-OE2 | -5.61 | 1.14        | 1.25     |
| 3   | 1-B   | 431 | GLU  | CD-OE1 | 5.51  | 1.35        | 1.25     |
| 3   | 2-B   | 431 | GLU  | CD-OE1 | 5.51  | 1.35        | 1.25     |

All (108) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 1-B   | 424 | ASN  | OD1-CG-ND2 | -8.42 | 114.18      | 122.60   |
| 3   | 2-B   | 424 | ASN  | OD1-CG-ND2 | -8.42 | 114.18      | 122.60   |
| 2   | 1-A   | 216 | ASN  | OD1-CG-ND2 | -8.39 | 114.21      | 122.60   |
| 2   | 2-A   | 216 | ASN  | OD1-CG-ND2 | -8.39 | 114.21      | 122.60   |
| 2   | 1-A   | 172 | TYR  | CB-CA-C    | 8.39  | 122.77      | 109.52   |
| 2   | 2-A   | 172 | TYR  | CB-CA-C    | 8.39  | 122.77      | 109.52   |
| 2   | 1-A   | 262 | TYR  | CA-C-N     | 8.21  | 127.93      | 119.56   |
| 2   | 1-A   | 262 | TYR  | C-N-CA     | 8.21  | 127.93      | 119.56   |
| 2   | 2-A   | 262 | TYR  | CA-C-N     | 8.21  | 127.93      | 119.56   |
| 2   | 2-A   | 262 | TYR  | C-N-CA     | 8.21  | 127.93      | 119.56   |
| 2   | 1-A   | 244 | PHE  | CA-CB-CG   | 7.87  | 121.67      | 113.80   |
| 2   | 2-A   | 244 | PHE  | CA-CB-CG   | 7.87  | 121.67      | 113.80   |
| 3   | 1-B   | 247 | GLN  | OE1-CD-NE2 | -7.60 | 115.00      | 122.60   |
| 3   | 2-B   | 247 | GLN  | OE1-CD-NE2 | -7.60 | 115.00      | 122.60   |
| 3   | 1-B   | 8   | GLN  | OE1-CD-NE2 | -7.33 | 115.27      | 122.60   |
| 3   | 2-B   | 8   | GLN  | OE1-CD-NE2 | -7.33 | 115.27      | 122.60   |
| 2   | 1-A   | 174 | ALA  | CA-C-N     | 7.30  | 127.31      | 119.28   |
| 2   | 1-A   | 174 | ALA  | C-N-CA     | 7.30  | 127.31      | 119.28   |
| 2   | 2-A   | 174 | ALA  | CA-C-N     | 7.30  | 127.31      | 119.28   |
| 2   | 2-A   | 174 | ALA  | C-N-CA     | 7.30  | 127.31      | 119.28   |
| 3   | 1-B   | 228 | ASN  | CA-CB-CG   | 6.98  | 119.58      | 112.60   |
| 3   | 2-B   | 228 | ASN  | CA-CB-CG   | 6.98  | 119.58      | 112.60   |
| 2   | 1-A   | 172 | TYR  | CA-C-N     | 6.76  | 128.29      | 119.84   |
| 2   | 1-A   | 172 | TYR  | C-N-CA     | 6.76  | 128.29      | 119.84   |
| 2   | 2-A   | 172 | TYR  | CA-C-N     | 6.76  | 128.29      | 119.84   |
| 2   | 2-A   | 172 | TYR  | C-N-CA     | 6.76  | 128.29      | 119.84   |
| 2   | 1-A   | 265 | GLY  | CA-C-N     | 6.58  | 134.11      | 121.54   |
| 2   | 1-A   | 265 | GLY  | C-N-CA     | 6.58  | 134.11      | 121.54   |
| 2   | 2-A   | 265 | GLY  | CA-C-N     | 6.58  | 134.11      | 121.54   |
| 2   | 2-A   | 265 | GLY  | C-N-CA     | 6.58  | 134.11      | 121.54   |
| 3   | 1-B   | 258 | ASN  | OD1-CG-ND2 | -6.56 | 116.04      | 122.60   |
| 3   | 2-B   | 258 | ASN  | OD1-CG-ND2 | -6.56 | 116.04      | 122.60   |
| 3   | 1-B   | 14  | ASN  | OD1-CG-ND2 | -6.34 | 116.26      | 122.60   |
| 3   | 2-B   | 14  | ASN  | OD1-CG-ND2 | -6.34 | 116.26      | 122.60   |
| 2   | 1-A   | 205 | ASP  | CA-CB-CG   | 6.29  | 118.89      | 112.60   |
| 2   | 2-A   | 205 | ASP  | CA-CB-CG   | 6.29  | 118.89      | 112.60   |
| 3   | 1-B   | 349 | ASN  | OD1-CG-ND2 | -6.29 | 116.31      | 122.60   |
| 3   | 2-B   | 349 | ASN  | OD1-CG-ND2 | -6.29 | 116.31      | 122.60   |
| 2   | 1-A   | 133 | GLN  | OE1-CD-NE2 | -6.26 | 116.34      | 122.60   |
| 2   | 2-A   | 133 | GLN  | OE1-CD-NE2 | -6.26 | 116.34      | 122.60   |
| 3   | 1-B   | 90  | ASP  | CA-CB-CG   | 6.24  | 118.84      | 112.60   |
| 3   | 2-B   | 90  | ASP  | CA-CB-CG   | 6.24  | 118.84      | 112.60   |
| 3   | 1-B   | 262 | PHE  | CA-C-N     | 6.20  | 127.58      | 119.84   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 1-B   | 262 | PHE  | C-N-CA     | 6.20  | 127.58      | 119.84   |
| 3   | 2-B   | 262 | PHE  | CA-C-N     | 6.20  | 127.58      | 119.84   |
| 3   | 2-B   | 262 | PHE  | C-N-CA     | 6.20  | 127.58      | 119.84   |
| 2   | 1-A   | 307 | PRO  | CA-C-N     | 6.14  | 130.43      | 120.60   |
| 2   | 1-A   | 307 | PRO  | C-N-CA     | 6.14  | 130.43      | 120.60   |
| 2   | 2-A   | 307 | PRO  | CA-C-N     | 6.14  | 130.43      | 120.60   |
| 2   | 2-A   | 307 | PRO  | C-N-CA     | 6.14  | 130.43      | 120.60   |
| 2   | 1-A   | 274 | PRO  | N-CA-CB    | 6.14  | 106.71      | 102.35   |
| 2   | 2-A   | 274 | PRO  | N-CA-CB    | 6.14  | 106.71      | 102.35   |
| 2   | 1-A   | 267 | PHE  | CA-CB-CG   | 6.05  | 119.85      | 113.80   |
| 2   | 2-A   | 267 | PHE  | CA-CB-CG   | 6.05  | 119.85      | 113.80   |
| 2   | 1-A   | 172 | TYR  | CA-CB-CG   | 5.97  | 124.65      | 113.90   |
| 2   | 2-A   | 172 | TYR  | CA-CB-CG   | 5.97  | 124.65      | 113.90   |
| 3   | 1-B   | 43  | GLN  | OE1-CD-NE2 | -5.94 | 116.66      | 122.60   |
| 3   | 2-B   | 43  | GLN  | OE1-CD-NE2 | -5.94 | 116.66      | 122.60   |
| 3   | 1-B   | 136 | GLN  | OE1-CD-NE2 | -5.87 | 116.73      | 122.60   |
| 3   | 2-B   | 136 | GLN  | OE1-CD-NE2 | -5.87 | 116.73      | 122.60   |
| 3   | 1-B   | 226 | ASP  | CA-CB-CG   | 5.86  | 118.46      | 112.60   |
| 3   | 2-B   | 226 | ASP  | CA-CB-CG   | 5.86  | 118.46      | 112.60   |
| 3   | 1-B   | 285 | ALA  | CA-C-N     | 5.76  | 129.85      | 120.23   |
| 3   | 1-B   | 285 | ALA  | C-N-CA     | 5.76  | 129.85      | 120.23   |
| 3   | 2-B   | 285 | ALA  | CA-C-N     | 5.76  | 129.85      | 120.23   |
| 3   | 2-B   | 285 | ALA  | C-N-CA     | 5.76  | 129.85      | 120.23   |
| 3   | 1-B   | 380 | ASN  | OD1-CG-ND2 | -5.67 | 116.93      | 122.60   |
| 3   | 2-B   | 380 | ASN  | OD1-CG-ND2 | -5.67 | 116.93      | 122.60   |
| 3   | 1-B   | 264 | ARG  | CA-C-N     | 5.67  | 132.36      | 121.54   |
| 3   | 1-B   | 264 | ARG  | C-N-CA     | 5.67  | 132.36      | 121.54   |
| 3   | 2-B   | 264 | ARG  | CA-C-N     | 5.67  | 132.36      | 121.54   |
| 3   | 2-B   | 264 | ARG  | C-N-CA     | 5.67  | 132.36      | 121.54   |
| 3   | 1-B   | 59  | ASN  | CA-CB-CG   | 5.51  | 118.11      | 112.60   |
| 3   | 2-B   | 59  | ASN  | CA-CB-CG   | 5.51  | 118.11      | 112.60   |
| 3   | 1-B   | 133 | GLN  | OE1-CD-NE2 | -5.42 | 117.18      | 122.60   |
| 3   | 2-B   | 133 | GLN  | OE1-CD-NE2 | -5.42 | 117.18      | 122.60   |
| 3   | 1-B   | 436 | GLN  | CA-C-N     | 5.42  | 131.46      | 121.70   |
| 3   | 1-B   | 436 | GLN  | C-N-CA     | 5.42  | 131.46      | 121.70   |
| 3   | 2-B   | 436 | GLN  | CA-C-N     | 5.42  | 131.46      | 121.70   |
| 3   | 2-B   | 436 | GLN  | C-N-CA     | 5.42  | 131.46      | 121.70   |
| 2   | 1-A   | 293 | ASN  | OD1-CG-ND2 | -5.40 | 117.20      | 122.60   |
| 2   | 2-A   | 293 | ASN  | OD1-CG-ND2 | -5.40 | 117.20      | 122.60   |
| 3   | 1-B   | 107 | HIS  | CB-CG-CD2  | -5.27 | 124.35      | 131.20   |
| 3   | 2-B   | 107 | HIS  | CB-CG-CD2  | -5.27 | 124.35      | 131.20   |
| 3   | 1-B   | 260 | VAL  | CB-CA-C    | 5.24  | 116.06      | 111.08   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 2-B   | 260 | VAL  | CB-CA-C    | 5.24  | 116.06      | 111.08   |
| 2   | 1-A   | 283 | HIS  | CA-C-N     | 5.22  | 131.52      | 121.54   |
| 2   | 1-A   | 283 | HIS  | C-N-CA     | 5.22  | 131.52      | 121.54   |
| 2   | 2-A   | 283 | HIS  | CA-C-N     | 5.22  | 131.52      | 121.54   |
| 2   | 2-A   | 283 | HIS  | C-N-CA     | 5.22  | 131.52      | 121.54   |
| 2   | 1-A   | 147 | SER  | CA-C-N     | 5.20  | 125.61      | 119.94   |
| 2   | 1-A   | 147 | SER  | C-N-CA     | 5.20  | 125.61      | 119.94   |
| 2   | 2-A   | 147 | SER  | CA-C-N     | 5.20  | 125.61      | 119.94   |
| 2   | 2-A   | 147 | SER  | C-N-CA     | 5.20  | 125.61      | 119.94   |
| 3   | 1-B   | 49  | ILE  | CB-CA-C    | -5.15 | 104.53      | 112.05   |
| 3   | 2-B   | 49  | ILE  | CB-CA-C    | -5.15 | 104.53      | 112.05   |
| 2   | 1-A   | 85  | GLN  | OE1-CD-NE2 | -5.12 | 117.48      | 122.60   |
| 2   | 2-A   | 85  | GLN  | OE1-CD-NE2 | -5.12 | 117.48      | 122.60   |
| 3   | 1-B   | 31  | ASP  | CA-C-N     | 5.11  | 126.23      | 119.84   |
| 3   | 1-B   | 31  | ASP  | C-N-CA     | 5.11  | 126.23      | 119.84   |
| 3   | 2-B   | 31  | ASP  | CA-C-N     | 5.11  | 126.23      | 119.84   |
| 3   | 2-B   | 31  | ASP  | C-N-CA     | 5.11  | 126.23      | 119.84   |
| 3   | 1-B   | 282 | GLN  | OE1-CD-NE2 | -5.10 | 117.50      | 122.60   |
| 3   | 2-B   | 282 | GLN  | OE1-CD-NE2 | -5.10 | 117.50      | 122.60   |
| 3   | 1-B   | 433 | GLN  | OE1-CD-NE2 | -5.08 | 117.52      | 122.60   |
| 3   | 2-B   | 433 | GLN  | OE1-CD-NE2 | -5.08 | 117.52      | 122.60   |
| 2   | 1-A   | 369 | ALA  | N-CA-C     | 5.01  | 117.12      | 111.11   |
| 2   | 2-A   | 369 | ALA  | N-CA-C     | 5.01  | 117.12      | 111.11   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | 2-K   | 47  | LYS  | CA   |

All (145) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 1-A   | 113 | GLU  | Sidechain |
| 2   | 1-A   | 120 | ASP  | Sidechain |
| 2   | 1-A   | 133 | GLN  | Sidechain |
| 2   | 1-A   | 151 | SER  | Mainchain |
| 2   | 1-A   | 166 | LYS  | Mainchain |
| 2   | 1-A   | 17  | GLY  | Mainchain |
| 2   | 1-A   | 179 | THR  | Mainchain |
| 2   | 1-A   | 199 | ASP  | Sidechain |
| 2   | 1-A   | 205 | ASP  | Sidechain |
| 2   | 1-A   | 211 | ASP  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 1-A   | 216 | ASN  | Sidechain |
| 2   | 1-A   | 218 | ASP  | Sidechain |
| 2   | 1-A   | 22  | GLU  | Sidechain |
| 2   | 1-A   | 227 | LEU  | Mainchain |
| 2   | 1-A   | 243 | ARG  | Sidechain |
| 2   | 1-A   | 262 | TYR  | Sidechain |
| 2   | 1-A   | 282 | TYR  | Sidechain |
| 2   | 1-A   | 286 | LEU  | Mainchain |
| 2   | 1-A   | 300 | ASN  | Sidechain |
| 2   | 1-A   | 345 | ASP  | Sidechain |
| 2   | 1-A   | 360 | PRO  | Mainchain |
| 2   | 1-A   | 392 | ASP  | Mainchain |
| 2   | 1-A   | 437 | VAL  | Mainchain |
| 2   | 1-A   | 71  | GLU  | Sidechain |
| 2   | 1-A   | 83  | TYR  | Sidechain |
| 2   | 1-A   | 97  | GLU  | Sidechain |
| 2   | 1-A   | 98  | ASP  | Sidechain |
| 3   | 1-B   | 11  | GLN  | Sidechain |
| 3   | 1-B   | 110 | GLU  | Sidechain |
| 3   | 1-B   | 136 | GLN  | Sidechain |
| 3   | 1-B   | 158 | ARG  | Sidechain |
| 3   | 1-B   | 171 | VAL  | Mainchain |
| 3   | 1-B   | 175 | PRO  | Mainchain |
| 3   | 1-B   | 2   | ARG  | Mainchain |
| 3   | 1-B   | 207 | GLU  | Sidechain |
| 3   | 1-B   | 216 | THR  | Mainchain |
| 3   | 1-B   | 247 | GLN  | Sidechain |
| 3   | 1-B   | 255 | LEU  | Mainchain |
| 3   | 1-B   | 285 | ALA  | Mainchain |
| 3   | 1-B   | 3   | GLU  | Sidechain |
| 3   | 1-B   | 306 | ASP  | Sidechain |
| 3   | 1-B   | 31  | ASP  | Sidechain |
| 3   | 1-B   | 312 | TYR  | Sidechain |
| 3   | 1-B   | 327 | GLU  | Sidechain |
| 3   | 1-B   | 388 | PHE  | Mainchain |
| 3   | 1-B   | 39  | ASP  | Sidechain |
| 3   | 1-B   | 393 | GLU  | Sidechain |
| 3   | 1-B   | 411 | GLU  | Sidechain |
| 3   | 1-B   | 414 | ASP  | Sidechain |
| 3   | 1-B   | 415 | GLU  | Sidechain |
| 3   | 1-B   | 420 | GLU  | Sidechain |
| 3   | 1-B   | 437 | ASP  | Sidechain |

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| Mol | Chain | Res | Type | Group               |
|-----|-------|-----|------|---------------------|
| 3   | 1-B   | 5   | VAL  | Mainchain           |
| 3   | 1-B   | 52  | TYR  | Sidechain           |
| 3   | 1-B   | 90  | ASP  | Sidechain           |
| 1   | 1-K   | 120 | THR  | Mainchain           |
| 1   | 1-K   | 141 | TYR  | Sidechain           |
| 1   | 1-K   | 145 | ASP  | Sidechain,Mainchain |
| 1   | 1-K   | 149 | GLU  | Mainchain           |
| 1   | 1-K   | 150 | GLU  | Sidechain           |
| 1   | 1-K   | 168 | ARG  | Sidechain           |
| 1   | 1-K   | 182 | ASP  | Sidechain           |
| 1   | 1-K   | 186 | GLY  | Mainchain           |
| 1   | 1-K   | 202 | GLU  | Sidechain           |
| 1   | 1-K   | 225 | SER  | Mainchain           |
| 1   | 1-K   | 228 | SER  | Mainchain           |
| 1   | 1-K   | 235 | TYR  | Sidechain           |
| 1   | 1-K   | 264 | ARG  | Mainchain           |
| 1   | 1-K   | 271 | LYS  | Mainchain           |
| 1   | 1-K   | 275 | PHE  | Mainchain           |
| 1   | 1-K   | 278 | GLY  | Mainchain           |
| 1   | 1-K   | 283 | ARG  | Sidechain           |
| 1   | 1-K   | 293 | ASN  | Mainchain           |
| 1   | 1-K   | 318 | ASP  | Sidechain           |
| 1   | 1-K   | 339 | TYR  | Sidechain           |
| 1   | 1-K   | 340 | ASP  | Sidechain           |
| 1   | 1-K   | 348 | TYR  | Sidechain           |
| 1   | 1-K   | 69  | ASN  | Sidechain           |
| 1   | 1-K   | 77  | ASP  | Peptide             |
| 1   | 1-K   | 81  | ASP  | Sidechain           |
| 1   | 1-K   | 86  | GLN  | Sidechain           |
| 2   | 2-A   | 108 | TYR  | Sidechain           |
| 2   | 2-A   | 113 | GLU  | Sidechain           |
| 2   | 2-A   | 120 | ASP  | Sidechain           |
| 2   | 2-A   | 133 | GLN  | Sidechain           |
| 2   | 2-A   | 151 | SER  | Mainchain           |
| 2   | 2-A   | 166 | LYS  | Mainchain           |
| 2   | 2-A   | 17  | GLY  | Mainchain           |
| 2   | 2-A   | 179 | THR  | Mainchain           |
| 2   | 2-A   | 199 | ASP  | Sidechain           |
| 2   | 2-A   | 205 | ASP  | Sidechain           |
| 2   | 2-A   | 211 | ASP  | Sidechain           |
| 2   | 2-A   | 216 | ASN  | Sidechain           |
| 2   | 2-A   | 218 | ASP  | Sidechain           |

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| Mol | Chain | Res | Type | Group               |
|-----|-------|-----|------|---------------------|
| 2   | 2-A   | 22  | GLU  | Sidechain           |
| 2   | 2-A   | 227 | LEU  | Mainchain           |
| 2   | 2-A   | 243 | ARG  | Sidechain           |
| 2   | 2-A   | 262 | TYR  | Sidechain           |
| 2   | 2-A   | 282 | TYR  | Sidechain           |
| 2   | 2-A   | 286 | LEU  | Mainchain           |
| 2   | 2-A   | 300 | ASN  | Sidechain           |
| 2   | 2-A   | 345 | ASP  | Sidechain           |
| 2   | 2-A   | 360 | PRO  | Mainchain           |
| 2   | 2-A   | 392 | ASP  | Mainchain           |
| 2   | 2-A   | 409 | VAL  | Mainchain           |
| 2   | 2-A   | 416 | GLY  | Mainchain           |
| 2   | 2-A   | 420 | GLU  | Sidechain,Mainchain |
| 2   | 2-A   | 437 | VAL  | Mainchain           |
| 2   | 2-A   | 71  | GLU  | Sidechain           |
| 2   | 2-A   | 83  | TYR  | Sidechain           |
| 2   | 2-A   | 97  | GLU  | Sidechain           |
| 2   | 2-A   | 98  | ASP  | Sidechain           |
| 3   | 2-B   | 11  | GLN  | Sidechain           |
| 3   | 2-B   | 110 | GLU  | Sidechain           |
| 3   | 2-B   | 136 | GLN  | Sidechain           |
| 3   | 2-B   | 158 | ARG  | Sidechain           |
| 3   | 2-B   | 171 | VAL  | Mainchain           |
| 3   | 2-B   | 175 | PRO  | Mainchain           |
| 3   | 2-B   | 2   | ARG  | Mainchain           |
| 3   | 2-B   | 207 | GLU  | Sidechain           |
| 3   | 2-B   | 216 | THR  | Mainchain           |
| 3   | 2-B   | 247 | GLN  | Sidechain           |
| 3   | 2-B   | 255 | LEU  | Mainchain           |
| 3   | 2-B   | 285 | ALA  | Mainchain           |
| 3   | 2-B   | 3   | GLU  | Sidechain           |
| 3   | 2-B   | 306 | ASP  | Sidechain           |
| 3   | 2-B   | 31  | ASP  | Sidechain           |
| 3   | 2-B   | 312 | TYR  | Sidechain           |
| 3   | 2-B   | 327 | GLU  | Sidechain           |
| 3   | 2-B   | 388 | PHE  | Mainchain           |
| 3   | 2-B   | 39  | ASP  | Sidechain           |
| 3   | 2-B   | 393 | GLU  | Sidechain           |
| 3   | 2-B   | 411 | GLU  | Sidechain           |
| 3   | 2-B   | 414 | ASP  | Sidechain           |
| 3   | 2-B   | 415 | GLU  | Sidechain           |
| 3   | 2-B   | 420 | GLU  | Sidechain           |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | 2-B   | 437 | ASP  | Sidechain |
| 3   | 2-B   | 5   | VAL  | Mainchain |
| 3   | 2-B   | 52  | TYR  | Sidechain |
| 3   | 2-B   | 90  | ASP  | Sidechain |
| 1   | 2-K   | 181 | GLU  | Sidechain |
| 1   | 2-K   | 343 | TYR  | Mainchain |
| 1   | 2-K   | 348 | TYR  | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1-K   | 2569  | 0        | 2587     | 157     | 0            |
| 1   | 2-K   | 2569  | 0        | 2587     | 65      | 0            |
| 2   | 1-A   | 3227  | 0        | 3143     | 130     | 0            |
| 2   | 2-A   | 3227  | 0        | 3143     | 137     | 0            |
| 3   | 1-B   | 3351  | 0        | 3229     | 136     | 0            |
| 3   | 2-B   | 3351  | 0        | 3229     | 133     | 0            |
| 4   | 1-K   | 19    | 0        | 0        | 0       | 0            |
| 4   | 2-K   | 19    | 0        | 0        | 5       | 0            |
| 5   | 1-A   | 1     | 0        | 0        | 0       | 0            |
| 5   | 2-A   | 1     | 0        | 0        | 0       | 0            |
| 6   | 1-A   | 1     | 0        | 0        | 0       | 0            |
| 6   | 2-A   | 1     | 0        | 0        | 0       | 0            |
| 7   | 1-A   | 32    | 0        | 12       | 10      | 0            |
| 7   | 2-A   | 32    | 0        | 12       | 10      | 0            |
| 8   | 1-B   | 28    | 0        | 12       | 2       | 0            |
| 8   | 2-B   | 28    | 0        | 12       | 2       | 0            |
| 9   | 1-B   | 62    | 0        | 51       | 7       | 0            |
| 9   | 2-B   | 62    | 0        | 51       | 7       | 0            |
| All | All   | 18580 | 0        | 18068    | 740     | 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 20.

All (740) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:33:VAL:HG13  | 1:K:34:VAL:H     | 1.05                     | 1.12              |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:HD21 | 1.32                     | 1.11              |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:HD21 | 1.32                     | 1.11              |
| 1:K:31:HIS:HE1   | 1:K:46:PRO:O     | 1.40                     | 1.02              |
| 1:K:291:VAL:HG13 | 1:K:305:ILE:HD11 | 1.41                     | 0.97              |
| 1:K:31:HIS:CE1   | 1:K:46:PRO:O     | 2.18                     | 0.96              |
| 1:K:33:VAL:HG23  | 1:K:339:TYR:HA   | 1.44                     | 0.96              |
| 3:B:323:MET:HE2  | 3:B:328:VAL:HG22 | 1.48                     | 0.95              |
| 3:B:323:MET:HE2  | 3:B:328:VAL:HG22 | 1.48                     | 0.95              |
| 1:K:19:ARG:HB2   | 1:K:119:LYS:HG3  | 1.48                     | 0.94              |
| 1:K:33:VAL:HG13  | 1:K:34:VAL:N     | 1.85                     | 0.91              |
| 1:K:110:LEU:HD23 | 1:K:257:ILE:HD11 | 1.55                     | 0.88              |
| 2:A:7:ILE:HG22   | 2:A:66:VAL:HG22  | 1.56                     | 0.87              |
| 2:A:7:ILE:HG22   | 2:A:66:VAL:HG22  | 1.56                     | 0.87              |
| 1:K:16:VAL:HG22  | 1:K:330:ALA:HB3  | 1.56                     | 0.86              |
| 3:B:234:THR:HG21 | 3:B:270:PRO:HB2  | 1.59                     | 0.85              |
| 3:B:234:THR:HG21 | 3:B:270:PRO:HB2  | 1.59                     | 0.85              |
| 1:K:286:LEU:HD13 | 2:A:409:VAL:HG21 | 1.59                     | 0.85              |
| 1:K:93:THR:HG21  | 1:K:329:ILE:HD11 | 1.56                     | 0.84              |
| 1:K:144:MET:HE3  | 1:K:155:THR:HG21 | 1.56                     | 0.84              |
| 1:K:97:ILE:HD11  | 1:K:327:ILE:HG22 | 1.59                     | 0.84              |
| 1:K:152:ILE:HG23 | 1:K:239:GLN:HB2  | 1.61                     | 0.83              |
| 3:B:325:MET:HE1  | 3:B:355:VAL:HG11 | 1.59                     | 0.83              |
| 3:B:325:MET:HE1  | 3:B:355:VAL:HG11 | 1.59                     | 0.83              |
| 4:K:401:9V5:O15  | 4:K:401:9V5:S18  | 2.38                     | 0.81              |
| 3:B:242:LEU:HD22 | 3:B:250:ALA:H    | 1.46                     | 0.80              |
| 3:B:242:LEU:HD22 | 3:B:250:ALA:H    | 1.46                     | 0.80              |
| 3:B:93:VAL:HG11  | 3:B:118:VAL:HG22 | 1.62                     | 0.80              |
| 3:B:93:VAL:HG11  | 3:B:118:VAL:HG22 | 1.62                     | 0.80              |
| 2:A:151:SER:HB3  | 2:A:193:THR:HG21 | 1.65                     | 0.78              |
| 2:A:151:SER:HB3  | 2:A:193:THR:HG21 | 1.65                     | 0.78              |
| 2:A:119:LEU:HD23 | 2:A:122:ILE:HD11 | 1.65                     | 0.78              |
| 2:A:119:LEU:HD23 | 2:A:122:ILE:HD11 | 1.65                     | 0.78              |
| 3:B:167:ASN:HD21 | 3:B:252:LEU:HD22 | 1.49                     | 0.77              |
| 3:B:167:ASN:HD21 | 3:B:252:LEU:HD22 | 1.49                     | 0.77              |
| 3:B:114:LEU:HD23 | 3:B:149:MET:CE   | 2.15                     | 0.77              |
| 3:B:114:LEU:HD23 | 3:B:149:MET:CE   | 2.15                     | 0.77              |
| 2:A:12:ALA:HB2   | 7:A:503:GTP:C8   | 2.20                     | 0.76              |
| 2:A:12:ALA:HB2   | 7:A:503:GTP:C8   | 2.20                     | 0.76              |
| 1:K:265:ALA:HB2  | 2:A:108:TYR:CD2  | 2.21                     | 0.76              |
| 2:A:69:ASP:HA    | 2:A:145:THR:HG21 | 1.68                     | 0.75              |
| 2:A:69:ASP:HA    | 2:A:145:THR:HG21 | 1.68                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:42:LEU:HD12  | 1:K:42:LEU:O     | 1.86                     | 0.75              |
| 1:K:86:GLN:HE21  | 1:K:132:VAL:H    | 1.34                     | 0.75              |
| 3:B:70:LEU:H     | 3:B:145:THR:HG21 | 1.52                     | 0.75              |
| 3:B:70:LEU:H     | 3:B:145:THR:HG21 | 1.52                     | 0.75              |
| 4:K:401:9V5:O15  | 4:K:401:9V5:C10  | 2.36                     | 0.74              |
| 3:B:114:LEU:HD23 | 3:B:149:MET:HE1  | 1.70                     | 0.73              |
| 3:B:114:LEU:HD23 | 3:B:149:MET:HE1  | 1.70                     | 0.73              |
| 3:B:319:PHE:CD2  | 3:B:323:MET:HE1  | 2.24                     | 0.73              |
| 3:B:319:PHE:CD2  | 3:B:323:MET:HE1  | 2.24                     | 0.73              |
| 2:A:204:VAL:HG11 | 2:A:231:ILE:HD12 | 1.69                     | 0.73              |
| 2:A:204:VAL:HG11 | 2:A:231:ILE:HD12 | 1.69                     | 0.73              |
| 2:A:101:ASN:ND2  | 7:A:503:GTP:O3G  | 2.23                     | 0.72              |
| 1:K:209:ASN:HA   | 1:K:212:LYS:HE2  | 1.70                     | 0.72              |
| 2:A:101:ASN:ND2  | 7:A:503:GTP:O3G  | 2.23                     | 0.72              |
| 2:A:204:VAL:HG13 | 2:A:209:ILE:HD11 | 1.72                     | 0.72              |
| 2:A:204:VAL:HG13 | 2:A:209:ILE:HD11 | 1.72                     | 0.72              |
| 1:K:93:THR:HG21  | 1:K:329:ILE:HD11 | 1.70                     | 0.72              |
| 2:A:7:ILE:HD12   | 2:A:153:LEU:HD21 | 1.70                     | 0.71              |
| 2:A:7:ILE:HD12   | 2:A:153:LEU:HD21 | 1.70                     | 0.71              |
| 3:B:66:ILE:CD1   | 3:B:122:VAL:HG12 | 2.21                     | 0.71              |
| 3:B:66:ILE:CD1   | 3:B:122:VAL:HG12 | 2.21                     | 0.71              |
| 2:A:243:ARG:NH2  | 2:A:252:LEU:H    | 1.88                     | 0.71              |
| 2:A:243:ARG:NH2  | 2:A:252:LEU:H    | 1.88                     | 0.71              |
| 1:K:31:HIS:NE2   | 1:K:46:PRO:HD2   | 2.06                     | 0.71              |
| 1:K:17:ARG:HD2   | 1:K:19:ARG:HD2   | 1.73                     | 0.70              |
| 1:K:108:THR:HG21 | 1:K:320:LEU:CD1  | 2.21                     | 0.70              |
| 1:K:118:GLY:H    | 1:K:121:HIS:HB2  | 1.57                     | 0.70              |
| 3:B:228:ASN:OD1  | 8:B:600:GDP:N1   | 2.18                     | 0.70              |
| 3:B:332:MET:HE3  | 3:B:351:VAL:HG11 | 1.73                     | 0.70              |
| 3:B:228:ASN:OD1  | 8:B:600:GDP:N1   | 2.18                     | 0.70              |
| 3:B:332:MET:HE3  | 3:B:351:VAL:HG11 | 1.73                     | 0.70              |
| 2:A:401:LYS:HZ2  | 3:B:346:TRP:CD1  | 2.10                     | 0.70              |
| 2:A:401:LYS:HZ2  | 3:B:346:TRP:CD1  | 2.10                     | 0.70              |
| 1:K:240:ASP:HB2  | 1:K:243:ALA:HB3  | 1.73                     | 0.70              |
| 2:A:259:LEU:HD11 | 2:A:378:LEU:HD13 | 1.74                     | 0.70              |
| 1:K:207:LEU:HD22 | 4:K:401:9V5:C2   | 2.22                     | 0.70              |
| 2:A:259:LEU:HD11 | 2:A:378:LEU:HD13 | 1.74                     | 0.70              |
| 2:A:115:ILE:HG13 | 2:A:152:LEU:HD13 | 1.73                     | 0.69              |
| 2:A:115:ILE:HG13 | 2:A:152:LEU:HD13 | 1.73                     | 0.69              |
| 3:B:66:ILE:HD13  | 3:B:122:VAL:HG12 | 1.73                     | 0.69              |
| 3:B:234:THR:HG21 | 3:B:270:PRO:CB   | 2.22                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:66:ILE:HD13  | 3:B:122:VAL:HG12 | 1.73                     | 0.69              |
| 3:B:234:THR:HG21 | 3:B:270:PRO:CB   | 2.22                     | 0.69              |
| 1:K:16:VAL:HG23  | 1:K:76:PHE:CE2   | 2.28                     | 0.68              |
| 1:K:155:THR:HG22 | 1:K:236:LEU:HA   | 1.76                     | 0.68              |
| 3:B:273:ALA:HB3  | 3:B:274:PRO:HD3  | 1.74                     | 0.68              |
| 3:B:273:ALA:HB3  | 3:B:274:PRO:HD3  | 1.74                     | 0.68              |
| 1:K:32:LYS:N     | 1:K:32:LYS:HD3   | 2.09                     | 0.68              |
| 2:A:273:ALA:HB3  | 2:A:274:PRO:HD3  | 1.76                     | 0.67              |
| 2:A:273:ALA:HB3  | 2:A:274:PRO:HD3  | 1.76                     | 0.67              |
| 1:K:33:VAL:CG1   | 1:K:34:VAL:H     | 1.92                     | 0.67              |
| 1:K:332:VAL:HG12 | 1:K:342:THR:HG23 | 1.76                     | 0.67              |
| 2:A:243:ARG:HH21 | 2:A:252:LEU:H    | 1.42                     | 0.67              |
| 2:A:276:ILE:HG23 | 2:A:369:ALA:CB   | 2.25                     | 0.67              |
| 2:A:243:ARG:HH21 | 2:A:252:LEU:H    | 1.42                     | 0.67              |
| 2:A:276:ILE:HG23 | 2:A:369:ALA:CB   | 2.25                     | 0.67              |
| 3:B:250:ALA:HA   | 3:B:254:LYS:HE2  | 1.77                     | 0.66              |
| 3:B:250:ALA:HA   | 3:B:254:LYS:HE2  | 1.77                     | 0.66              |
| 1:K:170:LEU:HD23 | 1:K:210:GLY:HA3  | 1.78                     | 0.66              |
| 3:B:209:LEU:HB3  | 3:B:227:LEU:HD22 | 1.78                     | 0.65              |
| 3:B:209:LEU:HB3  | 3:B:227:LEU:HD22 | 1.78                     | 0.65              |
| 1:K:115:THR:HA   | 1:K:261:GLY:HA3  | 1.78                     | 0.65              |
| 1:K:265:ALA:HB2  | 2:A:108:TYR:CD2  | 2.30                     | 0.65              |
| 1:K:187:VAL:HG21 | 1:K:314:ARG:HD2  | 1.79                     | 0.65              |
| 1:K:178:ALA:HB3  | 1:K:190:HIS:NE2  | 2.12                     | 0.65              |
| 1:K:22:ASN:OD1   | 1:K:23:THR:N     | 2.29                     | 0.64              |
| 1:K:31:HIS:HE1   | 1:K:46:PRO:C     | 2.06                     | 0.64              |
| 1:K:18:VAL:HG22  | 1:K:332:VAL:CG2  | 2.28                     | 0.64              |
| 3:B:108:TYR:CD1  | 3:B:413:MET:HE1  | 2.33                     | 0.64              |
| 3:B:108:TYR:CD1  | 3:B:413:MET:HE1  | 2.33                     | 0.64              |
| 1:K:15:VAL:HG12  | 1:K:327:ILE:HD11 | 1.80                     | 0.64              |
| 3:B:70:LEU:HD12  | 3:B:145:THR:HG23 | 1.79                     | 0.64              |
| 3:B:70:LEU:HD12  | 3:B:145:THR:HG23 | 1.79                     | 0.64              |
| 2:A:388:TRP:CE3  | 2:A:425:MET:HE1  | 2.33                     | 0.63              |
| 1:K:95:LYS:HB3   | 1:K:96:PRO:HD3   | 1.80                     | 0.63              |
| 1:K:197:PRO:HB3  | 1:K:203:ILE:HD11 | 1.80                     | 0.63              |
| 2:A:388:TRP:CE3  | 2:A:425:MET:HE1  | 2.33                     | 0.63              |
| 3:B:259:MET:HE1  | 3:B:378:ILE:HG21 | 1.81                     | 0.63              |
| 1:K:268:SER:HB3  | 1:K:274:ARG:HD2  | 1.81                     | 0.63              |
| 3:B:259:MET:HE1  | 3:B:378:ILE:HG21 | 1.81                     | 0.63              |
| 1:K:86:GLN:NE2   | 1:K:132:VAL:HG23 | 2.13                     | 0.63              |
| 3:B:243:ARG:HH21 | 3:B:252:LEU:H    | 1.44                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:243:ARG:HH21 | 3:B:252:LEU:H    | 1.44                     | 0.63              |
| 2:A:237:SER:HB2  | 2:A:376:CYS:SG   | 2.39                     | 0.63              |
| 2:A:237:SER:HB2  | 2:A:376:CYS:SG   | 2.39                     | 0.63              |
| 1:K:333:SER:HB3  | 1:K:338:PHE:CG   | 2.34                     | 0.62              |
| 2:A:7:ILE:HD11   | 2:A:137:VAL:HG22 | 1.81                     | 0.62              |
| 2:A:7:ILE:HD11   | 2:A:137:VAL:HG22 | 1.81                     | 0.62              |
| 1:K:33:VAL:CG2   | 1:K:339:TYR:HA   | 2.24                     | 0.62              |
| 1:K:93:THR:HG23  | 1:K:327:ILE:HG21 | 1.80                     | 0.62              |
| 2:A:234:ILE:HG13 | 2:A:270:ALA:HB1  | 1.81                     | 0.62              |
| 2:A:234:ILE:HG13 | 2:A:270:ALA:HB1  | 1.81                     | 0.62              |
| 9:B:601:TA1:H463 | 9:B:601:TA1:H261 | 1.80                     | 0.62              |
| 9:B:601:TA1:H463 | 9:B:601:TA1:H261 | 1.80                     | 0.62              |
| 3:B:325:MET:CE   | 3:B:355:VAL:HG21 | 2.30                     | 0.62              |
| 3:B:325:MET:CE   | 3:B:355:VAL:HG21 | 2.30                     | 0.62              |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:HD23 | 1.82                     | 0.62              |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:HD23 | 1.82                     | 0.62              |
| 1:K:14:VAL:HG21  | 1:K:76:PHE:CD1   | 2.35                     | 0.62              |
| 3:B:20:PHE:CZ    | 3:B:24:ILE:HD12  | 2.35                     | 0.61              |
| 3:B:20:PHE:CZ    | 3:B:24:ILE:HD12  | 2.35                     | 0.61              |
| 3:B:325:MET:CE   | 3:B:355:VAL:HG11 | 2.28                     | 0.61              |
| 3:B:325:MET:CE   | 3:B:355:VAL:HG11 | 2.28                     | 0.61              |
| 1:K:109:VAL:HB   | 1:K:256:LEU:HG   | 1.82                     | 0.61              |
| 1:K:171:LEU:HD13 | 1:K:206:LEU:HD22 | 1.83                     | 0.61              |
| 2:A:234:ILE:HG21 | 2:A:302:MET:HE1  | 1.83                     | 0.61              |
| 2:A:234:ILE:HG21 | 2:A:302:MET:HE1  | 1.83                     | 0.61              |
| 3:B:156:LYS:HE2  | 3:B:156:LYS:HA   | 1.82                     | 0.61              |
| 3:B:156:LYS:HE2  | 3:B:156:LYS:HA   | 1.82                     | 0.61              |
| 1:K:85:THR:HG23  | 1:K:87:SER:H     | 1.65                     | 0.61              |
| 1:K:163:TYR:O    | 1:K:166:GLN:HG2  | 2.01                     | 0.61              |
| 2:A:151:SER:CB   | 2:A:193:THR:HG21 | 2.30                     | 0.61              |
| 3:B:413:MET:HG3  | 3:B:414:ASP:H    | 1.64                     | 0.61              |
| 1:K:348:TYR:CE1  | 2:A:415:GLU:HG3  | 2.36                     | 0.61              |
| 2:A:151:SER:CB   | 2:A:193:THR:HG21 | 2.30                     | 0.61              |
| 3:B:413:MET:HG3  | 3:B:414:ASP:H    | 1.64                     | 0.61              |
| 2:A:7:ILE:HD12   | 2:A:153:LEU:CD2  | 2.31                     | 0.60              |
| 2:A:7:ILE:HD12   | 2:A:153:LEU:CD2  | 2.31                     | 0.60              |
| 3:B:259:MET:HA   | 3:B:314:THR:HG21 | 1.82                     | 0.60              |
| 3:B:259:MET:HA   | 3:B:314:THR:HG21 | 1.82                     | 0.60              |
| 1:K:32:LYS:HD3   | 1:K:32:LYS:H     | 1.67                     | 0.60              |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:CZ   | 2.37                     | 0.60              |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:CZ   | 2.37                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:333:SER:HB3  | 1:K:338:PHE:CD2  | 2.37                     | 0.60              |
| 3:B:287:THR:O    | 3:B:288:VAL:HG23 | 2.02                     | 0.60              |
| 3:B:287:THR:O    | 3:B:288:VAL:HG23 | 2.02                     | 0.60              |
| 3:B:66:ILE:C     | 3:B:67:LEU:HD23  | 2.26                     | 0.60              |
| 3:B:66:ILE:C     | 3:B:67:LEU:HD23  | 2.26                     | 0.60              |
| 1:K:18:VAL:HG21  | 1:K:36:VAL:HG21  | 1.82                     | 0.60              |
| 1:K:194:LEU:HD21 | 1:K:235:TYR:CE2  | 2.37                     | 0.60              |
| 3:B:242:LEU:CD1  | 3:B:255:LEU:HD11 | 2.32                     | 0.60              |
| 3:B:242:LEU:CD1  | 3:B:255:LEU:HD11 | 2.32                     | 0.60              |
| 1:K:102:LEU:HD11 | 1:K:147:ILE:HG21 | 1.81                     | 0.60              |
| 1:K:287:ALA:O    | 1:K:291:VAL:HG23 | 2.02                     | 0.60              |
| 2:A:223:THR:HB   | 2:A:225:THR:HG22 | 1.82                     | 0.60              |
| 2:A:223:THR:HB   | 2:A:225:THR:HG22 | 1.82                     | 0.60              |
| 1:K:152:ILE:HB   | 1:K:241:LYS:HE3  | 1.83                     | 0.59              |
| 2:A:276:ILE:HG23 | 2:A:369:ALA:HB2  | 1.83                     | 0.59              |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:CD2  | 2.33                     | 0.59              |
| 2:A:276:ILE:HG23 | 2:A:369:ALA:HB2  | 1.83                     | 0.59              |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:CD2  | 2.33                     | 0.59              |
| 1:K:259:LEU:HD12 | 1:K:259:LEU:N    | 2.18                     | 0.59              |
| 1:K:265:ALA:HB2  | 2:A:108:TYR:HD2  | 1.65                     | 0.59              |
| 1:K:144:MET:HE3  | 1:K:155:THR:CG2  | 2.30                     | 0.58              |
| 1:K:307:TYR:CE1  | 1:K:317:LYS:HG3  | 2.38                     | 0.58              |
| 2:A:68:VAL:HG11  | 2:A:149:PHE:CZ   | 2.39                     | 0.58              |
| 2:A:68:VAL:HG11  | 2:A:149:PHE:CZ   | 2.39                     | 0.58              |
| 2:A:231:ILE:HA   | 2:A:234:ILE:HG22 | 1.86                     | 0.58              |
| 2:A:231:ILE:HA   | 2:A:234:ILE:HG22 | 1.86                     | 0.58              |
| 2:A:115:ILE:CG1  | 2:A:152:LEU:HD13 | 2.33                     | 0.58              |
| 2:A:115:ILE:CG1  | 2:A:152:LEU:HD13 | 2.33                     | 0.58              |
| 3:B:250:ALA:HB1  | 3:B:254:LYS:HB2  | 1.84                     | 0.58              |
| 3:B:250:ALA:HB1  | 3:B:254:LYS:HB2  | 1.84                     | 0.58              |
| 3:B:93:VAL:HG11  | 3:B:118:VAL:CG2  | 2.32                     | 0.58              |
| 3:B:93:VAL:HG11  | 3:B:118:VAL:CG2  | 2.32                     | 0.58              |
| 3:B:10:GLY:HA2   | 3:B:145:THR:HB   | 1.85                     | 0.57              |
| 3:B:10:GLY:HA2   | 3:B:145:THR:HB   | 1.85                     | 0.57              |
| 2:A:11:GLN:HG3   | 2:A:74:VAL:HG11  | 1.87                     | 0.57              |
| 2:A:11:GLN:HG3   | 2:A:74:VAL:HG11  | 1.87                     | 0.57              |
| 3:B:182:VAL:HG23 | 3:B:186:ASN:HD21 | 1.69                     | 0.57              |
| 3:B:182:VAL:HG23 | 3:B:186:ASN:HD21 | 1.69                     | 0.57              |
| 3:B:137:LEU:HD22 | 3:B:154:ILE:HG21 | 1.87                     | 0.57              |
| 3:B:137:LEU:HD22 | 3:B:154:ILE:HG21 | 1.87                     | 0.57              |
| 1:K:119:LYS:HE3  | 1:K:119:LYS:HA   | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:K:401:9V5:O15  | 4:K:401:9V5:O16  | 2.23                     | 0.57              |
| 1:K:236:LEU:HD23 | 1:K:237:ARG:N    | 2.20                     | 0.56              |
| 2:A:7:ILE:HG22   | 2:A:66:VAL:CG2   | 2.33                     | 0.56              |
| 3:B:331:GLN:O    | 3:B:335:VAL:HG23 | 2.04                     | 0.56              |
| 2:A:7:ILE:HG22   | 2:A:66:VAL:CG2   | 2.33                     | 0.56              |
| 3:B:331:GLN:O    | 3:B:335:VAL:HG23 | 2.04                     | 0.56              |
| 2:A:104:ALA:CB   | 2:A:413:MET:HG3  | 2.35                     | 0.56              |
| 2:A:122:ILE:HD12 | 2:A:157:LEU:HD21 | 1.86                     | 0.56              |
| 2:A:104:ALA:CB   | 2:A:413:MET:HG3  | 2.35                     | 0.56              |
| 2:A:122:ILE:HD12 | 2:A:157:LEU:HD21 | 1.86                     | 0.56              |
| 2:A:250:VAL:HG22 | 2:A:352:LYS:NZ   | 2.21                     | 0.56              |
| 2:A:250:VAL:HG22 | 2:A:352:LYS:NZ   | 2.21                     | 0.56              |
| 1:K:170:LEU:HD23 | 1:K:210:GLY:CA   | 2.36                     | 0.56              |
| 3:B:209:LEU:HG   | 3:B:230:LEU:HD22 | 1.86                     | 0.56              |
| 1:K:203:ILE:O    | 1:K:207:LEU:HG   | 2.06                     | 0.56              |
| 3:B:209:LEU:HG   | 3:B:230:LEU:HD22 | 1.86                     | 0.56              |
| 1:K:158:SER:CB   | 1:K:192:LEU:HD21 | 2.36                     | 0.56              |
| 3:B:259:MET:HE1  | 3:B:378:ILE:CG2  | 2.36                     | 0.56              |
| 3:B:259:MET:HE1  | 3:B:378:ILE:CG2  | 2.36                     | 0.56              |
| 2:A:259:LEU:HD11 | 2:A:378:LEU:CD1  | 2.35                     | 0.56              |
| 3:B:8:GLN:CD     | 3:B:67:LEU:HD22  | 2.31                     | 0.56              |
| 2:A:259:LEU:HD11 | 2:A:378:LEU:CD1  | 2.35                     | 0.56              |
| 3:B:8:GLN:CD     | 3:B:67:LEU:HD22  | 2.31                     | 0.56              |
| 1:K:30:PHE:O     | 1:K:31:HIS:C     | 2.49                     | 0.55              |
| 1:K:138:LEU:HD23 | 1:K:138:LEU:O    | 2.06                     | 0.55              |
| 1:K:274:ARG:HE   | 1:K:275:PHE:HA   | 1.71                     | 0.55              |
| 1:K:16:VAL:HB    | 1:K:79:VAL:HG22  | 1.88                     | 0.55              |
| 1:K:202:GLU:O    | 1:K:206:LEU:HG   | 2.05                     | 0.55              |
| 1:K:351:ARG:HH21 | 2:A:419:SER:HB3  | 1.71                     | 0.55              |
| 1:K:101:PHE:CZ   | 1:K:236:LEU:HB2  | 2.42                     | 0.55              |
| 2:A:169:PHE:CE2  | 2:A:235:VAL:HG22 | 2.41                     | 0.55              |
| 3:B:132:LEU:HD23 | 3:B:164:ARG:HG3  | 1.89                     | 0.55              |
| 2:A:169:PHE:CE2  | 2:A:235:VAL:HG22 | 2.41                     | 0.55              |
| 3:B:132:LEU:HD23 | 3:B:164:ARG:HG3  | 1.89                     | 0.55              |
| 3:B:35:SER:HB3   | 3:B:59:ASN:HA    | 1.88                     | 0.55              |
| 1:K:171:LEU:HD23 | 1:K:193:THR:HB   | 1.89                     | 0.55              |
| 3:B:35:SER:HB3   | 3:B:59:ASN:HA    | 1.88                     | 0.55              |
| 3:B:259:MET:HG2  | 3:B:314:THR:HG21 | 1.87                     | 0.55              |
| 3:B:259:MET:HG2  | 3:B:314:THR:HG21 | 1.87                     | 0.55              |
| 3:B:204:ILE:HG21 | 3:B:231:VAL:HG22 | 1.88                     | 0.55              |
| 3:B:204:ILE:HG21 | 3:B:231:VAL:HG22 | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:209:ASN:HA   | 1:K:212:LYS:HE3  | 1.89                     | 0.54              |
| 1:K:219:THR:HG23 | 1:K:271:LYS:HE3  | 1.89                     | 0.54              |
| 1:K:305:ILE:HG23 | 1:K:307:TYR:CE1  | 2.42                     | 0.54              |
| 1:K:193:THR:C    | 1:K:194:LEU:HD12 | 2.33                     | 0.54              |
| 2:A:234:ILE:C    | 2:A:234:ILE:HD13 | 2.33                     | 0.54              |
| 2:A:234:ILE:C    | 2:A:234:ILE:HD13 | 2.33                     | 0.54              |
| 1:K:32:LYS:H     | 1:K:32:LYS:CD    | 2.19                     | 0.54              |
| 1:K:93:THR:HG21  | 1:K:329:ILE:CD1  | 2.35                     | 0.54              |
| 3:B:272:PHE:CE1  | 9:B:601:TA1:H391 | 2.43                     | 0.54              |
| 3:B:360:PRO:HB2  | 9:B:601:TA1:H281 | 1.90                     | 0.54              |
| 1:K:108:THR:HG21 | 1:K:320:LEU:HG   | 1.90                     | 0.54              |
| 3:B:272:PHE:CE1  | 9:B:601:TA1:H391 | 2.43                     | 0.54              |
| 3:B:360:PRO:HB2  | 9:B:601:TA1:H281 | 1.90                     | 0.54              |
| 1:K:33:VAL:HG23  | 1:K:339:TYR:CA   | 2.30                     | 0.54              |
| 1:K:37:VAL:HG21  | 1:K:43:VAL:HG23  | 1.89                     | 0.54              |
| 1:K:227:ARG:HA   | 1:K:260:ALA:HB2  | 1.90                     | 0.54              |
| 3:B:204:ILE:HD13 | 3:B:231:VAL:HG22 | 1.89                     | 0.54              |
| 3:B:204:ILE:HD13 | 3:B:231:VAL:HG22 | 1.89                     | 0.54              |
| 1:K:187:VAL:HG21 | 1:K:314:ARG:CD   | 2.38                     | 0.54              |
| 1:K:328:MET:HE1  | 1:K:349:ALA:HB2  | 1.88                     | 0.54              |
| 2:A:305:CYS:SG   | 2:A:384:ILE:HD13 | 2.48                     | 0.54              |
| 2:A:305:CYS:SG   | 2:A:384:ILE:HD13 | 2.48                     | 0.54              |
| 3:B:150:GLY:HA2  | 3:B:153:LEU:HD22 | 1.90                     | 0.54              |
| 3:B:150:GLY:HA2  | 3:B:153:LEU:HD22 | 1.90                     | 0.54              |
| 2:A:296:PHE:CD2  | 2:A:341:ILE:HD11 | 2.43                     | 0.53              |
| 3:B:20:PHE:CE1   | 3:B:24:ILE:HD12  | 2.43                     | 0.53              |
| 3:B:230:LEU:HD21 | 3:B:302:MET:HE2  | 1.89                     | 0.53              |
| 2:A:296:PHE:CD2  | 2:A:341:ILE:HD11 | 2.43                     | 0.53              |
| 3:B:20:PHE:CE1   | 3:B:24:ILE:HD12  | 2.43                     | 0.53              |
| 3:B:230:LEU:HD21 | 3:B:302:MET:HE2  | 1.89                     | 0.53              |
| 2:A:206:ASN:ND2  | 7:A:503:GTP:O2'  | 2.41                     | 0.53              |
| 2:A:206:ASN:ND2  | 7:A:503:GTP:O2'  | 2.41                     | 0.53              |
| 1:K:112:TYR:HB3  | 1:K:330:ALA:HA   | 1.91                     | 0.53              |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:HZ   | 1.73                     | 0.53              |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:HZ   | 1.73                     | 0.53              |
| 2:A:7:ILE:CG1    | 2:A:137:VAL:HG22 | 2.39                     | 0.53              |
| 2:A:11:GLN:N     | 7:A:503:GTP:O2B  | 2.42                     | 0.53              |
| 3:B:137:LEU:HD22 | 3:B:154:ILE:CG2  | 2.39                     | 0.53              |
| 1:K:119:LYS:N    | 1:K:119:LYS:HD2  | 2.22                     | 0.53              |
| 2:A:7:ILE:CG1    | 2:A:137:VAL:HG22 | 2.39                     | 0.53              |
| 2:A:11:GLN:N     | 7:A:503:GTP:O2B  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:137:LEU:HD22 | 3:B:154:ILE:CG2  | 2.39                     | 0.53              |
| 3:B:6:HIS:CE1    | 3:B:8:GLN:HG2    | 2.44                     | 0.53              |
| 3:B:396:THR:HG23 | 3:B:422:GLU:OE2  | 2.09                     | 0.53              |
| 3:B:6:HIS:CE1    | 3:B:8:GLN:HG2    | 2.44                     | 0.53              |
| 3:B:396:THR:HG23 | 3:B:422:GLU:OE2  | 2.09                     | 0.53              |
| 2:A:179:THR:HG21 | 3:B:248:LEU:CD2  | 2.37                     | 0.53              |
| 3:B:172:VAL:CG1  | 3:B:387:LEU:HD21 | 2.23                     | 0.53              |
| 2:A:179:THR:HG21 | 3:B:248:LEU:CD2  | 2.37                     | 0.53              |
| 3:B:172:VAL:CG1  | 3:B:387:LEU:HD21 | 2.23                     | 0.53              |
| 2:A:151:SER:HB3  | 2:A:193:THR:CG2  | 2.38                     | 0.52              |
| 2:A:184:PRO:HG2  | 2:A:398:MET:HE1  | 1.91                     | 0.52              |
| 2:A:388:TRP:CD2  | 2:A:425:MET:HE1  | 2.43                     | 0.52              |
| 1:K:106:ASN:OD1  | 1:K:319:SER:HA   | 2.09                     | 0.52              |
| 2:A:151:SER:HB3  | 2:A:193:THR:CG2  | 2.38                     | 0.52              |
| 2:A:184:PRO:HG2  | 2:A:398:MET:HE1  | 1.91                     | 0.52              |
| 2:A:388:TRP:CD2  | 2:A:425:MET:HE1  | 2.43                     | 0.52              |
| 1:K:108:THR:HG21 | 1:K:320:LEU:HG   | 1.91                     | 0.52              |
| 1:K:108:THR:HG21 | 1:K:320:LEU:HD12 | 1.91                     | 0.52              |
| 1:K:159:TYR:CD2  | 1:K:170:LEU:HD22 | 2.44                     | 0.52              |
| 2:A:316:CYS:HB3  | 2:A:378:LEU:HD11 | 1.90                     | 0.52              |
| 3:B:122:VAL:HG21 | 3:B:157:ILE:CD1  | 2.39                     | 0.52              |
| 1:K:108:THR:HG23 | 1:K:326:THR:HG23 | 1.91                     | 0.52              |
| 2:A:316:CYS:HB3  | 2:A:378:LEU:HD11 | 1.90                     | 0.52              |
| 3:B:122:VAL:HG21 | 3:B:157:ILE:CD1  | 2.39                     | 0.52              |
| 1:K:102:LEU:HD11 | 1:K:147:ILE:HG21 | 1.90                     | 0.52              |
| 1:K:19:ARG:HB2   | 1:K:119:LYS:CG   | 2.32                     | 0.52              |
| 1:K:42:LEU:HD12  | 1:K:42:LEU:C     | 2.34                     | 0.52              |
| 2:A:12:ALA:CB    | 7:A:503:GTP:C8   | 2.91                     | 0.52              |
| 2:A:172:TYR:OH   | 2:A:387:ALA:HB1  | 2.09                     | 0.52              |
| 2:A:344:VAL:HG11 | 2:A:346:TRP:CE2  | 2.45                     | 0.52              |
| 3:B:182:VAL:HG23 | 3:B:186:ASN:ND2  | 2.24                     | 0.52              |
| 2:A:12:ALA:CB    | 7:A:503:GTP:C8   | 2.91                     | 0.52              |
| 2:A:172:TYR:OH   | 2:A:387:ALA:HB1  | 2.09                     | 0.52              |
| 2:A:344:VAL:HG11 | 2:A:346:TRP:CE2  | 2.45                     | 0.52              |
| 3:B:182:VAL:HG23 | 3:B:186:ASN:ND2  | 2.24                     | 0.52              |
| 1:K:123:MET:HG2  | 1:K:124:LEU:HD22 | 1.92                     | 0.52              |
| 1:K:158:SER:OG   | 1:K:192:LEU:HD21 | 2.09                     | 0.52              |
| 1:K:32:LYS:N     | 1:K:32:LYS:CD    | 2.73                     | 0.52              |
| 1:K:133:MET:HA   | 1:K:136:THR:HG22 | 1.89                     | 0.52              |
| 1:K:152:ILE:HG22 | 1:K:241:LYS:NZ   | 2.24                     | 0.52              |
| 2:A:15:GLN:NE2   | 7:A:503:GTP:N7   | 2.57                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:24:TYR:CE1   | 2:A:240:ALA:HB2  | 2.45                     | 0.52              |
| 3:B:336:GLN:HE22 | 3:B:349:ASN:ND2  | 2.08                     | 0.52              |
| 2:A:15:GLN:NE2   | 7:A:503:GTP:N7   | 2.57                     | 0.52              |
| 2:A:24:TYR:CE1   | 2:A:240:ALA:HB2  | 2.45                     | 0.52              |
| 3:B:336:GLN:HE22 | 3:B:349:ASN:ND2  | 2.08                     | 0.52              |
| 1:K:22:ASN:HB3   | 1:K:25:GLU:CD    | 2.34                     | 0.51              |
| 2:A:103:TYR:CD2  | 2:A:189:LEU:HD13 | 2.45                     | 0.51              |
| 2:A:103:TYR:CD2  | 2:A:189:LEU:HD13 | 2.45                     | 0.51              |
| 1:K:335:SER:HB3  | 1:K:338:PHE:HD2  | 1.76                     | 0.51              |
| 2:A:205:ASP:HB3  | 2:A:303:VAL:HA   | 1.92                     | 0.51              |
| 2:A:317:LEU:HD23 | 2:A:377:MET:HB3  | 1.92                     | 0.51              |
| 2:A:205:ASP:HB3  | 2:A:303:VAL:HA   | 1.92                     | 0.51              |
| 2:A:317:LEU:HD23 | 2:A:377:MET:HB3  | 1.92                     | 0.51              |
| 2:A:204:VAL:CG1  | 2:A:231:ILE:HD12 | 2.41                     | 0.51              |
| 2:A:204:VAL:CG1  | 2:A:231:ILE:HD12 | 2.41                     | 0.51              |
| 1:K:90:PHE:CG    | 1:K:135:LEU:HB3  | 2.45                     | 0.51              |
| 1:K:204:LEU:HA   | 1:K:207:LEU:HD12 | 1.93                     | 0.51              |
| 1:K:113:GLY:HA2  | 1:K:331:ALA:HB3  | 1.92                     | 0.51              |
| 2:A:296:PHE:CE2  | 2:A:341:ILE:HD11 | 2.46                     | 0.51              |
| 2:A:296:PHE:CE2  | 2:A:341:ILE:HD11 | 2.46                     | 0.51              |
| 1:K:171:LEU:HD13 | 1:K:206:LEU:CD2  | 2.40                     | 0.51              |
| 3:B:141:LEU:HA   | 3:B:147:SER:HB3  | 1.93                     | 0.51              |
| 3:B:141:LEU:HA   | 3:B:147:SER:HB3  | 1.93                     | 0.51              |
| 1:K:86:GLN:HE21  | 1:K:132:VAL:N    | 2.07                     | 0.50              |
| 1:K:141:TYR:CZ   | 1:K:199:SER:HA   | 2.47                     | 0.50              |
| 1:K:234:ILE:HB   | 1:K:254:MET:HB3  | 1.92                     | 0.50              |
| 1:K:14:VAL:HG23  | 1:K:14:VAL:O     | 2.11                     | 0.50              |
| 1:K:194:LEU:HD12 | 1:K:194:LEU:N    | 2.27                     | 0.50              |
| 3:B:103:TRP:CE3  | 3:B:189:LEU:HD13 | 2.47                     | 0.50              |
| 3:B:103:TRP:CE3  | 3:B:189:LEU:HD13 | 2.47                     | 0.50              |
| 3:B:179:ASP:HB2  | 8:B:600:GDP:H3'  | 1.94                     | 0.50              |
| 3:B:179:ASP:HB2  | 8:B:600:GDP:H3'  | 1.94                     | 0.50              |
| 3:B:323:MET:HE2  | 3:B:328:VAL:CG2  | 2.32                     | 0.49              |
| 3:B:323:MET:HE2  | 3:B:328:VAL:CG2  | 2.32                     | 0.49              |
| 3:B:168:THR:HB   | 3:B:201:THR:HG23 | 1.94                     | 0.49              |
| 4:K:401:9V5:O15  | 4:K:401:9V5:C5   | 2.60                     | 0.49              |
| 3:B:168:THR:HB   | 3:B:201:THR:HG23 | 1.94                     | 0.49              |
| 3:B:369:ARG:C    | 3:B:369:ARG:HD2  | 2.38                     | 0.49              |
| 3:B:369:ARG:C    | 3:B:369:ARG:HD2  | 2.38                     | 0.49              |
| 1:K:253:LYS:HE2  | 1:K:319:SER:HA   | 1.95                     | 0.49              |
| 3:B:204:ILE:HG21 | 3:B:231:VAL:CG2  | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:274:PRO:O    | 9:B:601:TA1:H151 | 2.12                     | 0.49              |
| 3:B:204:ILE:HG21 | 3:B:231:VAL:CG2  | 2.42                     | 0.49              |
| 3:B:274:PRO:O    | 9:B:601:TA1:H151 | 2.12                     | 0.49              |
| 1:K:17:ARG:NH2   | 1:K:123:MET:HG3  | 2.27                     | 0.49              |
| 1:K:145:ASP:HA   | 1:K:148:LYS:HE3  | 1.93                     | 0.49              |
| 1:K:273:THR:O    | 1:K:277:GLU:HB3  | 2.13                     | 0.49              |
| 2:A:107:HIS:CD2  | 2:A:108:TYR:CE1  | 3.00                     | 0.49              |
| 1:K:45:ASP:N     | 1:K:46:PRO:HD3   | 2.28                     | 0.48              |
| 2:A:220:GLU:C    | 2:A:222:PRO:HD3  | 2.38                     | 0.48              |
| 2:A:220:GLU:C    | 2:A:222:PRO:HD3  | 2.38                     | 0.48              |
| 1:K:97:ILE:HD11  | 1:K:327:ILE:CG2  | 2.39                     | 0.48              |
| 2:A:114:ILE:O    | 2:A:118:VAL:HG23 | 2.13                     | 0.48              |
| 2:A:132:LEU:HD23 | 2:A:132:LEU:H    | 1.78                     | 0.48              |
| 2:A:114:ILE:O    | 2:A:118:VAL:HG23 | 2.13                     | 0.48              |
| 2:A:132:LEU:HD23 | 2:A:132:LEU:H    | 1.78                     | 0.48              |
| 3:B:285:ALA:HB1  | 3:B:290:GLU:HG2  | 1.95                     | 0.48              |
| 3:B:285:ALA:HB1  | 3:B:290:GLU:HG2  | 1.95                     | 0.48              |
| 1:K:18:VAL:HG22  | 1:K:332:VAL:HG23 | 1.96                     | 0.48              |
| 3:B:189:LEU:HD23 | 3:B:421:ALA:CB   | 2.44                     | 0.48              |
| 3:B:189:LEU:HD23 | 3:B:421:ALA:CB   | 2.44                     | 0.48              |
| 1:K:133:MET:O    | 1:K:137:MET:HB2  | 2.12                     | 0.48              |
| 1:K:241:LYS:NZ   | 1:K:241:LYS:HA   | 2.28                     | 0.48              |
| 2:A:179:THR:HG21 | 3:B:248:LEU:HD21 | 1.96                     | 0.48              |
| 3:B:20:PHE:HA    | 3:B:232:SER:HB2  | 1.96                     | 0.48              |
| 1:K:135:LEU:HD12 | 1:K:138:LEU:HD12 | 1.96                     | 0.48              |
| 1:K:306:PRO:HB2  | 1:K:309:ASN:HB2  | 1.96                     | 0.48              |
| 2:A:179:THR:HG21 | 3:B:248:LEU:HD21 | 1.96                     | 0.48              |
| 3:B:20:PHE:HA    | 3:B:232:SER:HB2  | 1.96                     | 0.48              |
| 2:A:102:ASN:HB2  | 2:A:408:TYR:CE1  | 2.49                     | 0.48              |
| 2:A:209:ILE:HG22 | 2:A:227:LEU:HD22 | 1.96                     | 0.48              |
| 2:A:250:VAL:HG22 | 2:A:352:LYS:HZ2  | 1.79                     | 0.48              |
| 2:A:102:ASN:HB2  | 2:A:408:TYR:CE1  | 2.49                     | 0.48              |
| 2:A:209:ILE:HG22 | 2:A:227:LEU:HD22 | 1.96                     | 0.48              |
| 2:A:250:VAL:HG22 | 2:A:352:LYS:HZ2  | 1.79                     | 0.48              |
| 1:K:14:VAL:HG23  | 1:K:77:ASP:H     | 1.78                     | 0.48              |
| 2:A:209:ILE:CG2  | 2:A:227:LEU:HD22 | 2.44                     | 0.48              |
| 2:A:209:ILE:CG2  | 2:A:227:LEU:HD22 | 2.44                     | 0.48              |
| 3:B:102:ASN:HD21 | 3:B:408:TYR:HA   | 1.77                     | 0.47              |
| 3:B:102:ASN:HD21 | 3:B:408:TYR:HA   | 1.77                     | 0.47              |
| 1:K:17:ARG:HH22  | 1:K:86:GLN:HE22  | 1.62                     | 0.47              |
| 2:A:14:VAL:HG21  | 2:A:75:ILE:CD1   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:203:CYS:SG   | 3:B:267:PHE:HB3  | 2.54                     | 0.47              |
| 3:B:250:ALA:CA   | 3:B:254:LYS:HE2  | 2.43                     | 0.47              |
| 1:K:119:LYS:HG2  | 1:K:333:SER:HB3  | 1.96                     | 0.47              |
| 1:K:312:LEU:O    | 1:K:316:LEU:HG   | 2.14                     | 0.47              |
| 2:A:14:VAL:HG21  | 2:A:75:ILE:CD1   | 2.44                     | 0.47              |
| 3:B:203:CYS:SG   | 3:B:267:PHE:HB3  | 2.54                     | 0.47              |
| 3:B:250:ALA:CA   | 3:B:254:LYS:HE2  | 2.43                     | 0.47              |
| 1:K:118:GLY:N    | 1:K:121:HIS:HB2  | 2.26                     | 0.47              |
| 2:A:7:ILE:HG21   | 2:A:122:ILE:HG21 | 1.96                     | 0.47              |
| 3:B:104:ALA:HB2  | 3:B:413:MET:SD   | 2.55                     | 0.47              |
| 3:B:274:PRO:HG2  | 3:B:371:LEU:HD21 | 1.95                     | 0.47              |
| 1:K:109:VAL:HB   | 1:K:256:LEU:HD12 | 1.96                     | 0.47              |
| 2:A:7:ILE:HG21   | 2:A:122:ILE:HG21 | 1.96                     | 0.47              |
| 3:B:104:ALA:HB2  | 3:B:413:MET:SD   | 2.55                     | 0.47              |
| 3:B:274:PRO:HG2  | 3:B:371:LEU:HD21 | 1.95                     | 0.47              |
| 1:K:178:ALA:HB3  | 1:K:190:HIS:CD2  | 2.49                     | 0.47              |
| 3:B:204:ILE:CD1  | 3:B:231:VAL:HG13 | 2.44                     | 0.47              |
| 1:K:39:LYS:HE2   | 1:K:80:PHE:HD1   | 1.79                     | 0.47              |
| 3:B:204:ILE:CD1  | 3:B:231:VAL:HG13 | 2.44                     | 0.47              |
| 1:K:253:LYS:HE2  | 1:K:319:SER:CA   | 2.45                     | 0.47              |
| 2:A:225:THR:O    | 2:A:229:ARG:HG3  | 2.15                     | 0.47              |
| 2:A:225:THR:O    | 2:A:229:ARG:HG3  | 2.15                     | 0.47              |
| 1:K:25:GLU:HB3   | 1:K:335:SER:HB2  | 1.96                     | 0.47              |
| 1:K:80:PHE:CZ    | 1:K:92:HIS:HB2   | 2.50                     | 0.47              |
| 1:K:164:ASN:HA   | 1:K:280:ASN:CG   | 2.39                     | 0.47              |
| 2:A:31:GLN:HB3   | 2:A:32:PRO:HD2   | 1.96                     | 0.47              |
| 2:A:154:MET:HE1  | 2:A:166:LYS:HB3  | 1.95                     | 0.47              |
| 3:B:67:LEU:HD23  | 3:B:67:LEU:N     | 2.30                     | 0.47              |
| 3:B:191:VAL:HG11 | 3:B:425:MET:HG3  | 1.96                     | 0.47              |
| 3:B:242:LEU:HD12 | 3:B:255:LEU:HD11 | 1.96                     | 0.47              |
| 3:B:325:MET:HE3  | 3:B:325:MET:HA   | 1.96                     | 0.47              |
| 2:A:31:GLN:HB3   | 2:A:32:PRO:HD2   | 1.96                     | 0.47              |
| 2:A:154:MET:HE1  | 2:A:166:LYS:HB3  | 1.95                     | 0.47              |
| 3:B:67:LEU:HD23  | 3:B:67:LEU:N     | 2.30                     | 0.47              |
| 3:B:191:VAL:HG11 | 3:B:425:MET:HG3  | 1.96                     | 0.47              |
| 3:B:242:LEU:HD12 | 3:B:255:LEU:HD11 | 1.96                     | 0.47              |
| 3:B:325:MET:HE3  | 3:B:325:MET:HA   | 1.96                     | 0.47              |
| 1:K:241:LYS:HA   | 1:K:241:LYS:CE   | 2.45                     | 0.47              |
| 2:A:209:ILE:HG23 | 2:A:230:LEU:HD23 | 1.96                     | 0.47              |
| 3:B:154:ILE:HG22 | 3:B:166:MET:HE2  | 1.97                     | 0.47              |
| 3:B:167:ASN:OD1  | 3:B:252:LEU:HD13 | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:209:ILE:HG23 | 2:A:230:LEU:HD23 | 1.96                     | 0.47              |
| 3:B:154:ILE:HG22 | 3:B:166:MET:HE2  | 1.97                     | 0.47              |
| 3:B:167:ASN:OD1  | 3:B:252:LEU:HD13 | 2.15                     | 0.47              |
| 2:A:234:ILE:CG2  | 2:A:302:MET:HE1  | 2.44                     | 0.47              |
| 2:A:234:ILE:CG2  | 2:A:302:MET:HE1  | 2.44                     | 0.47              |
| 2:A:7:ILE:CD1    | 2:A:137:VAL:HG22 | 2.44                     | 0.46              |
| 2:A:7:ILE:CD1    | 2:A:137:VAL:HG22 | 2.44                     | 0.46              |
| 1:K:127:ALA:HA   | 1:K:134:TYR:HE2  | 1.81                     | 0.46              |
| 1:K:295:LEU:HD21 | 1:K:320:LEU:HB3  | 1.96                     | 0.46              |
| 3:B:230:LEU:CD2  | 3:B:302:MET:HE2  | 2.46                     | 0.46              |
| 3:B:230:LEU:CD2  | 3:B:302:MET:HE2  | 2.46                     | 0.46              |
| 3:B:230:LEU:HD23 | 3:B:231:VAL:N    | 2.31                     | 0.46              |
| 3:B:230:LEU:HD23 | 3:B:231:VAL:N    | 2.31                     | 0.46              |
| 2:A:9:VAL:HG11   | 2:A:150:THR:OG1  | 2.15                     | 0.46              |
| 2:A:9:VAL:HG11   | 2:A:150:THR:OG1  | 2.15                     | 0.46              |
| 1:K:112:TYR:CZ   | 1:K:345:THR:HG22 | 2.51                     | 0.46              |
| 1:K:122:THR:HG22 | 1:K:129:GLU:HG3  | 1.96                     | 0.46              |
| 1:K:265:ALA:HB2  | 2:A:108:TYR:HD2  | 1.75                     | 0.46              |
| 1:K:304:HIS:HA   | 3:B:434:GLN:NE2  | 2.31                     | 0.46              |
| 2:A:343:PHE:CZ   | 2:A:351:PHE:CE2  | 3.03                     | 0.46              |
| 2:A:343:PHE:CZ   | 2:A:351:PHE:CE2  | 3.03                     | 0.46              |
| 1:K:114:ALA:CB   | 1:K:338:PHE:HD1  | 2.29                     | 0.46              |
| 2:A:93:ILE:HG21  | 2:A:118:VAL:HG22 | 1.98                     | 0.46              |
| 3:B:67:LEU:HD12  | 3:B:92:PHE:CE1   | 2.50                     | 0.46              |
| 1:K:227:ARG:HA   | 1:K:260:ALA:HB2  | 1.98                     | 0.46              |
| 2:A:93:ILE:HG21  | 2:A:118:VAL:HG22 | 1.98                     | 0.46              |
| 3:B:67:LEU:HD12  | 3:B:92:PHE:CE1   | 2.50                     | 0.46              |
| 2:A:264:ARG:HB2  | 2:A:266:HIS:CD2  | 2.51                     | 0.46              |
| 3:B:4:ILE:HG21   | 3:B:136:GLN:HG2  | 1.97                     | 0.46              |
| 3:B:264:ARG:O    | 3:B:265:LEU:HB3  | 2.15                     | 0.46              |
| 3:B:299:LYS:H    | 3:B:299:LYS:HD3  | 1.81                     | 0.46              |
| 2:A:264:ARG:HB2  | 2:A:266:HIS:CD2  | 2.51                     | 0.46              |
| 3:B:4:ILE:HG21   | 3:B:136:GLN:HG2  | 1.97                     | 0.46              |
| 3:B:299:LYS:H    | 3:B:299:LYS:HD3  | 1.81                     | 0.46              |
| 1:K:108:THR:HG21 | 1:K:320:LEU:CG   | 2.46                     | 0.45              |
| 1:K:189:VAL:HG23 | 1:K:192:LEU:HD23 | 1.97                     | 0.45              |
| 1:K:237:ARG:HG2  | 1:K:249:VAL:CG2  | 2.46                     | 0.45              |
| 1:K:305:ILE:C    | 1:K:305:ILE:HD13 | 2.40                     | 0.45              |
| 1:K:335:SER:HB3  | 1:K:338:PHE:CD2  | 2.51                     | 0.45              |
| 2:A:331:ALA:O    | 2:A:335:ILE:HG12 | 2.16                     | 0.45              |
| 2:A:331:ALA:O    | 2:A:335:ILE:HG12 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:101:PHE:CZ   | 1:K:236:LEU:HB2  | 2.52                     | 0.45              |
| 3:B:276:THR:O    | 9:B:601:TA1:H192 | 2.16                     | 0.45              |
| 1:K:163:TYR:CE1  | 1:K:277:GLU:HG3  | 2.51                     | 0.45              |
| 3:B:276:THR:O    | 9:B:601:TA1:H192 | 2.16                     | 0.45              |
| 2:A:23:LEU:HD23  | 2:A:236:SER:HB2  | 1.99                     | 0.45              |
| 2:A:184:PRO:HG2  | 2:A:398:MET:CE   | 2.46                     | 0.45              |
| 2:A:278:ALA:HB2  | 2:A:368:LEU:O    | 2.16                     | 0.45              |
| 2:A:23:LEU:HD23  | 2:A:236:SER:HB2  | 1.99                     | 0.45              |
| 2:A:184:PRO:HG2  | 2:A:398:MET:CE   | 2.46                     | 0.45              |
| 2:A:278:ALA:HB2  | 2:A:368:LEU:O    | 2.16                     | 0.45              |
| 2:A:112:LYS:O    | 2:A:115:ILE:HG22 | 2.17                     | 0.45              |
| 1:K:86:GLN:OE1   | 1:K:132:VAL:HG23 | 2.16                     | 0.45              |
| 2:A:112:LYS:O    | 2:A:115:ILE:HG22 | 2.17                     | 0.45              |
| 1:K:80:PHE:CE2   | 1:K:88:GLU:HG2   | 2.52                     | 0.45              |
| 3:B:315:VAL:HG13 | 3:B:377:PHE:CE1  | 2.52                     | 0.45              |
| 3:B:315:VAL:HG13 | 3:B:377:PHE:CE1  | 2.52                     | 0.45              |
| 2:A:313:MET:HB3  | 2:A:344:VAL:HG21 | 1.98                     | 0.45              |
| 2:A:313:MET:HB3  | 2:A:344:VAL:HG21 | 1.98                     | 0.45              |
| 3:B:319:PHE:CD2  | 3:B:375:ALA:HB2  | 2.51                     | 0.44              |
| 3:B:319:PHE:CD2  | 3:B:375:ALA:HB2  | 2.51                     | 0.44              |
| 1:K:157:VAL:HG21 | 1:K:203:ILE:HD12 | 2.00                     | 0.44              |
| 2:A:98:ASP:HB2   | 2:A:105:ARG:HH21 | 1.80                     | 0.44              |
| 3:B:325:MET:HE2  | 3:B:355:VAL:HG21 | 2.00                     | 0.44              |
| 1:K:286:LEU:CD1  | 2:A:409:VAL:HG21 | 2.41                     | 0.44              |
| 2:A:98:ASP:HB2   | 2:A:105:ARG:HH21 | 1.80                     | 0.44              |
| 3:B:325:MET:HE2  | 3:B:355:VAL:HG21 | 2.00                     | 0.44              |
| 1:K:22:ASN:O     | 1:K:23:THR:C     | 2.61                     | 0.44              |
| 1:K:37:VAL:CG2   | 1:K:43:VAL:HG23  | 2.48                     | 0.44              |
| 1:K:312:LEU:HD22 | 1:K:312:LEU:HA   | 1.82                     | 0.44              |
| 3:B:318:VAL:HA   | 3:B:354:ALA:HB3  | 1.98                     | 0.44              |
| 3:B:318:VAL:HA   | 3:B:354:ALA:HB3  | 1.98                     | 0.44              |
| 2:A:317:LEU:HD23 | 2:A:377:MET:CB   | 2.48                     | 0.44              |
| 3:B:67:LEU:HD12  | 3:B:92:PHE:CD1   | 2.53                     | 0.44              |
| 2:A:317:LEU:HD23 | 2:A:377:MET:CB   | 2.48                     | 0.44              |
| 3:B:67:LEU:HD12  | 3:B:92:PHE:CD1   | 2.53                     | 0.44              |
| 2:A:144:GLY:N    | 7:A:503:GTP:O3G  | 2.48                     | 0.44              |
| 2:A:144:GLY:N    | 7:A:503:GTP:O3G  | 2.48                     | 0.44              |
| 1:K:113:GLY:CA   | 1:K:331:ALA:HB3  | 2.47                     | 0.44              |
| 1:K:304:HIS:HA   | 3:B:434:GLN:HE22 | 1.83                     | 0.44              |
| 3:B:118:VAL:O    | 3:B:122:VAL:HG13 | 2.18                     | 0.44              |
| 1:K:17:ARG:HG3   | 1:K:89:VAL:CG2   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:271:LYS:H    | 1:K:271:LYS:HG2  | 1.59                     | 0.44              |
| 3:B:118:VAL:O    | 3:B:122:VAL:HG13 | 2.18                     | 0.44              |
| 2:A:231:ILE:O    | 2:A:235:VAL:HG23 | 2.17                     | 0.44              |
| 1:K:97:ILE:HG23  | 1:K:107:CYS:HB3  | 2.00                     | 0.44              |
| 2:A:231:ILE:O    | 2:A:235:VAL:HG23 | 2.17                     | 0.44              |
| 1:K:31:HIS:CE1   | 1:K:46:PRO:HB2   | 2.53                     | 0.43              |
| 1:K:133:MET:HG2  | 1:K:256:LEU:HD13 | 1.99                     | 0.43              |
| 1:K:307:TYR:CD1  | 1:K:317:LYS:HG3  | 2.53                     | 0.43              |
| 2:A:104:ALA:HB1  | 2:A:413:MET:HG3  | 1.99                     | 0.43              |
| 2:A:115:ILE:HD13 | 2:A:115:ILE:O    | 2.18                     | 0.43              |
| 2:A:231:ILE:HD13 | 2:A:231:ILE:N    | 2.34                     | 0.43              |
| 2:A:236:SER:O    | 2:A:240:ALA:HB3  | 2.18                     | 0.43              |
| 3:B:33:THR:HG22  | 3:B:33:THR:O     | 2.18                     | 0.43              |
| 9:B:601:TA1:H463 | 9:B:601:TA1:C26  | 2.46                     | 0.43              |
| 2:A:104:ALA:HB1  | 2:A:413:MET:HG3  | 1.99                     | 0.43              |
| 2:A:115:ILE:HD13 | 2:A:115:ILE:O    | 2.18                     | 0.43              |
| 2:A:231:ILE:HD13 | 2:A:231:ILE:N    | 2.34                     | 0.43              |
| 2:A:236:SER:O    | 2:A:240:ALA:HB3  | 2.18                     | 0.43              |
| 3:B:33:THR:HG22  | 3:B:33:THR:O     | 2.18                     | 0.43              |
| 9:B:601:TA1:H463 | 9:B:601:TA1:C26  | 2.46                     | 0.43              |
| 1:K:13:LYS:HE3   | 1:K:13:LYS:HB2   | 1.70                     | 0.43              |
| 1:K:151:LYS:HA   | 1:K:241:LYS:HG2  | 2.00                     | 0.43              |
| 2:A:109:THR:HG22 | 2:A:110:ILE:N    | 2.34                     | 0.43              |
| 3:B:147:SER:O    | 3:B:151:THR:HB   | 2.18                     | 0.43              |
| 3:B:319:PHE:HA   | 3:B:375:ALA:HA   | 2.00                     | 0.43              |
| 1:K:286:LEU:CD2  | 2:A:406:HIS:HA   | 2.48                     | 0.43              |
| 2:A:109:THR:HG22 | 2:A:110:ILE:N    | 2.34                     | 0.43              |
| 3:B:147:SER:O    | 3:B:151:THR:HB   | 2.18                     | 0.43              |
| 3:B:319:PHE:HA   | 3:B:375:ALA:HA   | 2.00                     | 0.43              |
| 2:A:238:ILE:HD11 | 2:A:378:LEU:HD23 | 1.99                     | 0.43              |
| 1:K:265:ALA:CB   | 2:A:108:TYR:HD2  | 2.31                     | 0.43              |
| 2:A:238:ILE:HD11 | 2:A:378:LEU:HD23 | 1.99                     | 0.43              |
| 3:B:101:ASN:ND2  | 3:B:143:GLY:HA2  | 2.33                     | 0.43              |
| 1:K:165:GLU:HG3  | 1:K:311:LYS:HE3  | 2.00                     | 0.43              |
| 3:B:101:ASN:ND2  | 3:B:143:GLY:HA2  | 2.33                     | 0.43              |
| 1:K:90:PHE:CD2   | 1:K:135:LEU:HB3  | 2.54                     | 0.43              |
| 1:K:152:ILE:HG22 | 1:K:241:LYS:HZ3  | 1.84                     | 0.43              |
| 2:A:191:THR:HG21 | 2:A:425:MET:SD   | 2.59                     | 0.43              |
| 3:B:27:GLU:CD    | 9:B:601:TA1:H411 | 2.44                     | 0.43              |
| 3:B:176:LYS:HE3  | 3:B:207:GLU:HG3  | 2.00                     | 0.43              |
| 2:A:191:THR:HG21 | 2:A:425:MET:SD   | 2.59                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:27:GLU:CD    | 9:B:601:TA1:H411 | 2.44                     | 0.43              |
| 3:B:176:LYS:HE3  | 3:B:207:GLU:HG3  | 2.00                     | 0.43              |
| 2:A:341:ILE:HG12 | 2:A:341:ILE:O    | 2.19                     | 0.43              |
| 1:K:237:ARG:HG2  | 1:K:249:VAL:HG21 | 1.99                     | 0.43              |
| 1:K:271:LYS:HG3  | 1:K:273:THR:HG23 | 2.00                     | 0.43              |
| 2:A:341:ILE:HG12 | 2:A:341:ILE:O    | 2.19                     | 0.43              |
| 2:A:16:ILE:HD12  | 2:A:171:ILE:HD11 | 2.01                     | 0.43              |
| 2:A:202:PHE:CE1  | 2:A:378:LEU:HD22 | 2.53                     | 0.43              |
| 2:A:224:TYR:OH   | 7:A:503:GTP:H2'  | 2.19                     | 0.43              |
| 2:A:407:TRP:HE1  | 3:B:260:VAL:HG23 | 1.83                     | 0.43              |
| 2:A:16:ILE:HD12  | 2:A:171:ILE:HD11 | 2.01                     | 0.43              |
| 2:A:202:PHE:CE1  | 2:A:378:LEU:HD22 | 2.53                     | 0.43              |
| 2:A:224:TYR:OH   | 7:A:503:GTP:H2'  | 2.19                     | 0.43              |
| 2:A:407:TRP:HE1  | 3:B:260:VAL:HG23 | 1.83                     | 0.43              |
| 1:K:265:ALA:HB2  | 2:A:108:TYR:CE2  | 2.54                     | 0.42              |
| 2:A:318:LEU:HB2  | 2:A:376:CYS:SG   | 2.59                     | 0.42              |
| 3:B:210:TYR:CD1  | 3:B:227:LEU:HD21 | 2.53                     | 0.42              |
| 1:K:46:PRO:HB2   | 1:K:47:LYS:H     | 1.66                     | 0.42              |
| 2:A:318:LEU:HB2  | 2:A:376:CYS:SG   | 2.59                     | 0.42              |
| 3:B:210:TYR:CD1  | 3:B:227:LEU:HD21 | 2.53                     | 0.42              |
| 1:K:14:VAL:HB    | 1:K:76:PHE:CE2   | 2.54                     | 0.42              |
| 1:K:113:GLY:HA3  | 1:K:120:THR:HG22 | 2.01                     | 0.42              |
| 1:K:158:SER:HB2  | 1:K:192:LEU:HD11 | 2.00                     | 0.42              |
| 1:K:254:MET:HE3  | 1:K:254:MET:HB3  | 1.77                     | 0.42              |
| 1:K:236:LEU:O    | 1:K:251:ILE:HA   | 2.20                     | 0.42              |
| 2:A:144:GLY:H    | 7:A:503:GTP:PG   | 2.42                     | 0.42              |
| 2:A:144:GLY:H    | 7:A:503:GTP:PG   | 2.42                     | 0.42              |
| 2:A:104:ALA:HB2  | 2:A:413:MET:HG3  | 1.99                     | 0.42              |
| 2:A:132:LEU:CD2  | 2:A:164:LYS:HE3  | 2.50                     | 0.42              |
| 2:A:152:LEU:HA   | 2:A:155:GLU:HB2  | 1.99                     | 0.42              |
| 2:A:269:LEU:HD22 | 2:A:384:ILE:HD11 | 2.00                     | 0.42              |
| 2:A:104:ALA:HB2  | 2:A:413:MET:HG3  | 1.99                     | 0.42              |
| 2:A:132:LEU:CD2  | 2:A:164:LYS:HE3  | 2.50                     | 0.42              |
| 2:A:152:LEU:HA   | 2:A:155:GLU:HB2  | 1.99                     | 0.42              |
| 2:A:269:LEU:HD22 | 2:A:384:ILE:HD11 | 2.00                     | 0.42              |
| 2:A:315:CYS:HB3  | 2:A:377:MET:HE1  | 2.02                     | 0.42              |
| 2:A:315:CYS:HB3  | 2:A:377:MET:HE1  | 2.02                     | 0.42              |
| 1:K:11:HIS:CE1   | 1:K:299:LYS:HE3  | 2.55                     | 0.42              |
| 1:K:107:CYS:O    | 1:K:254:MET:HA   | 2.19                     | 0.42              |
| 3:B:297:ASP:OD2  | 3:B:299:LYS:HE2  | 2.20                     | 0.42              |
| 3:B:332:MET:CE   | 3:B:351:VAL:HG11 | 2.46                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:413:MET:CG   | 3:B:414:ASP:H    | 2.32                     | 0.42              |
| 1:K:217:HIS:CD2  | 1:K:225:SER:HA   | 2.54                     | 0.42              |
| 1:K:232:PHE:HB3  | 1:K:256:LEU:HB3  | 2.02                     | 0.42              |
| 1:K:265:ALA:HB2  | 2:A:108:TYR:CE2  | 2.54                     | 0.42              |
| 3:B:297:ASP:OD2  | 3:B:299:LYS:HE2  | 2.20                     | 0.42              |
| 3:B:332:MET:CE   | 3:B:351:VAL:HG11 | 2.46                     | 0.42              |
| 3:B:413:MET:CG   | 3:B:414:ASP:H    | 2.32                     | 0.42              |
| 2:A:344:VAL:HG12 | 2:A:345:ASP:N    | 2.34                     | 0.42              |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:CD2  | 2.24                     | 0.42              |
| 1:K:160:LEU:HD13 | 1:K:167:ILE:HG23 | 2.02                     | 0.42              |
| 1:K:163:TYR:HE1  | 1:K:277:GLU:HG3  | 1.84                     | 0.42              |
| 2:A:344:VAL:HG12 | 2:A:345:ASP:N    | 2.34                     | 0.42              |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:CD2  | 2.24                     | 0.42              |
| 1:K:101:PHE:CD1  | 1:K:252:ALA:HB3  | 2.55                     | 0.42              |
| 2:A:141:PHE:HB3  | 2:A:173:PRO:HD3  | 2.02                     | 0.42              |
| 3:B:3:GLU:HA     | 3:B:51:VAL:HA    | 2.01                     | 0.42              |
| 3:B:288:VAL:HG22 | 3:B:323:MET:HE3  | 2.02                     | 0.42              |
| 2:A:141:PHE:HB3  | 2:A:173:PRO:HD3  | 2.02                     | 0.42              |
| 3:B:3:GLU:HA     | 3:B:51:VAL:HA    | 2.01                     | 0.42              |
| 3:B:288:VAL:HG22 | 3:B:323:MET:HE3  | 2.02                     | 0.42              |
| 1:K:94:THR:HG21  | 1:K:136:THR:HB   | 2.01                     | 0.42              |
| 2:A:11:GLN:HB3   | 7:A:503:GTP:O2B  | 2.20                     | 0.42              |
| 2:A:179:THR:HG21 | 3:B:248:LEU:HD22 | 2.00                     | 0.42              |
| 2:A:11:GLN:HB3   | 7:A:503:GTP:O2B  | 2.20                     | 0.42              |
| 2:A:179:THR:HG21 | 3:B:248:LEU:HD22 | 2.00                     | 0.42              |
| 1:K:140:LEU:HG   | 1:K:144:MET:SD   | 2.60                     | 0.41              |
| 1:K:144:MET:O    | 1:K:148:LYS:HG3  | 2.20                     | 0.41              |
| 3:B:44:LEU:HD12  | 3:B:49:ILE:HD13  | 2.01                     | 0.41              |
| 3:B:191:VAL:HG11 | 3:B:425:MET:HE2  | 2.02                     | 0.41              |
| 3:B:191:VAL:CG1  | 3:B:425:MET:HG3  | 2.50                     | 0.41              |
| 3:B:44:LEU:HD12  | 3:B:49:ILE:HD13  | 2.01                     | 0.41              |
| 3:B:191:VAL:HG11 | 3:B:425:MET:HE2  | 2.02                     | 0.41              |
| 3:B:191:VAL:CG1  | 3:B:425:MET:HG3  | 2.50                     | 0.41              |
| 1:K:151:LYS:HB3  | 1:K:239:GLN:O    | 2.20                     | 0.41              |
| 1:K:204:LEU:HD13 | 1:K:207:LEU:HD12 | 2.01                     | 0.41              |
| 2:A:21:TRP:HE1   | 2:A:63:PRO:HB3   | 1.85                     | 0.41              |
| 2:A:99:ALA:H     | 3:B:2:ARG:HH22   | 1.68                     | 0.41              |
| 3:B:93:VAL:CG1   | 3:B:118:VAL:HG22 | 2.42                     | 0.41              |
| 3:B:147:SER:HB2  | 3:B:190:SER:HB3  | 2.01                     | 0.41              |
| 3:B:154:ILE:HG22 | 3:B:166:MET:CE   | 2.51                     | 0.41              |
| 2:A:21:TRP:HE1   | 2:A:63:PRO:HB3   | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:99:ALA:H     | 3:B:2:ARG:HH22   | 1.68                     | 0.41              |
| 3:B:93:VAL:CG1   | 3:B:118:VAL:HG22 | 2.42                     | 0.41              |
| 3:B:147:SER:HB2  | 3:B:190:SER:HB3  | 2.01                     | 0.41              |
| 3:B:154:ILE:HG22 | 3:B:166:MET:CE   | 2.51                     | 0.41              |
| 3:B:24:ILE:HD11  | 3:B:52:TYR:CE2   | 2.56                     | 0.41              |
| 3:B:269:MET:HE2  | 3:B:381:SER:OG   | 2.20                     | 0.41              |
| 3:B:24:ILE:HD11  | 3:B:52:TYR:CE2   | 2.56                     | 0.41              |
| 3:B:269:MET:HE2  | 3:B:381:SER:OG   | 2.20                     | 0.41              |
| 1:K:86:GLN:CG    | 1:K:129:GLU:HB3  | 2.50                     | 0.41              |
| 1:K:159:TYR:CE2  | 1:K:170:LEU:HD22 | 2.55                     | 0.41              |
| 2:A:152:LEU:HD12 | 2:A:153:LEU:N    | 2.35                     | 0.41              |
| 2:A:274:PRO:HB2  | 2:A:371:VAL:HG21 | 2.03                     | 0.41              |
| 2:A:152:LEU:HD12 | 2:A:153:LEU:N    | 2.35                     | 0.41              |
| 2:A:274:PRO:HB2  | 2:A:371:VAL:HG21 | 2.03                     | 0.41              |
| 1:K:272:GLY:HA2  | 1:K:275:PHE:HB2  | 2.02                     | 0.41              |
| 2:A:172:TYR:C    | 2:A:172:TYR:HD1  | 2.29                     | 0.41              |
| 2:A:210:TYR:CD1  | 2:A:227:LEU:HD21 | 2.56                     | 0.41              |
| 3:B:63:PRO:HD2   | 3:B:86:ILE:HG12  | 2.03                     | 0.41              |
| 1:K:73:LYS:H     | 1:K:73:LYS:HG3   | 1.70                     | 0.41              |
| 2:A:172:TYR:C    | 2:A:172:TYR:HD1  | 2.29                     | 0.41              |
| 2:A:210:TYR:CD1  | 2:A:227:LEU:HD21 | 2.56                     | 0.41              |
| 3:B:63:PRO:HD2   | 3:B:86:ILE:HG12  | 2.03                     | 0.41              |
| 1:K:159:TYR:CD2  | 1:K:231:VAL:O    | 2.73                     | 0.41              |
| 1:K:33:VAL:HG21  | 1:K:339:TYR:HA   | 2.01                     | 0.41              |
| 1:K:232:PHE:O    | 1:K:255:SER:HA   | 2.20                     | 0.41              |
| 1:K:217:HIS:NE2  | 1:K:225:SER:HA   | 2.36                     | 0.41              |
| 2:A:212:ILE:HD11 | 2:A:302:MET:H    | 1.86                     | 0.41              |
| 3:B:35:SER:HB3   | 3:B:59:ASN:CA    | 2.51                     | 0.41              |
| 3:B:165:ILE:HD13 | 3:B:165:ILE:H    | 1.85                     | 0.41              |
| 1:K:152:ILE:HG23 | 1:K:239:GLN:HB3  | 2.03                     | 0.41              |
| 2:A:212:ILE:HD11 | 2:A:302:MET:H    | 1.86                     | 0.41              |
| 3:B:35:SER:HB3   | 3:B:59:ASN:CA    | 2.51                     | 0.41              |
| 3:B:165:ILE:HD13 | 3:B:165:ILE:H    | 1.85                     | 0.41              |
| 2:A:97:GLU:HB2   | 2:A:110:ILE:HD11 | 2.03                     | 0.41              |
| 3:B:212:ILE:HG12 | 3:B:300:ASN:H    | 1.86                     | 0.41              |
| 3:B:236:SER:O    | 3:B:240:THR:HG23 | 2.20                     | 0.41              |
| 2:A:97:GLU:HB2   | 2:A:110:ILE:HD11 | 2.03                     | 0.41              |
| 3:B:212:ILE:HG12 | 3:B:300:ASN:H    | 1.86                     | 0.41              |
| 3:B:236:SER:O    | 3:B:240:THR:HG23 | 2.20                     | 0.41              |
| 1:K:18:VAL:HG22  | 1:K:332:VAL:HG21 | 2.03                     | 0.41              |
| 2:A:229:ARG:NH1  | 2:A:363:VAL:HG21 | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:163:TYR:HB2  | 1:K:228:SER:OG   | 2.20                     | 0.41              |
| 2:A:229:ARG:NH1  | 2:A:363:VAL:HG21 | 2.36                     | 0.41              |
| 1:K:17:ARG:HE    | 1:K:17:ARG:HB3   | 1.72                     | 0.40              |
| 1:K:332:VAL:HG11 | 1:K:346:LEU:HD21 | 2.03                     | 0.40              |
| 3:B:76:ASP:HA    | 3:B:79:ARG:HG2   | 2.03                     | 0.40              |
| 1:K:33:VAL:CG2   | 1:K:339:TYR:HA   | 2.51                     | 0.40              |
| 1:K:119:LYS:HD2  | 1:K:119:LYS:H    | 1.84                     | 0.40              |
| 1:K:196:GLN:HA   | 1:K:197:PRO:HD3  | 1.90                     | 0.40              |
| 3:B:76:ASP:HA    | 3:B:79:ARG:HG2   | 2.03                     | 0.40              |
| 1:K:17:ARG:NE    | 1:K:89:VAL:HG21  | 2.36                     | 0.40              |
| 1:K:227:ARG:HA   | 1:K:260:ALA:CB   | 2.50                     | 0.40              |
| 2:A:9:VAL:HG21   | 2:A:149:PHE:HD1  | 1.86                     | 0.40              |
| 2:A:63:PRO:HD3   | 2:A:86:LEU:O     | 2.21                     | 0.40              |
| 2:A:115:ILE:CD1  | 2:A:119:LEU:HG   | 2.50                     | 0.40              |
| 2:A:295:CYS:HB3  | 2:A:377:MET:HG2  | 2.02                     | 0.40              |
| 3:B:133:GLN:HE21 | 3:B:243:ARG:NH2  | 2.18                     | 0.40              |
| 1:K:17:ARG:HG3   | 1:K:89:VAL:HG22  | 2.03                     | 0.40              |
| 2:A:9:VAL:HG21   | 2:A:149:PHE:HD1  | 1.86                     | 0.40              |
| 2:A:63:PRO:HD3   | 2:A:86:LEU:O     | 2.21                     | 0.40              |
| 2:A:115:ILE:CD1  | 2:A:119:LEU:HG   | 2.50                     | 0.40              |
| 2:A:295:CYS:HB3  | 2:A:377:MET:HG2  | 2.02                     | 0.40              |
| 3:B:133:GLN:HE21 | 3:B:243:ARG:NH2  | 2.18                     | 0.40              |
| 1:K:90:PHE:CG    | 1:K:135:LEU:CB   | 3.03                     | 0.40              |
| 2:A:133:GLN:HB3  | 2:A:243:ARG:HH12 | 1.86                     | 0.40              |
| 3:B:70:LEU:H     | 3:B:145:THR:CG2  | 2.29                     | 0.40              |
| 3:B:242:LEU:HD23 | 3:B:242:LEU:HA   | 1.90                     | 0.40              |
| 2:A:133:GLN:HB3  | 2:A:243:ARG:HH12 | 1.86                     | 0.40              |
| 3:B:70:LEU:H     | 3:B:145:THR:CG2  | 2.29                     | 0.40              |
| 3:B:242:LEU:HD23 | 3:B:242:LEU:HA   | 1.90                     | 0.40              |
| 1:K:241:LYS:HA   | 1:K:241:LYS:HE3  | 2.03                     | 0.40              |
| 1:K:17:ARG:HH21  | 1:K:123:MET:HG3  | 1.86                     | 0.40              |
| 1:K:152:ILE:HG13 | 1:K:237:ARG:HH22 | 1.87                     | 0.40              |
| 2:A:155:GLU:HA   | 2:A:197:HIS:ND1  | 2.36                     | 0.40              |
| 2:A:298:PRO:HB3  | 2:A:307:PRO:HD2  | 2.03                     | 0.40              |
| 3:B:269:MET:HB2  | 3:B:301:MET:HE3  | 2.04                     | 0.40              |
| 3:B:311:ARG:HD3  | 3:B:342:TYR:HA   | 2.04                     | 0.40              |
| 1:K:21:GLU:HG2   | 1:K:335:SER:HB2  | 2.04                     | 0.40              |
| 1:K:152:ILE:HG22 | 1:K:241:LYS:HG3  | 2.03                     | 0.40              |
| 2:A:155:GLU:HA   | 2:A:197:HIS:ND1  | 2.36                     | 0.40              |
| 2:A:298:PRO:HB3  | 2:A:307:PRO:HD2  | 2.03                     | 0.40              |
| 3:B:269:MET:HB2  | 3:B:301:MET:HE3  | 2.04                     | 0.40              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 3:B:311:ARG:HD3 | 3:B:342:TYR:HA | 2.04                     | 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   | 1-K   | 324/377 (86%)   | 288 (89%)  | 28 (9%)   | 8 (2%)   | 4           | 26 |
| 1   | 2-K   | 324/377 (86%)   | 292 (90%)  | 28 (9%)   | 4 (1%)   | 10          | 42 |
| 2   | 1-A   | 408/451 (90%)   | 316 (78%)  | 66 (16%)  | 26 (6%)  | 1           | 13 |
| 2   | 2-A   | 408/451 (90%)   | 317 (78%)  | 65 (16%)  | 26 (6%)  | 1           | 13 |
| 3   | 1-B   | 424/445 (95%)   | 338 (80%)  | 66 (16%)  | 20 (5%)  | 2           | 16 |
| 3   | 2-B   | 424/445 (95%)   | 338 (80%)  | 66 (16%)  | 20 (5%)  | 2           | 16 |
| All | All   | 2312/2546 (91%) | 1889 (82%) | 319 (14%) | 104 (4%) | 3           | 17 |

All (104) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-K   | 33  | VAL  |
| 1   | 1-K   | 268 | SER  |
| 2   | 1-A   | 97  | GLU  |
| 2   | 1-A   | 108 | TYR  |
| 2   | 1-A   | 109 | THR  |
| 2   | 1-A   | 141 | PHE  |
| 2   | 1-A   | 183 | GLU  |
| 2   | 1-A   | 245 | ASP  |
| 2   | 1-A   | 266 | HIS  |
| 2   | 1-A   | 280 | LYS  |
| 2   | 1-A   | 284 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1-A   | 285 | GLN  |
| 2   | 1-A   | 437 | VAL  |
| 3   | 1-B   | 82  | PRO  |
| 3   | 1-B   | 97  | SER  |
| 3   | 1-B   | 183 | GLU  |
| 3   | 1-B   | 278 | ARG  |
| 3   | 1-B   | 282 | GLN  |
| 3   | 1-B   | 288 | VAL  |
| 3   | 1-B   | 344 | VAL  |
| 3   | 1-B   | 369 | ARG  |
| 3   | 1-B   | 403 | ALA  |
| 2   | 2-A   | 97  | GLU  |
| 2   | 2-A   | 109 | THR  |
| 2   | 2-A   | 141 | PHE  |
| 2   | 2-A   | 183 | GLU  |
| 2   | 2-A   | 245 | ASP  |
| 2   | 2-A   | 266 | HIS  |
| 2   | 2-A   | 280 | LYS  |
| 2   | 2-A   | 284 | GLU  |
| 2   | 2-A   | 285 | GLN  |
| 2   | 2-A   | 437 | VAL  |
| 3   | 2-B   | 82  | PRO  |
| 3   | 2-B   | 97  | SER  |
| 3   | 2-B   | 183 | GLU  |
| 3   | 2-B   | 265 | LEU  |
| 3   | 2-B   | 278 | ARG  |
| 3   | 2-B   | 282 | GLN  |
| 3   | 2-B   | 288 | VAL  |
| 3   | 2-B   | 344 | VAL  |
| 3   | 2-B   | 369 | ARG  |
| 3   | 2-B   | 403 | ALA  |
| 1   | 1-K   | 69  | ASN  |
| 1   | 1-K   | 224 | THR  |
| 2   | 1-A   | 100 | ALA  |
| 2   | 1-A   | 251 | ASP  |
| 2   | 1-A   | 342 | GLN  |
| 3   | 1-B   | 38  | GLY  |
| 3   | 1-B   | 175 | PRO  |
| 3   | 1-B   | 265 | LEU  |
| 3   | 1-B   | 266 | HIS  |
| 1   | 2-K   | 46  | PRO  |
| 2   | 2-A   | 100 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2-A   | 108 | TYR  |
| 2   | 2-A   | 251 | ASP  |
| 2   | 2-A   | 342 | GLN  |
| 3   | 2-B   | 38  | GLY  |
| 3   | 2-B   | 175 | PRO  |
| 3   | 2-B   | 266 | HIS  |
| 2   | 1-A   | 309 | HIS  |
| 2   | 1-A   | 330 | ALA  |
| 2   | 1-A   | 339 | ARG  |
| 3   | 1-B   | 32  | PRO  |
| 3   | 1-B   | 273 | ALA  |
| 1   | 2-K   | 40  | HIS  |
| 2   | 2-A   | 309 | HIS  |
| 2   | 2-A   | 330 | ALA  |
| 2   | 2-A   | 339 | ARG  |
| 3   | 2-B   | 32  | PRO  |
| 3   | 2-B   | 273 | ALA  |
| 1   | 1-K   | 37  | VAL  |
| 1   | 1-K   | 301 | LYS  |
| 1   | 1-K   | 302 | ASN  |
| 2   | 1-A   | 173 | PRO  |
| 2   | 1-A   | 255 | PHE  |
| 2   | 1-A   | 287 | SER  |
| 2   | 1-A   | 366 | GLY  |
| 3   | 1-B   | 43  | GLN  |
| 3   | 1-B   | 99  | ALA  |
| 3   | 1-B   | 298 | ALA  |
| 1   | 2-K   | 220 | ASP  |
| 2   | 2-A   | 173 | PRO  |
| 2   | 2-A   | 255 | PHE  |
| 2   | 2-A   | 287 | SER  |
| 2   | 2-A   | 366 | GLY  |
| 3   | 2-B   | 43  | GLN  |
| 3   | 2-B   | 99  | ALA  |
| 3   | 2-B   | 298 | ALA  |
| 2   | 1-A   | 403 | ALA  |
| 3   | 1-B   | 343 | PHE  |
| 3   | 1-B   | 386 | GLU  |
| 2   | 2-A   | 403 | ALA  |
| 3   | 2-B   | 343 | PHE  |
| 3   | 2-B   | 386 | GLU  |
| 2   | 1-A   | 221 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1-A   | 273 | ALA  |
| 2   | 2-A   | 221 | ARG  |
| 2   | 2-A   | 273 | ALA  |
| 1   | 1-K   | 29  | GLY  |
| 1   | 2-K   | 104 | GLY  |
| 2   | 1-A   | 238 | ILE  |
| 2   | 2-A   | 238 | ILE  |
| 2   | 1-A   | 275 | VAL  |
| 2   | 2-A   | 275 | VAL  |

### 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   | 1-K   | 287/334 (86%)   | 258 (90%)  | 29 (10%)  | 7           | 23 |
| 1   | 2-K   | 287/334 (86%)   | 258 (90%)  | 29 (10%)  | 7           | 23 |
| 2   | 1-A   | 347/377 (92%)   | 302 (87%)  | 45 (13%)  | 4           | 16 |
| 2   | 2-A   | 347/377 (92%)   | 302 (87%)  | 45 (13%)  | 4           | 16 |
| 3   | 1-B   | 367/381 (96%)   | 311 (85%)  | 56 (15%)  | 3           | 13 |
| 3   | 2-B   | 367/381 (96%)   | 311 (85%)  | 56 (15%)  | 3           | 13 |
| All | All   | 2002/2184 (92%) | 1742 (87%) | 260 (13%) | 6           | 16 |

All (260) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-K   | 17  | ARG  |
| 1   | 1-K   | 24  | LYS  |
| 1   | 1-K   | 68  | GLN  |
| 1   | 1-K   | 76  | PHE  |
| 1   | 1-K   | 102 | LEU  |
| 1   | 1-K   | 110 | LEU  |
| 1   | 1-K   | 119 | LYS  |
| 1   | 1-K   | 121 | HIS  |
| 1   | 1-K   | 124 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-K   | 133 | MET  |
| 1   | 1-K   | 137 | MET  |
| 1   | 1-K   | 151 | LYS  |
| 1   | 1-K   | 168 | ARG  |
| 1   | 1-K   | 198 | LYS  |
| 1   | 1-K   | 204 | LEU  |
| 1   | 1-K   | 211 | ASN  |
| 1   | 1-K   | 214 | ARG  |
| 1   | 1-K   | 224 | THR  |
| 1   | 1-K   | 225 | SER  |
| 1   | 1-K   | 241 | LYS  |
| 1   | 1-K   | 248 | ASN  |
| 1   | 1-K   | 254 | MET  |
| 1   | 1-K   | 256 | LEU  |
| 1   | 1-K   | 259 | LEU  |
| 1   | 1-K   | 274 | ARG  |
| 1   | 1-K   | 302 | ASN  |
| 1   | 1-K   | 305 | ILE  |
| 1   | 1-K   | 312 | LEU  |
| 1   | 1-K   | 341 | ASP  |
| 2   | 1-A   | 6   | SER  |
| 2   | 1-A   | 16  | ILE  |
| 2   | 1-A   | 25  | CYS  |
| 2   | 1-A   | 32  | PRO  |
| 2   | 1-A   | 98  | ASP  |
| 2   | 1-A   | 115 | ILE  |
| 2   | 1-A   | 120 | ASP  |
| 2   | 1-A   | 130 | THR  |
| 2   | 1-A   | 135 | PHE  |
| 2   | 1-A   | 141 | PHE  |
| 2   | 1-A   | 150 | THR  |
| 2   | 1-A   | 152 | LEU  |
| 2   | 1-A   | 154 | MET  |
| 2   | 1-A   | 155 | GLU  |
| 2   | 1-A   | 172 | TYR  |
| 2   | 1-A   | 173 | PRO  |
| 2   | 1-A   | 183 | GLU  |
| 2   | 1-A   | 190 | THR  |
| 2   | 1-A   | 192 | HIS  |
| 2   | 1-A   | 194 | THR  |
| 2   | 1-A   | 204 | VAL  |
| 2   | 1-A   | 219 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1-A   | 224 | TYR  |
| 2   | 1-A   | 231 | ILE  |
| 2   | 1-A   | 234 | ILE  |
| 2   | 1-A   | 237 | SER  |
| 2   | 1-A   | 253 | THR  |
| 2   | 1-A   | 260 | VAL  |
| 2   | 1-A   | 267 | PHE  |
| 2   | 1-A   | 269 | LEU  |
| 2   | 1-A   | 276 | ILE  |
| 2   | 1-A   | 280 | LYS  |
| 2   | 1-A   | 284 | GLU  |
| 2   | 1-A   | 303 | VAL  |
| 2   | 1-A   | 328 | VAL  |
| 2   | 1-A   | 334 | THR  |
| 2   | 1-A   | 345 | ASP  |
| 2   | 1-A   | 352 | LYS  |
| 2   | 1-A   | 368 | LEU  |
| 2   | 1-A   | 376 | CYS  |
| 2   | 1-A   | 377 | MET  |
| 2   | 1-A   | 415 | GLU  |
| 2   | 1-A   | 417 | GLU  |
| 2   | 1-A   | 425 | MET  |
| 2   | 1-A   | 433 | GLU  |
| 3   | 1-B   | 24  | ILE  |
| 3   | 1-B   | 26  | ASP  |
| 3   | 1-B   | 32  | PRO  |
| 3   | 1-B   | 41  | ASP  |
| 3   | 1-B   | 48  | ARG  |
| 3   | 1-B   | 59  | ASN  |
| 3   | 1-B   | 67  | LEU  |
| 3   | 1-B   | 68  | VAL  |
| 3   | 1-B   | 90  | ASP  |
| 3   | 1-B   | 94  | PHE  |
| 3   | 1-B   | 121 | VAL  |
| 3   | 1-B   | 122 | VAL  |
| 3   | 1-B   | 129 | CYS  |
| 3   | 1-B   | 135 | PHE  |
| 3   | 1-B   | 145 | THR  |
| 3   | 1-B   | 149 | MET  |
| 3   | 1-B   | 151 | THR  |
| 3   | 1-B   | 153 | LEU  |
| 3   | 1-B   | 158 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1-B   | 161 | TYR  |
| 3   | 1-B   | 163 | ASP  |
| 3   | 1-B   | 165 | ILE  |
| 3   | 1-B   | 174 | SER  |
| 3   | 1-B   | 193 | GLN  |
| 3   | 1-B   | 195 | VAL  |
| 3   | 1-B   | 198 | THR  |
| 3   | 1-B   | 201 | THR  |
| 3   | 1-B   | 203 | CYS  |
| 3   | 1-B   | 207 | GLU  |
| 3   | 1-B   | 214 | PHE  |
| 3   | 1-B   | 226 | ASP  |
| 3   | 1-B   | 227 | LEU  |
| 3   | 1-B   | 229 | HIS  |
| 3   | 1-B   | 230 | LEU  |
| 3   | 1-B   | 240 | THR  |
| 3   | 1-B   | 265 | LEU  |
| 3   | 1-B   | 267 | PHE  |
| 3   | 1-B   | 275 | LEU  |
| 3   | 1-B   | 282 | GLN  |
| 3   | 1-B   | 284 | ARG  |
| 3   | 1-B   | 299 | LYS  |
| 3   | 1-B   | 300 | ASN  |
| 3   | 1-B   | 306 | ASP  |
| 3   | 1-B   | 309 | HIS  |
| 3   | 1-B   | 322 | ARG  |
| 3   | 1-B   | 324 | SER  |
| 3   | 1-B   | 343 | PHE  |
| 3   | 1-B   | 344 | VAL  |
| 3   | 1-B   | 349 | ASN  |
| 3   | 1-B   | 352 | LYS  |
| 3   | 1-B   | 369 | ARG  |
| 3   | 1-B   | 413 | MET  |
| 3   | 1-B   | 424 | ASN  |
| 3   | 1-B   | 427 | ASP  |
| 3   | 1-B   | 432 | TYR  |
| 3   | 1-B   | 437 | ASP  |
| 1   | 2-K   | 17  | ARG  |
| 1   | 2-K   | 24  | LYS  |
| 1   | 2-K   | 68  | GLN  |
| 1   | 2-K   | 76  | PHE  |
| 1   | 2-K   | 102 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2-K   | 110 | LEU  |
| 1   | 2-K   | 119 | LYS  |
| 1   | 2-K   | 121 | HIS  |
| 1   | 2-K   | 124 | LEU  |
| 1   | 2-K   | 133 | MET  |
| 1   | 2-K   | 137 | MET  |
| 1   | 2-K   | 151 | LYS  |
| 1   | 2-K   | 168 | ARG  |
| 1   | 2-K   | 198 | LYS  |
| 1   | 2-K   | 204 | LEU  |
| 1   | 2-K   | 211 | ASN  |
| 1   | 2-K   | 214 | ARG  |
| 1   | 2-K   | 224 | THR  |
| 1   | 2-K   | 225 | SER  |
| 1   | 2-K   | 241 | LYS  |
| 1   | 2-K   | 248 | ASN  |
| 1   | 2-K   | 254 | MET  |
| 1   | 2-K   | 256 | LEU  |
| 1   | 2-K   | 259 | LEU  |
| 1   | 2-K   | 274 | ARG  |
| 1   | 2-K   | 302 | ASN  |
| 1   | 2-K   | 305 | ILE  |
| 1   | 2-K   | 312 | LEU  |
| 1   | 2-K   | 341 | ASP  |
| 2   | 2-A   | 6   | SER  |
| 2   | 2-A   | 16  | ILE  |
| 2   | 2-A   | 25  | CYS  |
| 2   | 2-A   | 32  | PRO  |
| 2   | 2-A   | 98  | ASP  |
| 2   | 2-A   | 115 | ILE  |
| 2   | 2-A   | 120 | ASP  |
| 2   | 2-A   | 130 | THR  |
| 2   | 2-A   | 135 | PHE  |
| 2   | 2-A   | 141 | PHE  |
| 2   | 2-A   | 150 | THR  |
| 2   | 2-A   | 152 | LEU  |
| 2   | 2-A   | 154 | MET  |
| 2   | 2-A   | 155 | GLU  |
| 2   | 2-A   | 172 | TYR  |
| 2   | 2-A   | 173 | PRO  |
| 2   | 2-A   | 183 | GLU  |
| 2   | 2-A   | 190 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2-A   | 192 | HIS  |
| 2   | 2-A   | 194 | THR  |
| 2   | 2-A   | 204 | VAL  |
| 2   | 2-A   | 219 | ILE  |
| 2   | 2-A   | 224 | TYR  |
| 2   | 2-A   | 231 | ILE  |
| 2   | 2-A   | 234 | ILE  |
| 2   | 2-A   | 237 | SER  |
| 2   | 2-A   | 253 | THR  |
| 2   | 2-A   | 260 | VAL  |
| 2   | 2-A   | 267 | PHE  |
| 2   | 2-A   | 269 | LEU  |
| 2   | 2-A   | 276 | ILE  |
| 2   | 2-A   | 280 | LYS  |
| 2   | 2-A   | 284 | GLU  |
| 2   | 2-A   | 303 | VAL  |
| 2   | 2-A   | 328 | VAL  |
| 2   | 2-A   | 334 | THR  |
| 2   | 2-A   | 345 | ASP  |
| 2   | 2-A   | 352 | LYS  |
| 2   | 2-A   | 368 | LEU  |
| 2   | 2-A   | 376 | CYS  |
| 2   | 2-A   | 377 | MET  |
| 2   | 2-A   | 415 | GLU  |
| 2   | 2-A   | 417 | GLU  |
| 2   | 2-A   | 425 | MET  |
| 2   | 2-A   | 433 | GLU  |
| 3   | 2-B   | 24  | ILE  |
| 3   | 2-B   | 26  | ASP  |
| 3   | 2-B   | 32  | PRO  |
| 3   | 2-B   | 41  | ASP  |
| 3   | 2-B   | 48  | ARG  |
| 3   | 2-B   | 59  | ASN  |
| 3   | 2-B   | 67  | LEU  |
| 3   | 2-B   | 68  | VAL  |
| 3   | 2-B   | 90  | ASP  |
| 3   | 2-B   | 94  | PHE  |
| 3   | 2-B   | 121 | VAL  |
| 3   | 2-B   | 122 | VAL  |
| 3   | 2-B   | 129 | CYS  |
| 3   | 2-B   | 135 | PHE  |
| 3   | 2-B   | 145 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2-B   | 149 | MET  |
| 3   | 2-B   | 151 | THR  |
| 3   | 2-B   | 153 | LEU  |
| 3   | 2-B   | 158 | ARG  |
| 3   | 2-B   | 161 | TYR  |
| 3   | 2-B   | 163 | ASP  |
| 3   | 2-B   | 165 | ILE  |
| 3   | 2-B   | 174 | SER  |
| 3   | 2-B   | 193 | GLN  |
| 3   | 2-B   | 195 | VAL  |
| 3   | 2-B   | 198 | THR  |
| 3   | 2-B   | 201 | THR  |
| 3   | 2-B   | 203 | CYS  |
| 3   | 2-B   | 207 | GLU  |
| 3   | 2-B   | 214 | PHE  |
| 3   | 2-B   | 226 | ASP  |
| 3   | 2-B   | 227 | LEU  |
| 3   | 2-B   | 229 | HIS  |
| 3   | 2-B   | 230 | LEU  |
| 3   | 2-B   | 240 | THR  |
| 3   | 2-B   | 265 | LEU  |
| 3   | 2-B   | 267 | PHE  |
| 3   | 2-B   | 275 | LEU  |
| 3   | 2-B   | 282 | GLN  |
| 3   | 2-B   | 284 | ARG  |
| 3   | 2-B   | 299 | LYS  |
| 3   | 2-B   | 300 | ASN  |
| 3   | 2-B   | 306 | ASP  |
| 3   | 2-B   | 309 | HIS  |
| 3   | 2-B   | 322 | ARG  |
| 3   | 2-B   | 324 | SER  |
| 3   | 2-B   | 343 | PHE  |
| 3   | 2-B   | 344 | VAL  |
| 3   | 2-B   | 349 | ASN  |
| 3   | 2-B   | 352 | LYS  |
| 3   | 2-B   | 369 | ARG  |
| 3   | 2-B   | 413 | MET  |
| 3   | 2-B   | 424 | ASN  |
| 3   | 2-B   | 427 | ASP  |
| 3   | 2-B   | 432 | TYR  |
| 3   | 2-B   | 437 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-K   | 31  | HIS  |
| 1   | 1-K   | 40  | HIS  |
| 1   | 1-K   | 106 | ASN  |
| 1   | 1-K   | 121 | HIS  |
| 1   | 1-K   | 164 | ASN  |
| 1   | 1-K   | 205 | HIS  |
| 1   | 1-K   | 209 | ASN  |
| 1   | 1-K   | 211 | ASN  |
| 1   | 1-K   | 222 | ASN  |
| 1   | 1-K   | 233 | GLN  |
| 1   | 1-K   | 302 | ASN  |
| 1   | 1-K   | 309 | ASN  |
| 1   | 1-K   | 325 | GLN  |
| 2   | 1-A   | 8   | HIS  |
| 2   | 1-A   | 11  | GLN  |
| 2   | 1-A   | 139 | HIS  |
| 2   | 1-A   | 206 | ASN  |
| 2   | 1-A   | 216 | ASN  |
| 2   | 1-A   | 226 | ASN  |
| 3   | 1-B   | 43  | GLN  |
| 3   | 1-B   | 102 | ASN  |
| 3   | 1-B   | 133 | GLN  |
| 3   | 1-B   | 186 | ASN  |
| 3   | 1-B   | 282 | GLN  |
| 3   | 1-B   | 309 | HIS  |
| 3   | 1-B   | 349 | ASN  |
| 3   | 1-B   | 380 | ASN  |
| 3   | 1-B   | 385 | GLN  |
| 3   | 1-B   | 394 | GLN  |
| 3   | 1-B   | 433 | GLN  |
| 3   | 1-B   | 434 | GLN  |
| 3   | 1-B   | 436 | GLN  |
| 1   | 2-K   | 103 | ASN  |
| 1   | 2-K   | 303 | GLN  |
| 1   | 2-K   | 344 | ASN  |
| 2   | 2-A   | 8   | HIS  |
| 2   | 2-A   | 11  | GLN  |
| 2   | 2-A   | 139 | HIS  |
| 2   | 2-A   | 206 | ASN  |
| 2   | 2-A   | 216 | ASN  |
| 2   | 2-A   | 226 | ASN  |
| 3   | 2-B   | 43  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2-B   | 102 | ASN  |
| 3   | 2-B   | 133 | GLN  |
| 3   | 2-B   | 186 | ASN  |
| 3   | 2-B   | 282 | GLN  |
| 3   | 2-B   | 309 | HIS  |
| 3   | 2-B   | 349 | ASN  |
| 3   | 2-B   | 380 | ASN  |
| 3   | 2-B   | 385 | GLN  |
| 3   | 2-B   | 394 | GLN  |
| 3   | 2-B   | 433 | GLN  |
| 3   | 2-B   | 436 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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 | $\# Z  > 2$ |
| 9   | TA1  | 1-B   | 601 | -    | 68,68,68     | 2.20 | 26 (38%)    | 105,105,105 | 1.50 | 13 (12%)    |
| 7   | GTP  | 2-A   | 503 | 6    | 33,34,34     | 1.91 | 3 (9%)      | 50,54,54    | 0.94 | 4 (8%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | GDP  | 1-B   | 600 | -    | 29,30,30     | 2.86 | 11 (37%) | 45,47,47    | 3.48 | 16 (35%) |
| 8   | GDP  | 2-B   | 600 | -    | 29,30,30     | 2.86 | 11 (37%) | 45,47,47    | 3.48 | 16 (35%) |
| 9   | TA1  | 2-B   | 601 | -    | 68,68,68     | 2.20 | 26 (38%) | 105,105,105 | 1.50 | 13 (12%) |
| 4   | 9V5  | 2-K   | 401 | -    | 20,20,20     | 3.22 | 5 (25%)  | 25,29,29    | 1.68 | 4 (16%)  |
| 7   | GTP  | 1-A   | 503 | 6    | 33,34,34     | 1.91 | 3 (9%)   | 50,54,54    | 0.94 | 4 (8%)   |
| 4   | 9V5  | 1-K   | 401 | -    | 20,20,20     | 0.83 | 0        | 25,29,29    | 1.37 | 4 (16%)  |

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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 9   | TA1  | 1-B   | 601 | -    | -       | 9/41/127/127 | 0/7/7/7 |
| 7   | GTP  | 2-A   | 503 | 6    | -       | 3/22/38/38   | 0/3/3/3 |
| 8   | GDP  | 1-B   | 600 | -    | -       | 4/16/32/32   | 0/3/3/3 |
| 8   | GDP  | 2-B   | 600 | -    | -       | 4/16/32/32   | 0/3/3/3 |
| 9   | TA1  | 2-B   | 601 | -    | -       | 9/41/127/127 | 0/7/7/7 |
| 4   | 9V5  | 2-K   | 401 | -    | -       | 4/14/16/16   | 0/2/2/2 |
| 7   | GTP  | 1-A   | 503 | 6    | -       | 3/22/38/38   | 0/3/3/3 |
| 4   | 9V5  | 1-K   | 401 | -    | -       | 6/14/16/16   | 0/2/2/2 |

All (85) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | 2-K   | 401 | 9V5  | O15-N13 | 11.33 | 1.42        | 1.22     |
| 8   | 1-B   | 600 | GDP  | PA-O3A  | 7.57  | 1.67        | 1.59     |
| 8   | 2-B   | 600 | GDP  | PA-O3A  | 7.57  | 1.67        | 1.59     |
| 4   | 2-K   | 401 | 9V5  | C9-N13  | -6.62 | 1.33        | 1.45     |
| 9   | 1-B   | 601 | TA1  | C06-C05 | 6.52  | 1.50        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C06-C05 | 6.52  | 1.50        | 1.38     |
| 7   | 1-A   | 503 | GTP  | PA-O3A  | -5.94 | 1.53        | 1.59     |
| 7   | 2-A   | 503 | GTP  | PA-O3A  | -5.94 | 1.53        | 1.59     |
| 8   | 1-B   | 600 | GDP  | O6-C6   | 5.93  | 1.34        | 1.23     |
| 8   | 2-B   | 600 | GDP  | O6-C6   | 5.93  | 1.34        | 1.23     |
| 8   | 1-B   | 600 | GDP  | C8-N9   | 5.90  | 1.50        | 1.37     |
| 8   | 2-B   | 600 | GDP  | C8-N9   | 5.90  | 1.50        | 1.37     |
| 7   | 1-A   | 503 | GTP  | PB-O3A  | -5.73 | 1.53        | 1.59     |
| 7   | 2-A   | 503 | GTP  | PB-O3A  | -5.73 | 1.53        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | 1-B   | 601 | TA1  | C08-C07 | -5.67 | 1.25        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C08-C07 | -5.67 | 1.25        | 1.38     |
| 7   | 1-A   | 503 | GTP  | PB-O3B  | 5.39  | 1.65        | 1.59     |
| 7   | 2-A   | 503 | GTP  | PB-O3B  | 5.39  | 1.65        | 1.59     |
| 9   | 1-B   | 601 | TA1  | C18-C10 | 5.36  | 1.69        | 1.57     |
| 9   | 2-B   | 601 | TA1  | C18-C10 | 5.36  | 1.69        | 1.57     |
| 9   | 1-B   | 601 | TA1  | C05-C04 | 4.82  | 1.46        | 1.39     |
| 9   | 2-B   | 601 | TA1  | C05-C04 | 4.82  | 1.46        | 1.39     |
| 8   | 1-B   | 600 | GDP  | C2-N1   | 4.76  | 1.49        | 1.37     |
| 8   | 2-B   | 600 | GDP  | C2-N1   | 4.76  | 1.49        | 1.37     |
| 9   | 1-B   | 601 | TA1  | C45-C24 | 4.33  | 1.61        | 1.54     |
| 9   | 2-B   | 601 | TA1  | C45-C24 | 4.33  | 1.61        | 1.54     |
| 8   | 1-B   | 600 | GDP  | PB-O2B  | -3.92 | 1.40        | 1.54     |
| 8   | 2-B   | 600 | GDP  | PB-O2B  | -3.92 | 1.40        | 1.54     |
| 9   | 1-B   | 601 | TA1  | C36-C31 | 3.74  | 1.45        | 1.39     |
| 9   | 2-B   | 601 | TA1  | C36-C31 | 3.74  | 1.45        | 1.39     |
| 4   | 2-K   | 401 | 9V5  | O17-S18 | 3.57  | 1.50        | 1.44     |
| 9   | 1-B   | 601 | TA1  | O02-C03 | 3.53  | 1.41        | 1.34     |
| 9   | 2-B   | 601 | TA1  | O02-C03 | 3.53  | 1.41        | 1.34     |
| 4   | 2-K   | 401 | 9V5  | O16-S18 | 3.43  | 1.50        | 1.44     |
| 8   | 1-B   | 600 | GDP  | O4'-C1' | 3.37  | 1.49        | 1.42     |
| 8   | 2-B   | 600 | GDP  | O4'-C1' | 3.37  | 1.49        | 1.42     |
| 9   | 1-B   | 601 | TA1  | C25-C24 | 3.36  | 1.39        | 1.34     |
| 9   | 2-B   | 601 | TA1  | C25-C24 | 3.36  | 1.39        | 1.34     |
| 9   | 1-B   | 601 | TA1  | C46-C45 | 3.21  | 1.60        | 1.53     |
| 9   | 2-B   | 601 | TA1  | C46-C45 | 3.21  | 1.60        | 1.53     |
| 9   | 1-B   | 601 | TA1  | C43-C01 | 3.19  | 1.60        | 1.54     |
| 9   | 2-B   | 601 | TA1  | C43-C01 | 3.19  | 1.60        | 1.54     |
| 9   | 1-B   | 601 | TA1  | C11-C10 | 3.10  | 1.61        | 1.54     |
| 9   | 2-B   | 601 | TA1  | C11-C10 | 3.10  | 1.61        | 1.54     |
| 8   | 1-B   | 600 | GDP  | C8-N7   | 3.01  | 1.41        | 1.32     |
| 8   | 2-B   | 600 | GDP  | C8-N7   | 3.01  | 1.41        | 1.32     |
| 8   | 1-B   | 600 | GDP  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 8   | 2-B   | 600 | GDP  | C5-N7   | -2.85 | 1.33        | 1.39     |
| 9   | 1-B   | 601 | TA1  | C43-C26 | 2.80  | 1.58        | 1.52     |
| 9   | 2-B   | 601 | TA1  | C43-C26 | 2.80  | 1.58        | 1.52     |
| 8   | 1-B   | 600 | GDP  | C5-C4   | 2.64  | 1.45        | 1.38     |
| 8   | 2-B   | 600 | GDP  | C5-C4   | 2.64  | 1.45        | 1.38     |
| 9   | 1-B   | 601 | TA1  | C26-C25 | 2.58  | 1.56        | 1.51     |
| 9   | 2-B   | 601 | TA1  | C26-C25 | 2.58  | 1.56        | 1.51     |
| 9   | 1-B   | 601 | TA1  | C01-C45 | 2.54  | 1.66        | 1.56     |
| 9   | 2-B   | 601 | TA1  | C01-C45 | 2.54  | 1.66        | 1.56     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | 1-B   | 601 | TA1  | C18-C20 | 2.49  | 1.62        | 1.55     |
| 9   | 2-B   | 601 | TA1  | C18-C20 | 2.49  | 1.62        | 1.55     |
| 8   | 1-B   | 600 | GDP  | PB-O3B  | 2.45  | 1.63        | 1.54     |
| 8   | 2-B   | 600 | GDP  | PB-O3B  | 2.45  | 1.63        | 1.54     |
| 9   | 1-B   | 601 | TA1  | C04-C03 | -2.44 | 1.44        | 1.50     |
| 9   | 2-B   | 601 | TA1  | C04-C03 | -2.44 | 1.44        | 1.50     |
| 8   | 1-B   | 600 | GDP  | C2-N3   | -2.42 | 1.27        | 1.33     |
| 8   | 2-B   | 600 | GDP  | C2-N3   | -2.42 | 1.27        | 1.33     |
| 9   | 1-B   | 601 | TA1  | C41-C42 | 2.36  | 1.42        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C41-C42 | 2.36  | 1.42        | 1.38     |
| 9   | 1-B   | 601 | TA1  | C16-C15 | 2.31  | 1.56        | 1.52     |
| 9   | 2-B   | 601 | TA1  | C16-C15 | 2.31  | 1.56        | 1.52     |
| 4   | 2-K   | 401 | 9V5  | C11-S18 | -2.24 | 1.75        | 1.78     |
| 9   | 1-B   | 601 | TA1  | O09-C21 | 2.14  | 1.49        | 1.44     |
| 9   | 2-B   | 601 | TA1  | O09-C21 | 2.14  | 1.49        | 1.44     |
| 9   | 1-B   | 601 | TA1  | C08-C09 | 2.14  | 1.42        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C08-C09 | 2.14  | 1.42        | 1.38     |
| 9   | 1-B   | 601 | TA1  | C33-C32 | 2.14  | 1.42        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C33-C32 | 2.14  | 1.42        | 1.38     |
| 9   | 1-B   | 601 | TA1  | C37-C29 | 2.14  | 1.54        | 1.52     |
| 9   | 2-B   | 601 | TA1  | C37-C29 | 2.14  | 1.54        | 1.52     |
| 9   | 1-B   | 601 | TA1  | C10-C02 | 2.10  | 1.62        | 1.57     |
| 9   | 2-B   | 601 | TA1  | C10-C02 | 2.10  | 1.62        | 1.57     |
| 9   | 1-B   | 601 | TA1  | C07-C06 | 2.04  | 1.42        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C07-C06 | 2.04  | 1.42        | 1.38     |
| 9   | 1-B   | 601 | TA1  | C39-C38 | 2.03  | 1.42        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C39-C38 | 2.03  | 1.42        | 1.38     |
| 9   | 1-B   | 601 | TA1  | C34-C33 | 2.01  | 1.42        | 1.38     |
| 9   | 2-B   | 601 | TA1  | C34-C33 | 2.01  | 1.42        | 1.38     |

All (74) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 8   | 1-B   | 600 | GDP  | N9-C8-N7 | -10.78 | 93.42       | 113.40   |
| 8   | 2-B   | 600 | GDP  | N9-C8-N7 | -10.78 | 93.42       | 113.40   |
| 8   | 1-B   | 600 | GDP  | C8-N7-C5 | 9.25   | 120.74      | 104.26   |
| 8   | 2-B   | 600 | GDP  | C8-N7-C5 | 9.25   | 120.74      | 104.26   |
| 8   | 1-B   | 600 | GDP  | C6-C5-N7 | 8.60   | 145.94      | 130.29   |
| 8   | 2-B   | 600 | GDP  | C6-C5-N7 | 8.60   | 145.94      | 130.29   |
| 8   | 1-B   | 600 | GDP  | N2-C2-N3 | 6.28   | 131.94      | 119.67   |
| 8   | 2-B   | 600 | GDP  | N2-C2-N3 | 6.28   | 131.94      | 119.67   |
| 8   | 1-B   | 600 | GDP  | C6-C5-C4 | -6.18  | 109.54      | 118.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | 2-B   | 600 | GDP  | C6-C5-C4    | -6.18 | 109.54      | 118.83   |
| 9   | 1-B   | 601 | TA1  | C06-C05-C04 | -5.88 | 114.59      | 120.36   |
| 9   | 2-B   | 601 | TA1  | C06-C05-C04 | -5.88 | 114.59      | 120.36   |
| 8   | 1-B   | 600 | GDP  | C8-N9-C4    | 5.86  | 117.00      | 106.03   |
| 8   | 2-B   | 600 | GDP  | C8-N9-C4    | 5.86  | 117.00      | 106.03   |
| 9   | 1-B   | 601 | TA1  | C07-C08-C09 | 5.82  | 127.42      | 120.24   |
| 9   | 2-B   | 601 | TA1  | C07-C08-C09 | 5.82  | 127.42      | 120.24   |
| 4   | 2-K   | 401 | 9V5  | O17-S18-O16 | -5.45 | 108.24      | 119.25   |
| 8   | 1-B   | 600 | GDP  | C5-C6-N1    | 4.50  | 124.70      | 113.25   |
| 8   | 2-B   | 600 | GDP  | C5-C6-N1    | 4.50  | 124.70      | 113.25   |
| 8   | 1-B   | 600 | GDP  | N2-C2-N1    | -4.24 | 107.82      | 116.76   |
| 8   | 2-B   | 600 | GDP  | N2-C2-N1    | -4.24 | 107.82      | 116.76   |
| 8   | 1-B   | 600 | GDP  | C2-N3-C4    | 4.10  | 119.36      | 112.30   |
| 8   | 2-B   | 600 | GDP  | C2-N3-C4    | 4.10  | 119.36      | 112.30   |
| 9   | 1-B   | 601 | TA1  | C05-C04-C03 | -4.05 | 111.47      | 120.40   |
| 9   | 2-B   | 601 | TA1  | C05-C04-C03 | -4.05 | 111.47      | 120.40   |
| 8   | 1-B   | 600 | GDP  | O6-C6-C5    | -3.95 | 116.11      | 126.53   |
| 8   | 2-B   | 600 | GDP  | O6-C6-C5    | -3.95 | 116.11      | 126.53   |
| 8   | 1-B   | 600 | GDP  | C4-C5-N7    | -3.88 | 104.53      | 110.67   |
| 8   | 2-B   | 600 | GDP  | C4-C5-N7    | -3.88 | 104.53      | 110.67   |
| 8   | 1-B   | 600 | GDP  | C2-N1-C6    | -3.80 | 118.22      | 125.11   |
| 8   | 2-B   | 600 | GDP  | C2-N1-C6    | -3.80 | 118.22      | 125.11   |
| 9   | 1-B   | 601 | TA1  | C09-C04-C03 | 3.60  | 128.34      | 120.40   |
| 9   | 2-B   | 601 | TA1  | C09-C04-C03 | 3.60  | 128.34      | 120.40   |
| 4   | 2-K   | 401 | 9V5  | C10-S18-C11 | 3.56  | 110.81      | 105.33   |
| 8   | 1-B   | 600 | GDP  | C2'-C3'-C4' | 3.44  | 109.26      | 102.61   |
| 8   | 2-B   | 600 | GDP  | C2'-C3'-C4' | 3.44  | 109.26      | 102.61   |
| 9   | 1-B   | 601 | TA1  | C17-C18-C20 | 3.23  | 109.83      | 102.58   |
| 9   | 2-B   | 601 | TA1  | C17-C18-C20 | 3.23  | 109.83      | 102.58   |
| 4   | 1-K   | 401 | 9V5  | O17-S18-O16 | 3.04  | 125.40      | 119.25   |
| 9   | 1-B   | 601 | TA1  | O04-C11-C14 | -3.01 | 101.75      | 108.13   |
| 9   | 2-B   | 601 | TA1  | O04-C11-C14 | -3.01 | 101.75      | 108.13   |
| 9   | 1-B   | 601 | TA1  | C45-C01-C02 | 2.95  | 115.17      | 111.93   |
| 9   | 2-B   | 601 | TA1  | C45-C01-C02 | 2.95  | 115.17      | 111.93   |
| 4   | 1-K   | 401 | 9V5  | C6-C11-S18  | 2.73  | 120.03      | 116.38   |
| 8   | 1-B   | 600 | GDP  | C1'-N9-C8   | -2.67 | 119.16      | 126.73   |
| 8   | 2-B   | 600 | GDP  | C1'-N9-C8   | -2.67 | 119.16      | 126.73   |
| 4   | 2-K   | 401 | 9V5  | C6-C11-S18  | 2.62  | 119.88      | 116.38   |
| 4   | 1-K   | 401 | 9V5  | C9-C11-S18  | -2.58 | 119.97      | 123.11   |
| 9   | 1-B   | 601 | TA1  | O01-C01-C43 | 2.50  | 113.42      | 107.04   |
| 9   | 2-B   | 601 | TA1  | O01-C01-C43 | 2.50  | 113.42      | 107.04   |
| 7   | 1-A   | 503 | GTP  | O3A-PB-O1B  | -2.44 | 103.36      | 110.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | 2-A   | 503 | GTP  | O3A-PB-O1B  | -2.44 | 103.36      | 110.70   |
| 9   | 1-B   | 601 | TA1  | C08-C09-C04 | -2.42 | 117.98      | 120.36   |
| 9   | 2-B   | 601 | TA1  | C08-C09-C04 | -2.42 | 117.98      | 120.36   |
| 8   | 1-B   | 600 | GDP  | O2'-C2'-C3' | 2.29  | 119.17      | 111.82   |
| 8   | 2-B   | 600 | GDP  | O2'-C2'-C3' | 2.29  | 119.17      | 111.82   |
| 9   | 1-B   | 601 | TA1  | C14-C11-C15 | -2.25 | 83.06       | 85.38    |
| 9   | 2-B   | 601 | TA1  | C14-C11-C15 | -2.25 | 83.06       | 85.38    |
| 9   | 1-B   | 601 | TA1  | C10-C18-C17 | -2.22 | 102.33      | 106.55   |
| 9   | 2-B   | 601 | TA1  | C10-C18-C17 | -2.22 | 102.33      | 106.55   |
| 9   | 1-B   | 601 | TA1  | O06-C15-C11 | 2.21  | 93.00       | 90.58    |
| 9   | 2-B   | 601 | TA1  | O06-C15-C11 | 2.21  | 93.00       | 90.58    |
| 4   | 2-K   | 401 | 9V5  | C9-C11-S18  | -2.20 | 120.43      | 123.11   |
| 7   | 1-A   | 503 | GTP  | O2B-PB-O3A  | 2.18  | 113.17      | 107.27   |
| 7   | 2-A   | 503 | GTP  | O2B-PB-O3A  | 2.18  | 113.17      | 107.27   |
| 4   | 1-K   | 401 | 9V5  | C8-C9-C11   | -2.11 | 120.02      | 122.24   |
| 7   | 1-A   | 503 | GTP  | O5'-C5'-C4' | 2.09  | 116.10      | 108.99   |
| 7   | 2-A   | 503 | GTP  | O5'-C5'-C4' | 2.09  | 116.10      | 108.99   |
| 8   | 1-B   | 600 | GDP  | C4'-O4'-C1' | 2.09  | 114.07      | 109.47   |
| 8   | 2-B   | 600 | GDP  | C4'-O4'-C1' | 2.09  | 114.07      | 109.47   |
| 9   | 1-B   | 601 | TA1  | C21-O09-C22 | 2.03  | 120.15      | 115.95   |
| 9   | 2-B   | 601 | TA1  | C21-O09-C22 | 2.03  | 120.15      | 115.95   |
| 7   | 1-A   | 503 | GTP  | O3G-PG-O3B  | 2.02  | 111.40      | 104.64   |
| 7   | 2-A   | 503 | GTP  | O3G-PG-O3B  | 2.02  | 111.40      | 104.64   |

There are no chirality outliers.

All (42) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | 1-K   | 401 | 9V5  | C9-C11-S18-C10  |
| 4   | 1-K   | 401 | 9V5  | C8-C9-N13-O15   |
| 4   | 1-K   | 401 | 9V5  | C11-C9-N13-O15  |
| 8   | 1-B   | 600 | GDP  | PA-O3A-PB-O2B   |
| 8   | 1-B   | 600 | GDP  | C5'-O5'-PA-O3A  |
| 8   | 1-B   | 600 | GDP  | C5'-O5'-PA-O1A  |
| 8   | 2-B   | 600 | GDP  | PA-O3A-PB-O2B   |
| 8   | 2-B   | 600 | GDP  | C5'-O5'-PA-O3A  |
| 8   | 2-B   | 600 | GDP  | C5'-O5'-PA-O1A  |
| 9   | 1-B   | 601 | TA1  | O02-C03-C04-C05 |
| 9   | 2-B   | 601 | TA1  | O02-C03-C04-C05 |
| 9   | 1-B   | 601 | TA1  | O02-C03-C04-C09 |
| 9   | 2-B   | 601 | TA1  | O02-C03-C04-C09 |
| 4   | 1-K   | 401 | 9V5  | C6-C11-S18-C10  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | 1-B   | 601 | TA1  | O03-C03-C04-C09 |
| 9   | 2-B   | 601 | TA1  | O03-C03-C04-C09 |
| 9   | 1-B   | 601 | TA1  | O03-C03-C04-C05 |
| 9   | 2-B   | 601 | TA1  | O03-C03-C04-C05 |
| 9   | 1-B   | 601 | TA1  | N01-C30-C31-C36 |
| 9   | 2-B   | 601 | TA1  | N01-C30-C31-C36 |
| 9   | 1-B   | 601 | TA1  | O14-C30-C31-C36 |
| 9   | 2-B   | 601 | TA1  | O14-C30-C31-C36 |
| 4   | 2-K   | 401 | 9V5  | C4-C10-S18-O17  |
| 4   | 2-K   | 401 | 9V5  | C5-C10-S18-O17  |
| 9   | 1-B   | 601 | TA1  | N01-C30-C31-C32 |
| 9   | 2-B   | 601 | TA1  | N01-C30-C31-C32 |
| 9   | 1-B   | 601 | TA1  | O14-C30-C31-C32 |
| 9   | 2-B   | 601 | TA1  | O14-C30-C31-C32 |
| 7   | 1-A   | 503 | GTP  | C3'-C4'-C5'-O5' |
| 7   | 2-A   | 503 | GTP  | C3'-C4'-C5'-O5' |
| 4   | 2-K   | 401 | 9V5  | C4-C10-S18-C11  |
| 4   | 2-K   | 401 | 9V5  | C5-C10-S18-C11  |
| 7   | 1-A   | 503 | GTP  | O4'-C4'-C5'-O5' |
| 7   | 2-A   | 503 | GTP  | O4'-C4'-C5'-O5' |
| 4   | 1-K   | 401 | 9V5  | C9-C11-S18-O16  |
| 4   | 1-K   | 401 | 9V5  | C9-C11-S18-O17  |
| 8   | 1-B   | 600 | GDP  | PA-O3A-PB-O3B   |
| 8   | 2-B   | 600 | GDP  | PA-O3A-PB-O3B   |
| 7   | 1-A   | 503 | GTP  | PG-O3B-PB-O1B   |
| 7   | 2-A   | 503 | GTP  | PG-O3B-PB-O1B   |
| 9   | 1-B   | 601 | TA1  | C15-C11-O04-C12 |
| 9   | 2-B   | 601 | TA1  | C15-C11-O04-C12 |

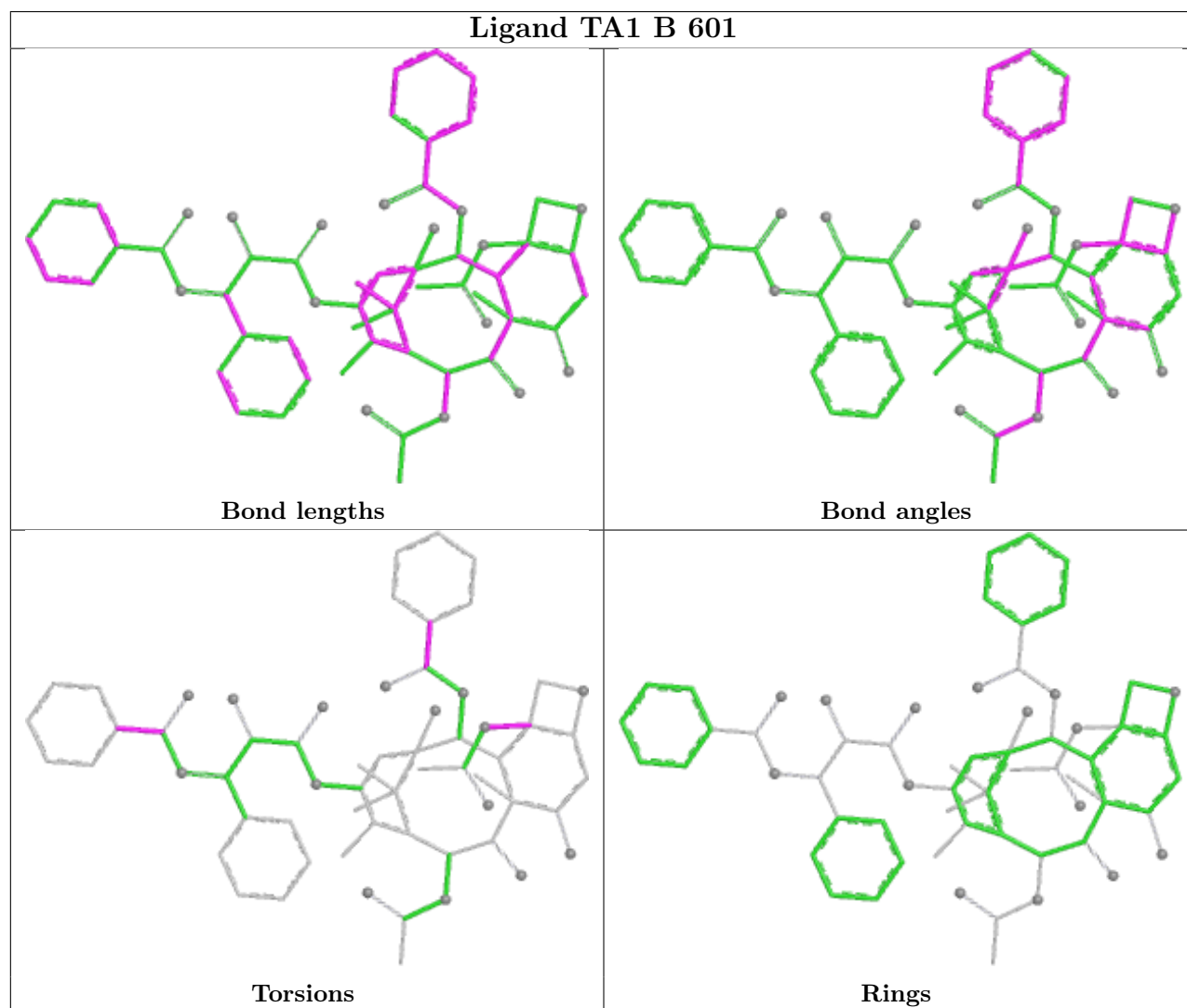
There are no ring outliers.

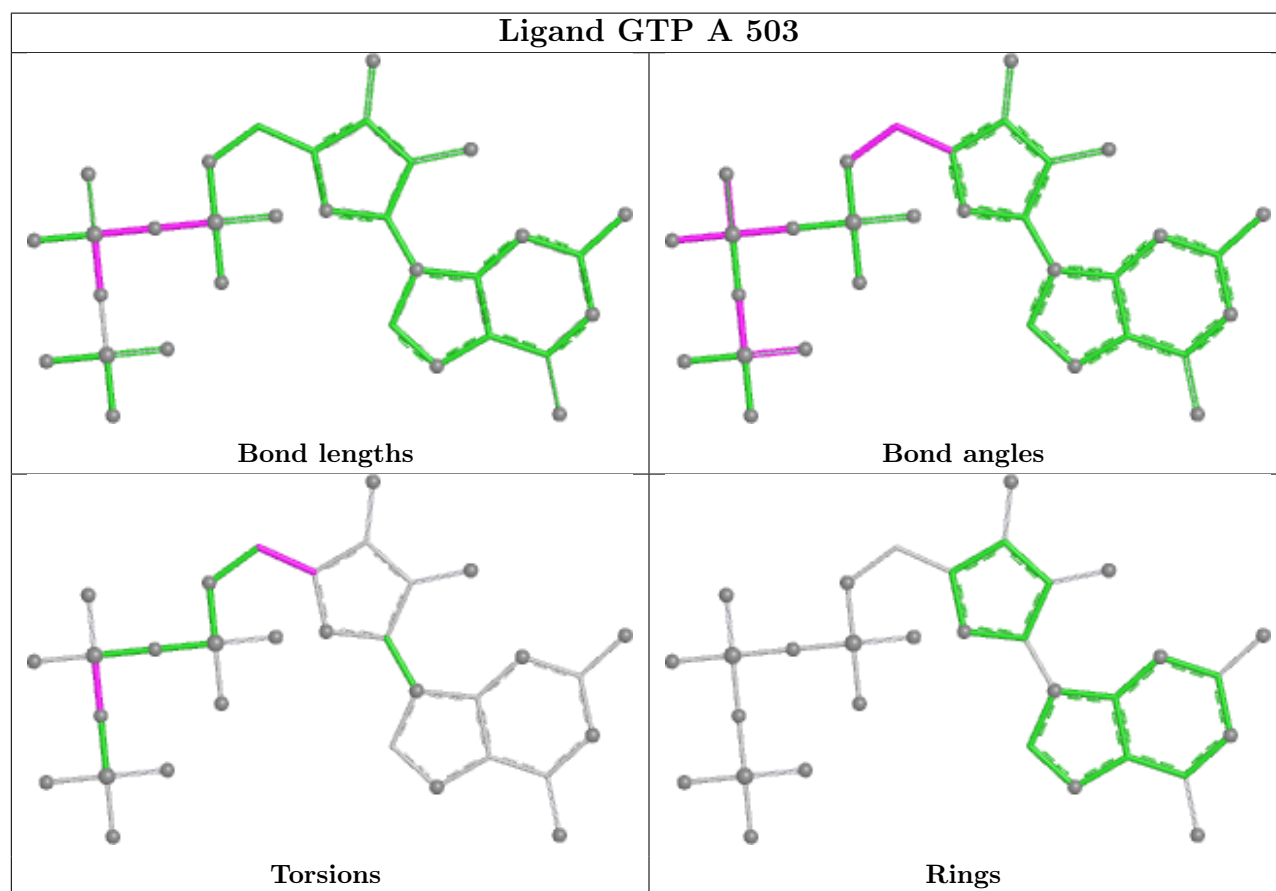
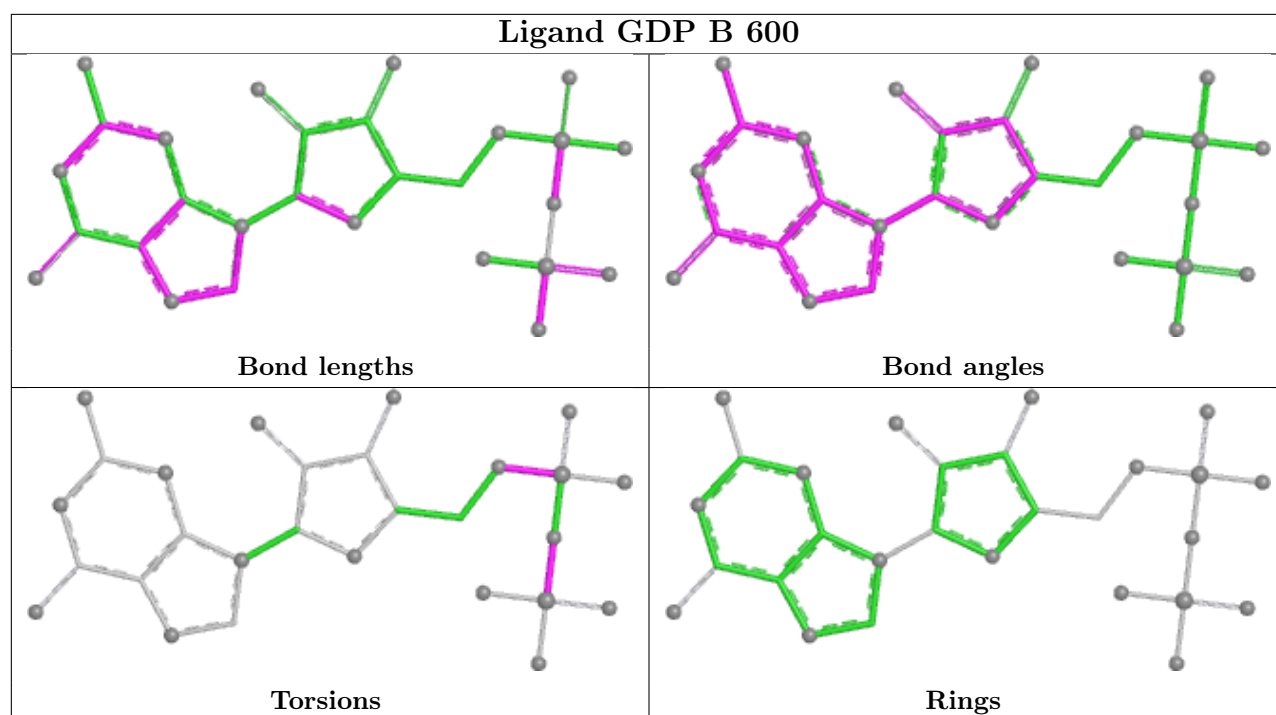
7 monomers are involved in 43 short contacts:

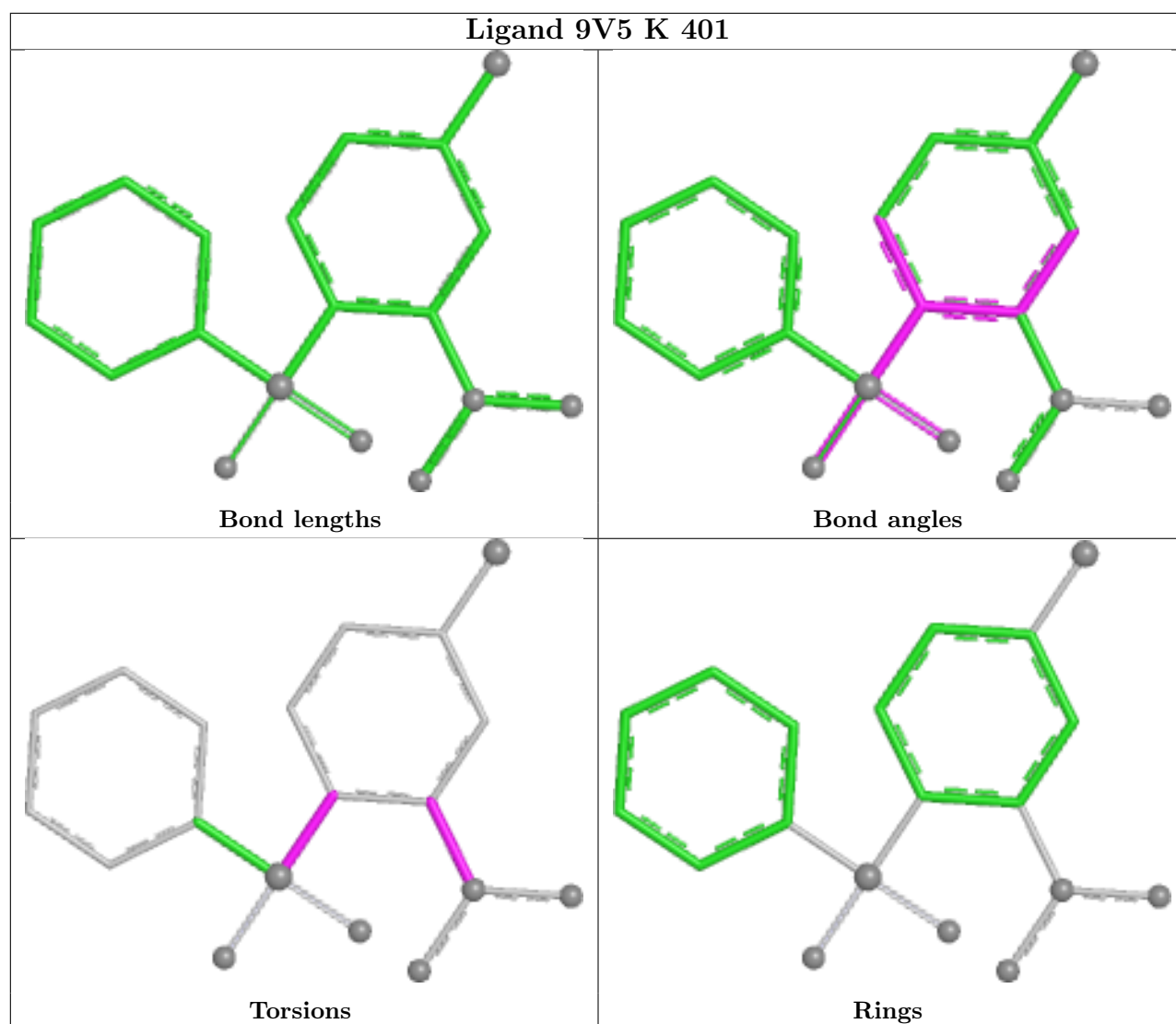
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | 1-B   | 601 | TA1  | 7       | 0            |
| 7   | 2-A   | 503 | GTP  | 10      | 0            |
| 8   | 1-B   | 600 | GDP  | 2       | 0            |
| 8   | 2-B   | 600 | GDP  | 2       | 0            |
| 9   | 2-B   | 601 | TA1  | 7       | 0            |
| 4   | 2-K   | 401 | 9V5  | 5       | 0            |
| 7   | 1-A   | 503 | GTP  | 10      | 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.

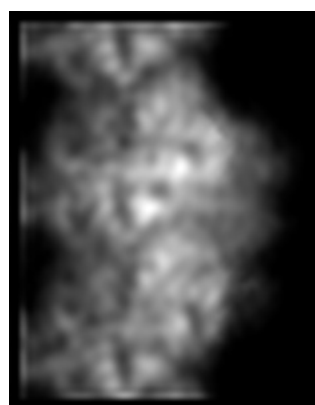
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3803. These allow visual inspection of the internal detail of the map and identification of artifacts.

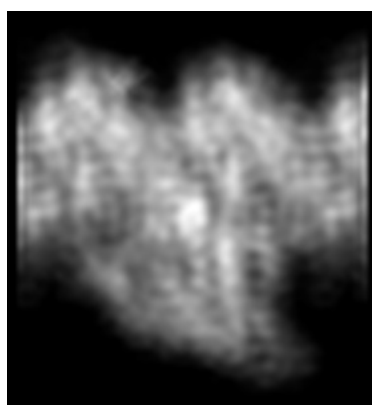
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

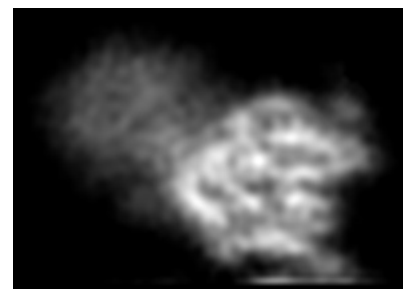
#### 6.1.1 Primary map



X



Y



Z

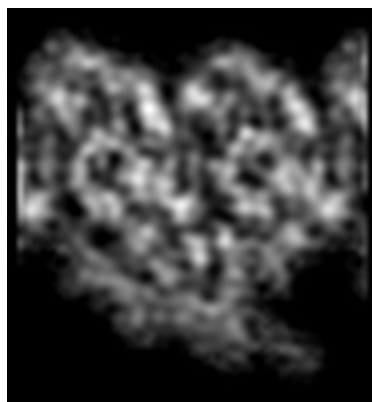
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 40



Y Index: 29



Z Index: 37

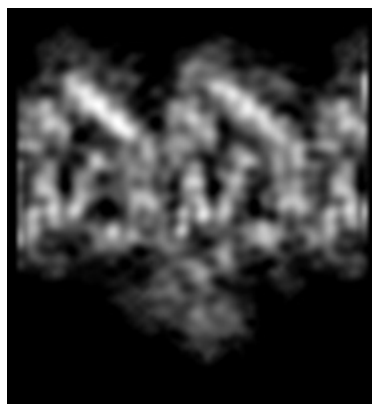
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 56



Y Index: 24

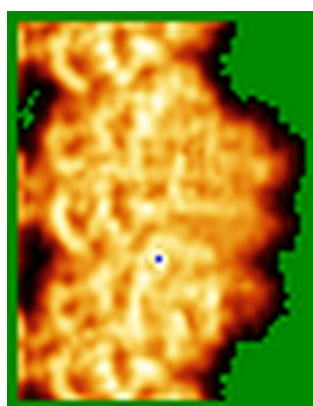


Z Index: 45

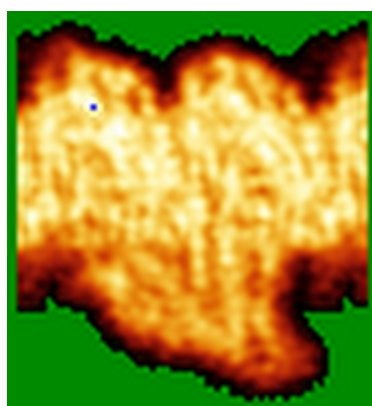
The images above show the largest variance slices of the map in three orthogonal directions.

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

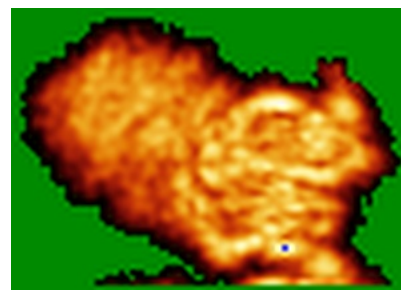
### 6.4.1 Primary map



X



Y

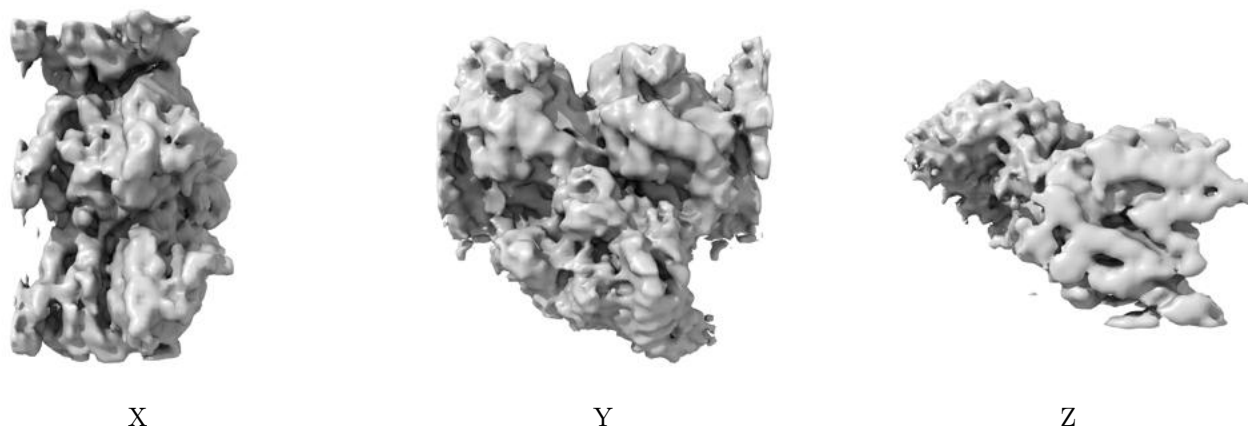


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

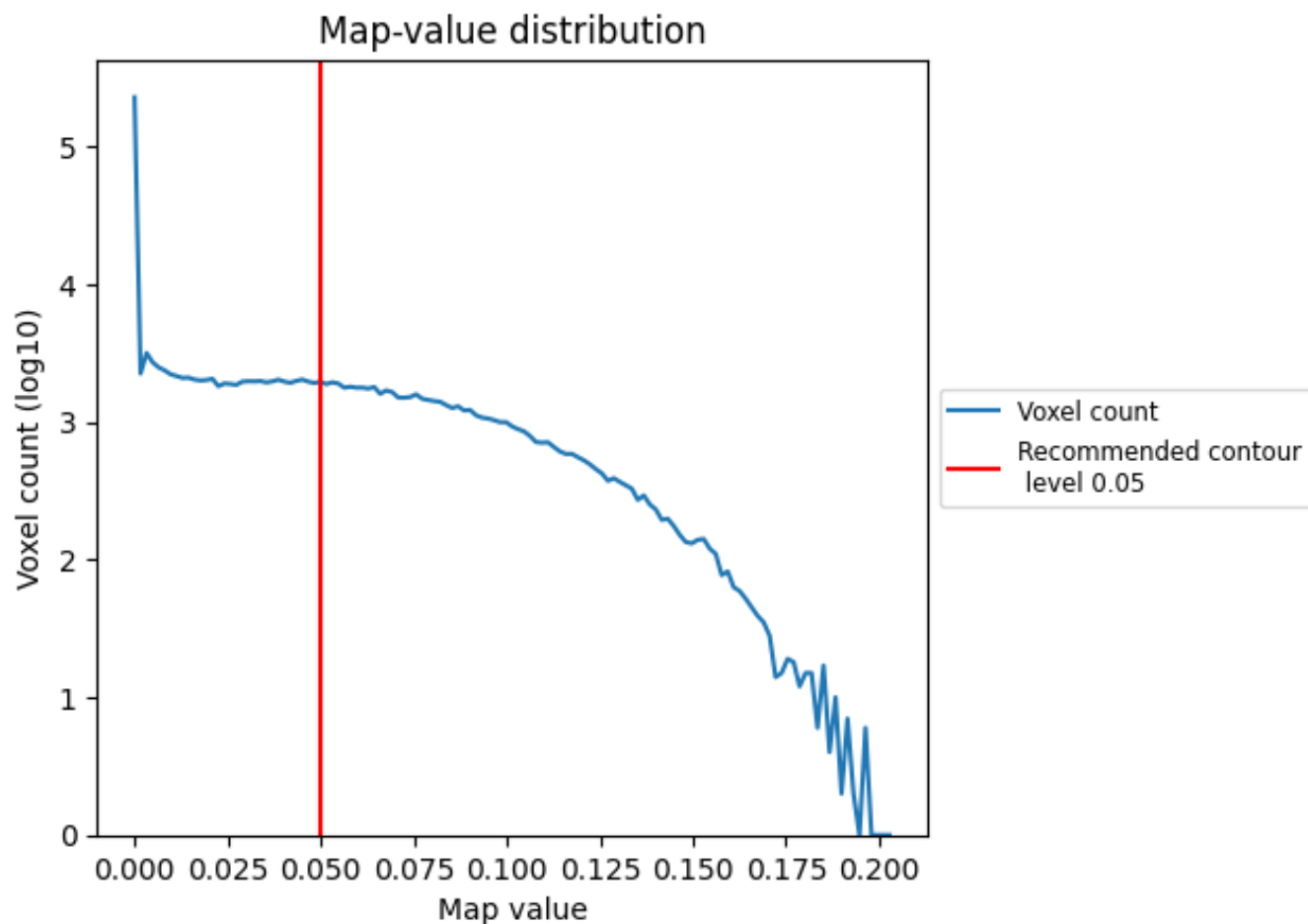
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

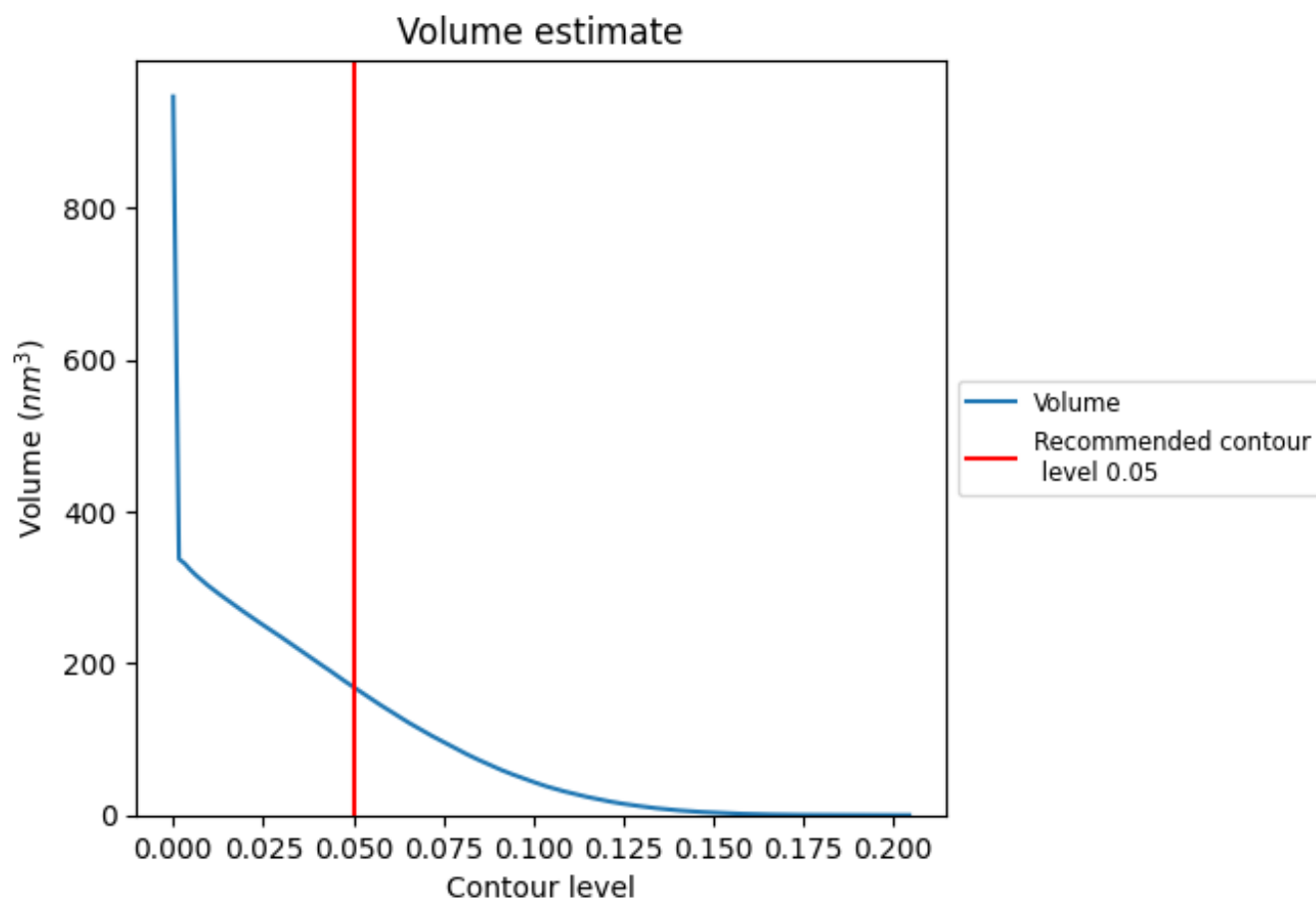
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $169 \text{ nm}^3$ ; this corresponds to an approximate mass of 153 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.

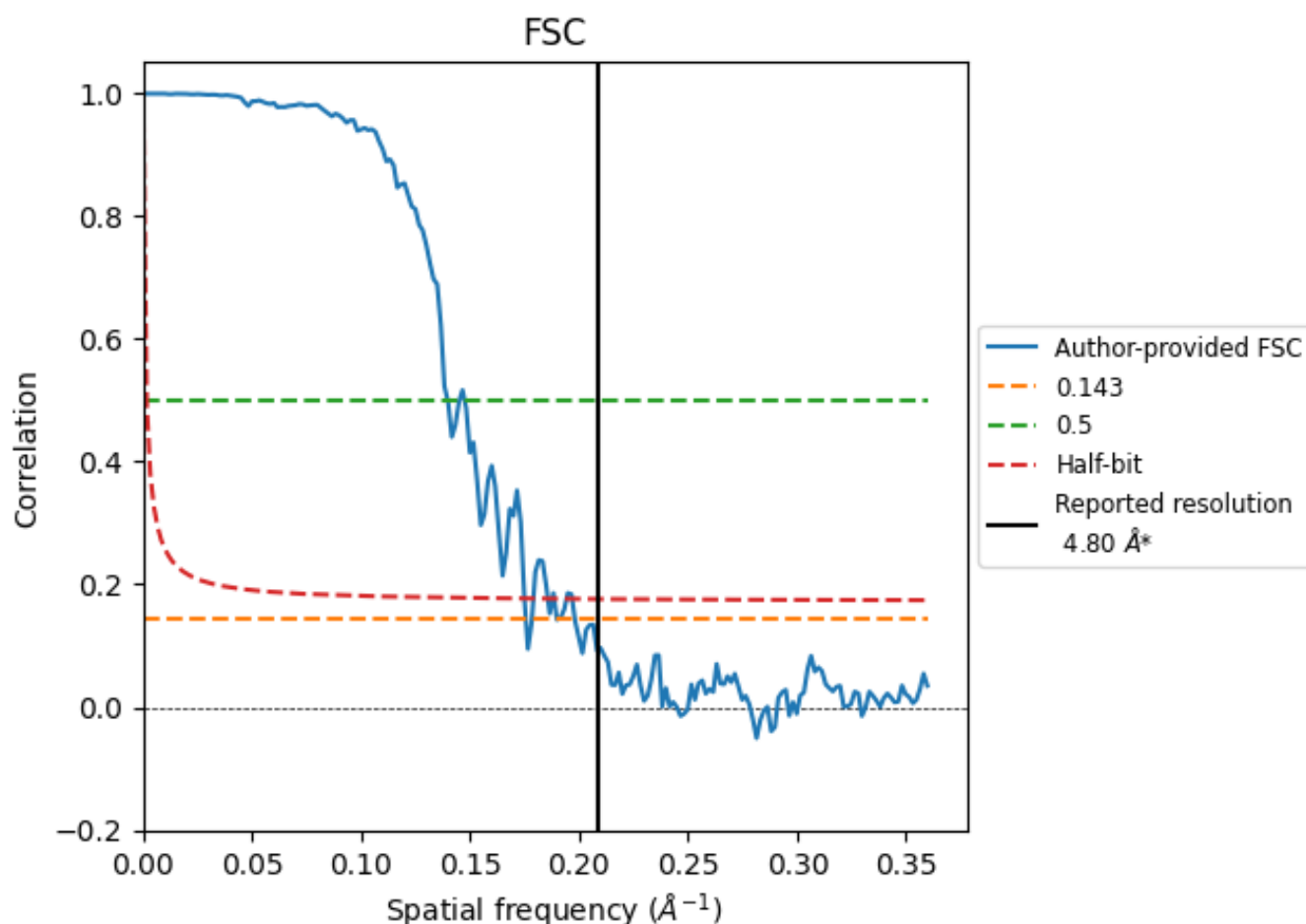
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.208 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

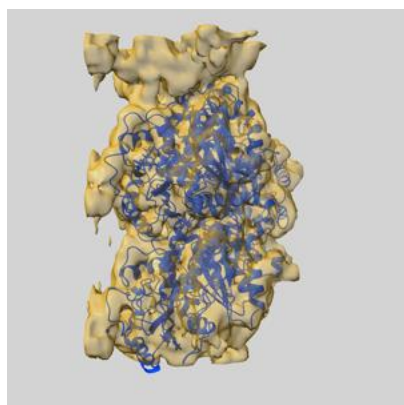
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.80                               | -    | -        |
| Author-provided FSC curve | 5.70                               | 7.16 | 5.72     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 5.70 differs from the reported value 4.8 by more than 10 %

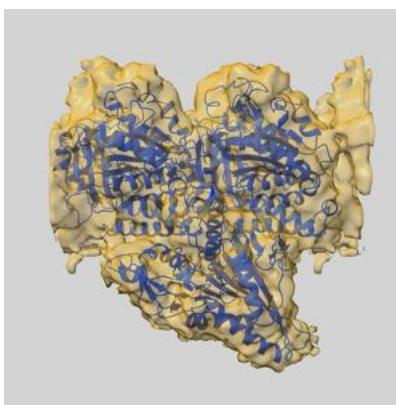
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3803 and PDB model 5OGC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

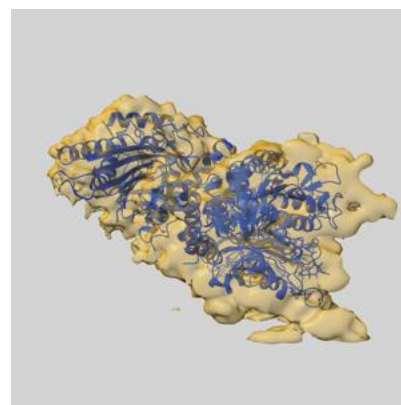
### 9.1 Map-model overlay [i](#)



X



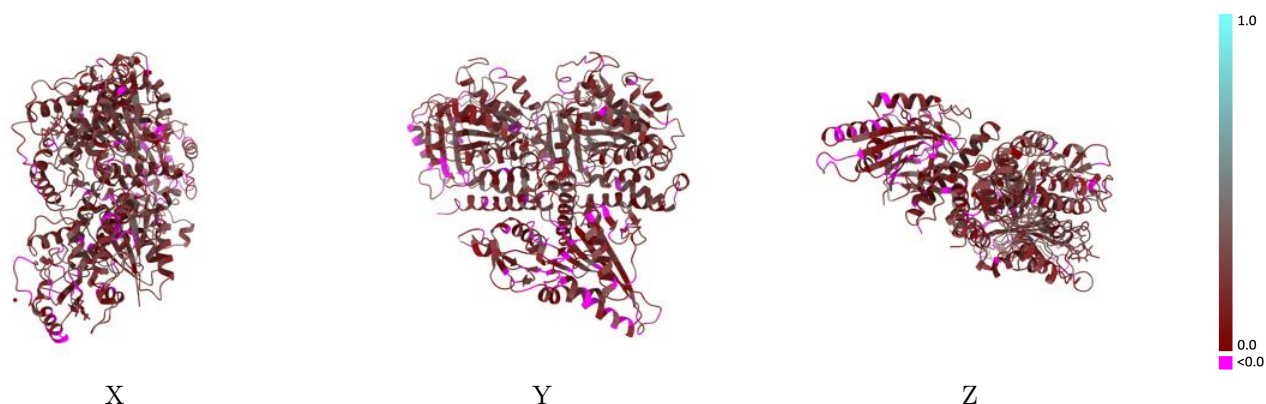
Y



Z

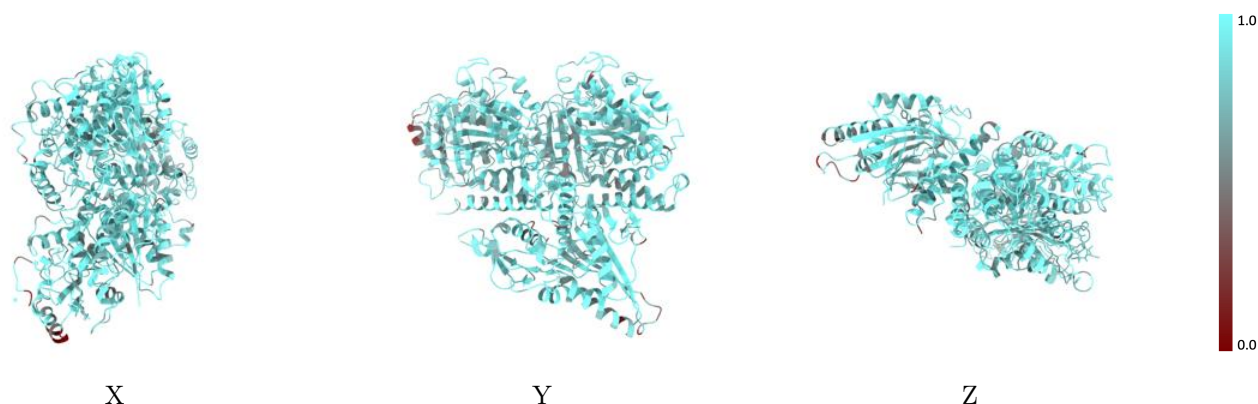
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



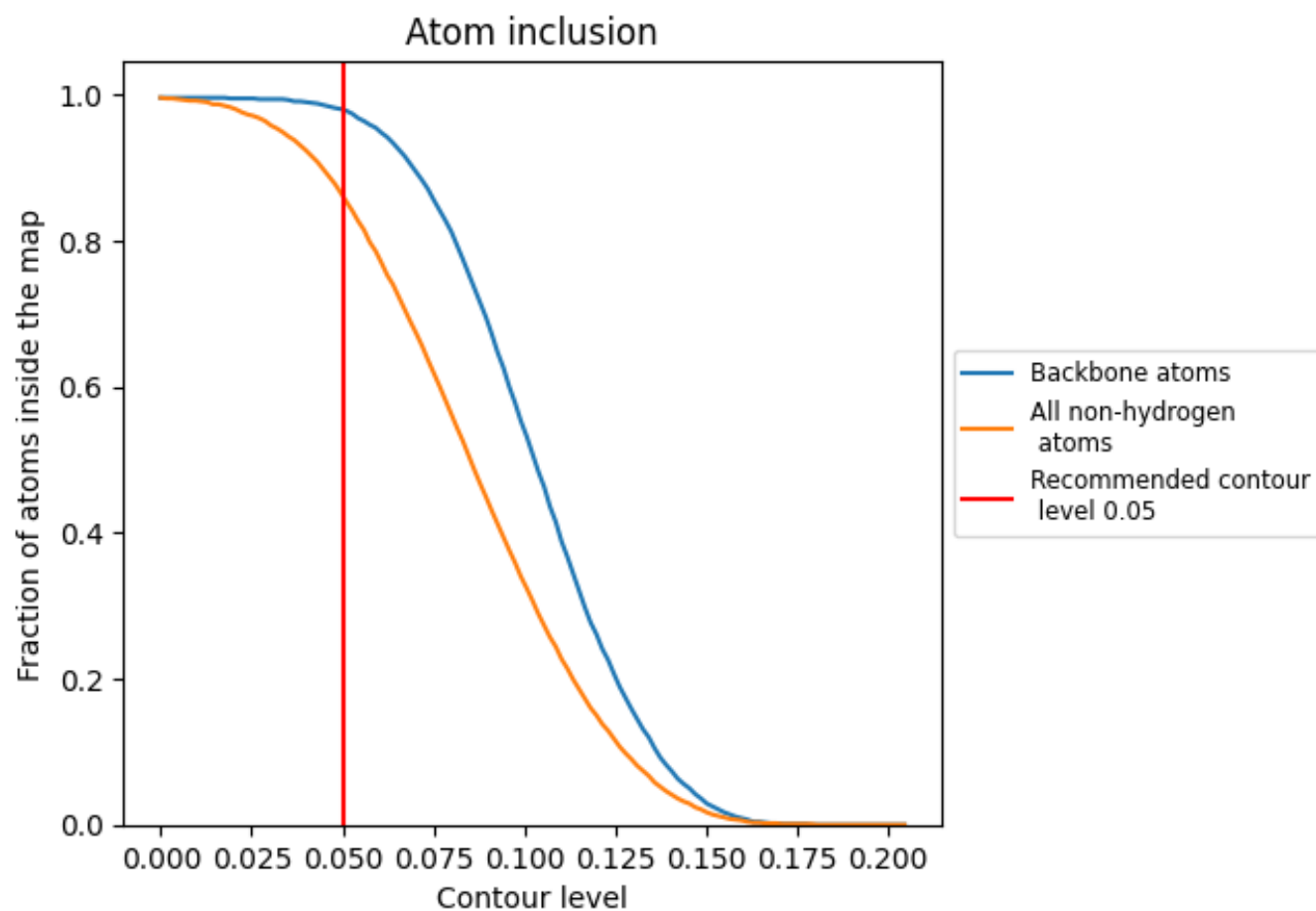
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.8620 | <div></div> 0.1780 |
| A     | <div></div> 0.8490 | <div></div> 0.1820 |
| B     | <div></div> 0.8800 | <div></div> 0.2050 |
| K     | <div></div> 0.8530 | <div></div> 0.1370 |

