



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:56 PM UTC

PDB ID : 8QYO / pdb\_00008qyo  
EMDB ID : EMD-18760  
Title : Human proteasome 20S core particle  
Authors : Schulman, B.A.; Hanna, J.W.; Harper, J.W.; Adolf, F.; Du, J.; Rawson, S.D.;  
Walsh Jr, R.M.; Goodall, E.A.  
Deposited on : 2023-10-26  
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

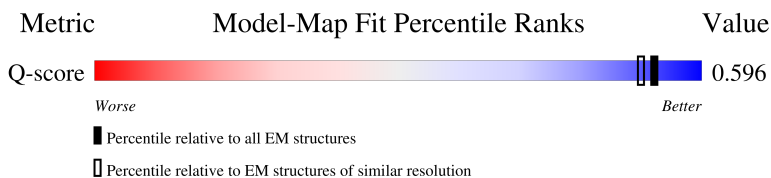
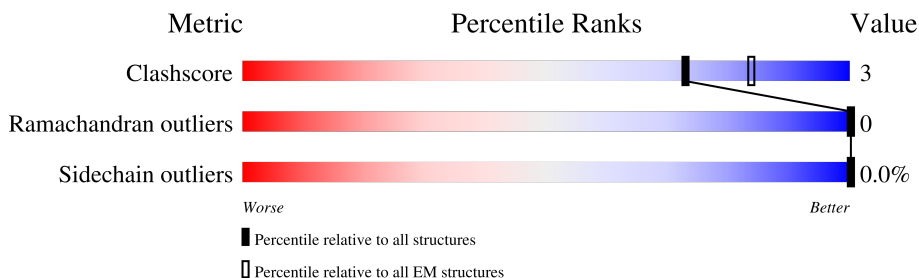
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.84 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                       | 11884 ( 2.34 - 3.34 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 234    | <div> <div>22%</div> <div>88%</div> <div>10%</div> <div>.</div> </div> |
| 1   | O     | 234    | <div> <div>23%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>  |
| 2   | B     | 261    | <div> <div>23%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div> |
| 2   | P     | 261    | <div> <div>23%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 248    |                  |
| 3   | Q     | 248    |                  |
| 4   | D     | 241    |                  |
| 4   | R     | 241    |                  |
| 5   | E     | 263    |                  |
| 5   | S     | 263    |                  |
| 6   | F     | 255    |                  |
| 6   | T     | 255    |                  |
| 7   | G     | 246    |                  |
| 7   | U     | 246    |                  |
| 8   | H     | 277    |                  |
| 8   | V     | 277    |                  |
| 9   | I     | 205    |                  |
| 9   | W     | 205    |                  |
| 10  | J     | 201    |                  |
| 10  | X     | 201    |                  |
| 11  | K     | 263    |                  |
| 11  | Y     | 263    |                  |
| 12  | L     | 241    |                  |
| 12  | Z     | 241    |                  |
| 13  | M     | 264    |                  |
| 13  | a     | 264    |                  |
| 14  | N     | 239    |                  |
| 14  | b     | 239    |                  |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 47940 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 Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1783  | 1141 | 300 | 336 | 6 |         |       |
| 1   | O     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1783  | 1141 | 300 | 336 | 6 |         |       |

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 245      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1922  | 1212 | 332 | 368 | 10 |         |       |
| 2   | P     | 245      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1922  | 1212 | 332 | 368 | 10 |         |       |

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1171 | 331 | 360 | 5 |         |       |
| 3   | Q     | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1171 | 331 | 360 | 5 |         |       |

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1736  | 1093 | 288 | 344 | 11 |         |       |
| 4   | R     | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1736  | 1093 | 288 | 344 | 11 |         |       |

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1837  | 1151 | 329 | 346 | 11 |         |       |
| 5   | S     | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1837  | 1151 | 329 | 346 | 11 |         |       |

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | F     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1870  | 1187 | 320 | 352 | 11 |         |       |
| 6   | T     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1870  | 1187 | 320 | 352 | 11 |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | G     | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1839  | 1163 | 310 | 353 | 13 |         |       |
| 7   | U     | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1839  | 1163 | 310 | 353 | 13 |         |       |

- Molecule 8 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | H     | 219      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1650  | 1039 | 282 | 317 | 12 |         |       |
| 8   | V     | 219      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1650  | 1039 | 282 | 317 | 12 |         |       |

- Molecule 9 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | I     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1591  | 1013 | 265 | 294 | 19 |         |       |
| 9   | W     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1591  | 1013 | 265 | 294 | 19 |         |       |

- Molecule 10 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | J     | 196      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1561  | 1001 | 264 | 287 | 9 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | X     | 196      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1561  | 1001 | 264 | 287 | 9 |         |       |

- Molecule 11 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 979 | 271 | 294 | 9 |         |       |
| 11  | Y     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 979 | 271 | 294 | 9 |         |       |

- Molecule 12 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | L     | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1613  | 1022 | 276 | 305 | 10 |         |       |
| 12  | Z     | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1613  | 1022 | 276 | 305 | 10 |         |       |

- Molecule 13 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | M     | 215      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1680  | 1059 | 290 | 319 | 12 |         |       |
| 13  | a     | 215      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1680  | 1059 | 290 | 319 | 12 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| M     | 234     | THR      | ILE    | variant | UNP P28070 |
| a     | 234     | THR      | ILE    | variant | UNP P28070 |

- Molecule 14 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14  | N     | 196      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1468  | 916 | 252 | 288 | 12 |         |       |
| 14  | b     | 196      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1468  | 916 | 252 | 288 | 12 |         |       |

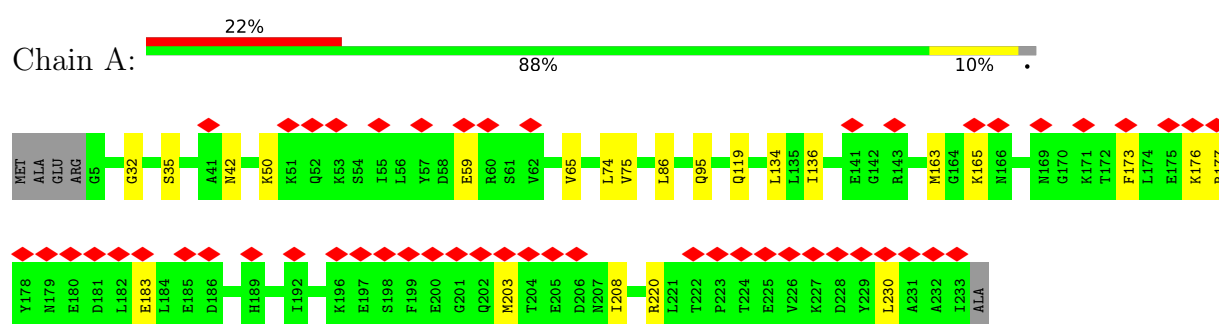
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| N     | 145     | GLY      | VAL    | variant | UNP P28072 |
| b     | 145     | GLY      | VAL    | variant | UNP P28072 |

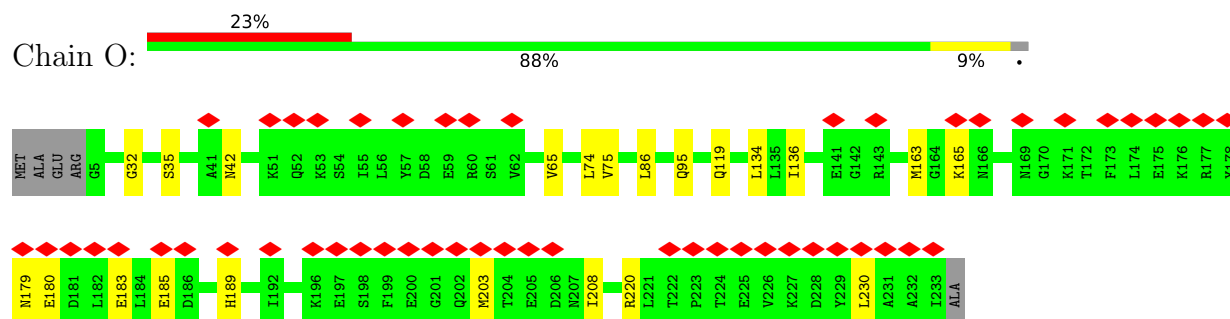
### 3 Residue-property plots [i](#)

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.

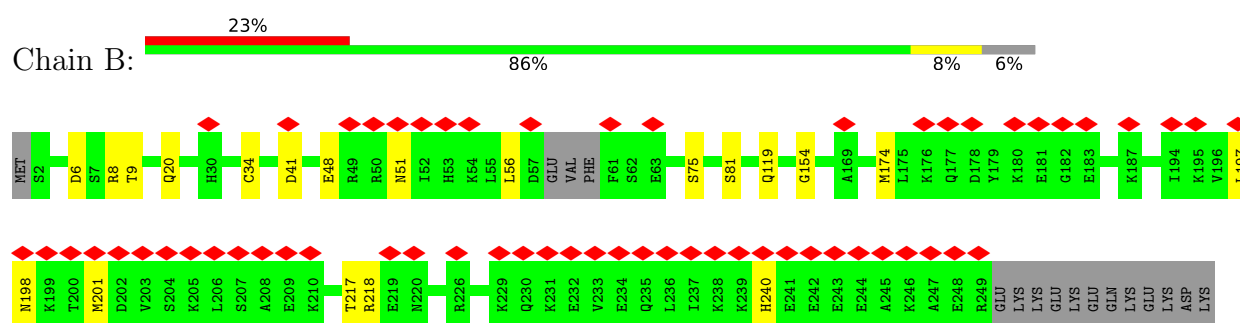
- Molecule 1: Proteasome subunit alpha type-2



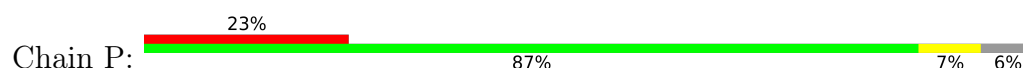
- Molecule 1: Proteasome subunit alpha type-2



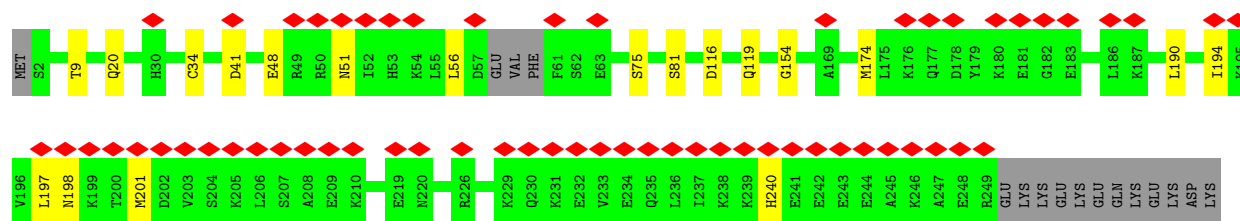
- Molecule 2: Proteasome subunit alpha type-4



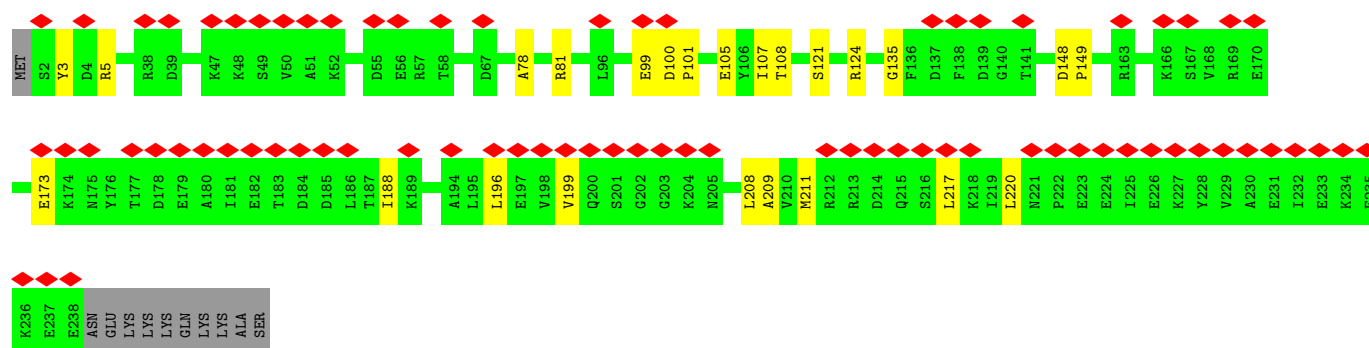
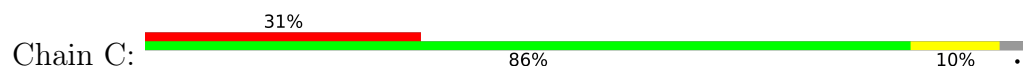
- Molecule 2: Proteasome subunit alpha type-4



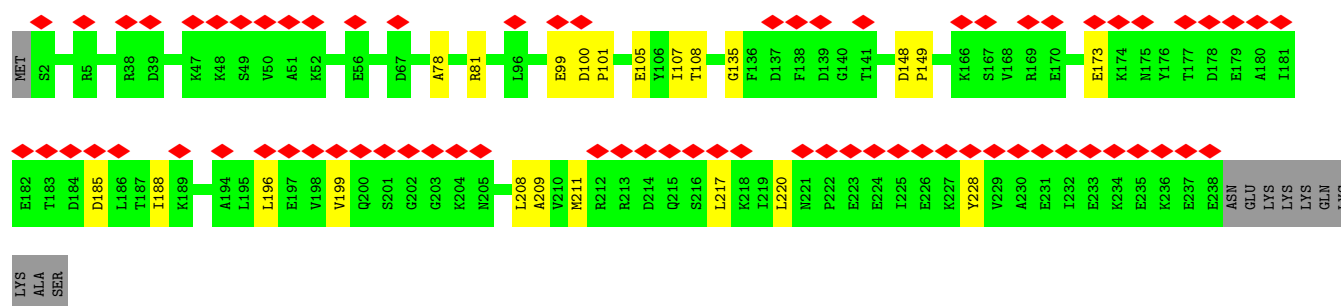
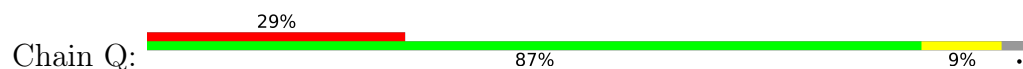




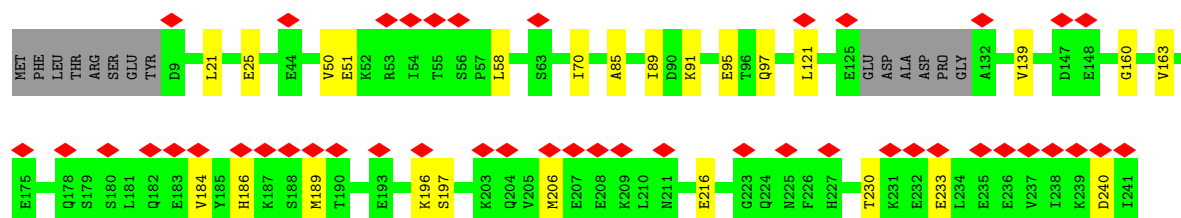
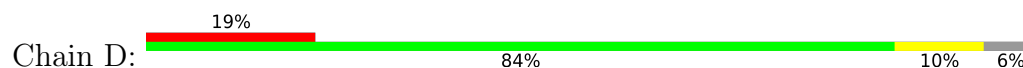
• Molecule 3: Proteasome subunit alpha type-7



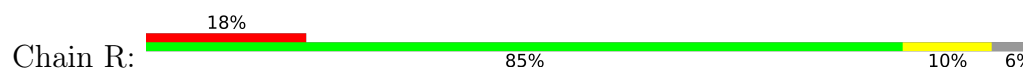
• Molecule 3: Proteasome subunit alpha type-7

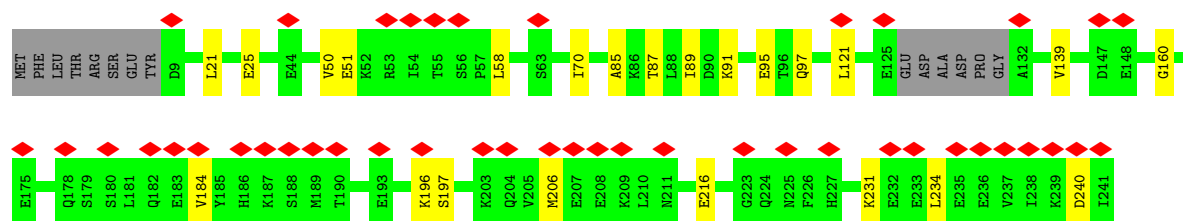


• Molecule 4: Proteasome subunit alpha type-5

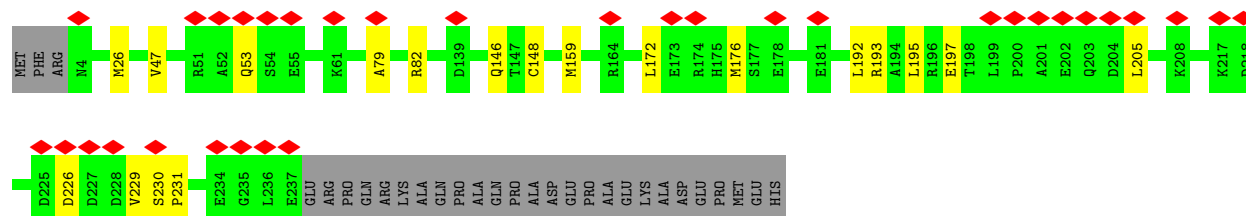
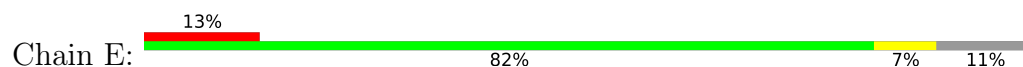


• Molecule 4: Proteasome subunit alpha type-5

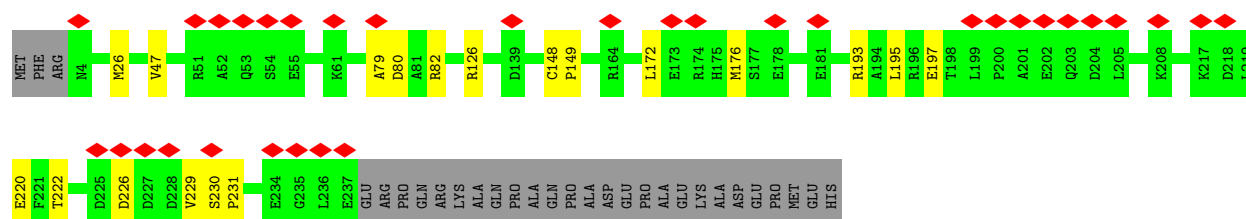
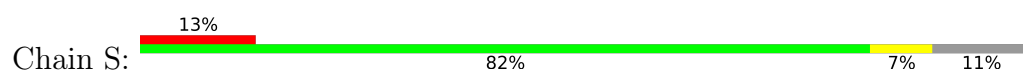




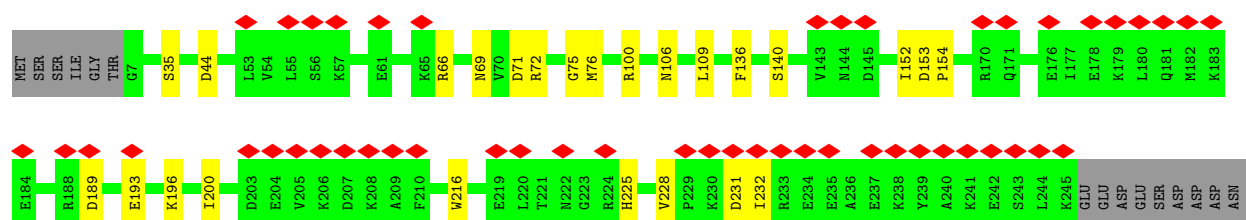
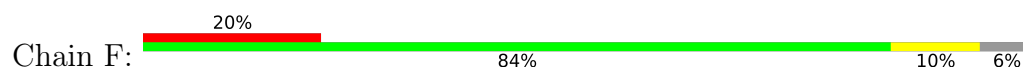
• Molecule 5: Proteasome subunit alpha type-1



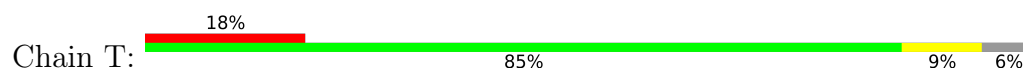
• Molecule 5: Proteasome subunit alpha type-1

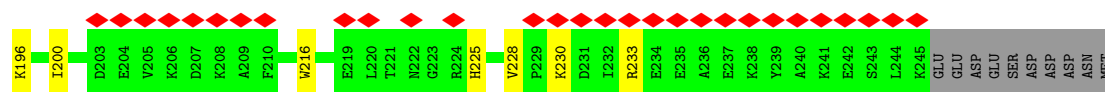


• Molecule 6: Proteasome subunit alpha type-3

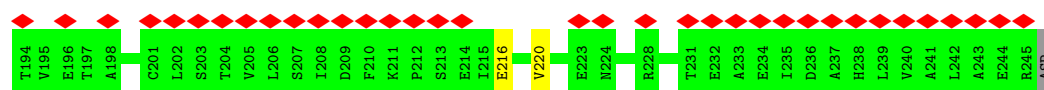
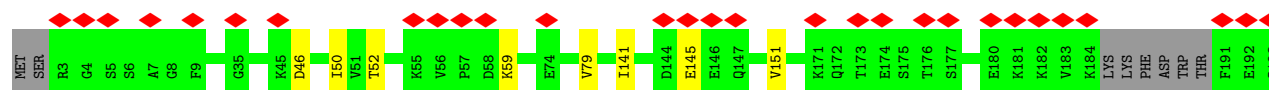


• Molecule 6: Proteasome subunit alpha type-3

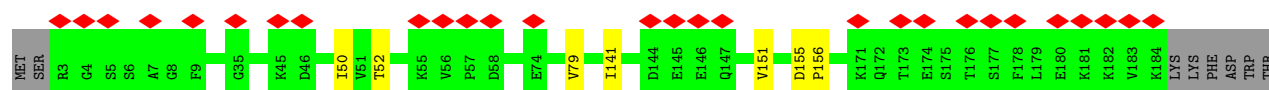




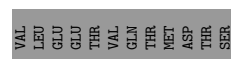
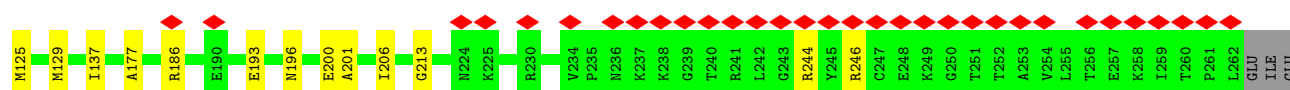
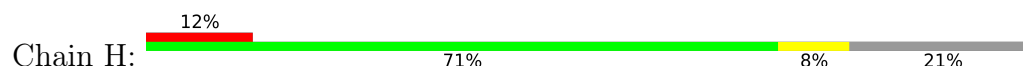
• Molecule 7: Proteasome subunit alpha type-6



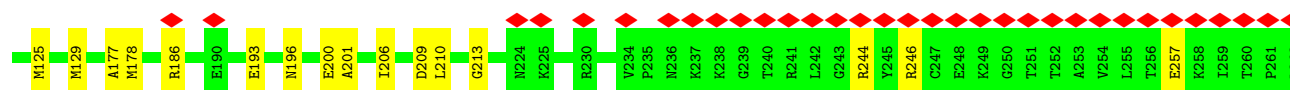
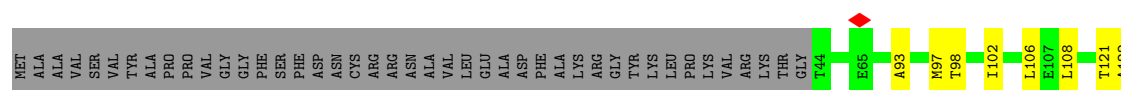
• Molecule 7: Proteasome subunit alpha type-6



• Molecule 8: Proteasome subunit beta type-7



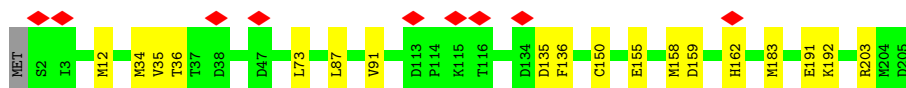
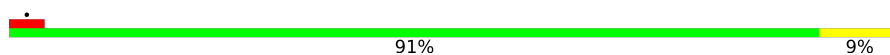
• Molecule 8: Proteasome subunit beta type-7



GLU  
ILE  
GLU  
VAL  
LEU  
GLU  
GLU  
THR  
GLN  
THR  
MET  
ASP  
THR  
SER

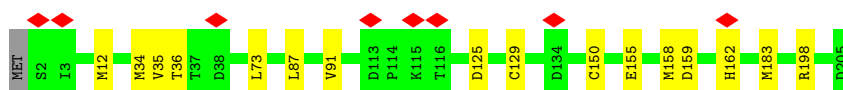
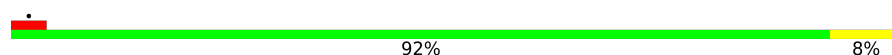
• Molecule 9: Proteasome subunit beta type-3

Chain I:



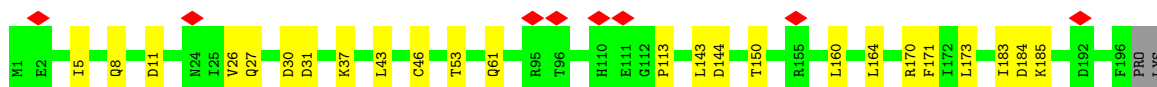
• Molecule 9: Proteasome subunit beta type-3

Chain W:



• Molecule 10: Proteasome subunit beta type-2

Chain J:



GLN  
GLY  
SER

• Molecule 10: Proteasome subunit beta type-2

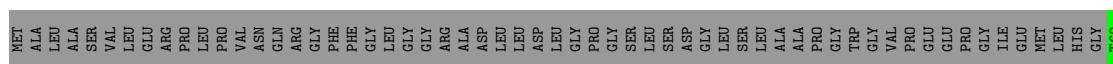
Chain X:



GLY  
SER

• Molecule 11: Proteasome subunit beta type-5

Chain K:



• Molecule 11: Proteasome subunit beta type-5

Chain Y:  71% 5% 24%

MET ALA LEU SER ALA VAL LEU ARG PRO LEU PRO VAL ASN GLN ARG GLY PHE PHE GLY LEU ARG ALA ASP LEU LEU LEU LEU PRO GLY SER LEU ASP GLY LEU ALA ALA PRO GLY TRP VAL PRO GLU GLU PRO PRO ILE GLY MET LEU HIS GLY T60

A79 V90 I94 M104 R123 I124 Y125 E126 E131 K140 L141 M145 K165 R166 D174 S175 E176 G177 N178 D205 R225 D249 N250 D253 S259 G260 THR PRO

• Molecule 12: Proteasome subunit beta type-1

Chain L:  7% 81% 5% 14%

MET LEU SER THR ALA MET TYR SER ALA PRO GLY ARG ASP LEU GLY MET GLU PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R29 A44 G45 E46 D47 F48 R56 F61 D67 K73 L74 T75 D76 E143 E144 G145 K146 V149 M172 F183 M186 Q187

ASN VAL GLU HIS VAL P193 R198 R213 D219 K228 E229 G230 I231 D241

• Molecule 12: Proteasome subunit beta type-1

Chain Z:  7% 82% 5% 14%

MET LEU SER THR ALA MET TYR SER ALA PRO GLY ARG ASP LEU GLY MET GLU PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R29 A44 G45 E46 D47 F48 R56 F61 D67 K73 D76 E143 E144 G145 K146 V149 K164 M172 F183 M186

Q187 ASN VAL GLU HIS VAL P193 R198 R213 D219 K228 E229 G230 I231 D241

• Molecule 13: Proteasome subunit beta type-4

Chain M:  5% 71% 11% 19%

MET GLU ALA PHE LEU GLY SER ARG SER GLY LEU TRP ALA GLY GLY PRO PRO ALA PRO PRO GLN PHE TYR ARG ILE PRO SER THR PRO ASP PHE MET ASP PRO ALA SER ALA LEU TYR ARG GLY PRO ILE THR ARG T46 Q47 N48 P49 M50 L57 D70 M83 M88 R89 V90

M96 K109 L112 D124 W152 D162 L167 G168 Y169 V170 D171 M172 L182 A183 T184 K201 Q202 R211 E215 M218 R224 R231 F232 V237 T238 E239 K240 E251 T252 D255 T256 A257 H258 M259 I260 SER GLY PHE GLU

• Molecule 13: Proteasome subunit beta type-4

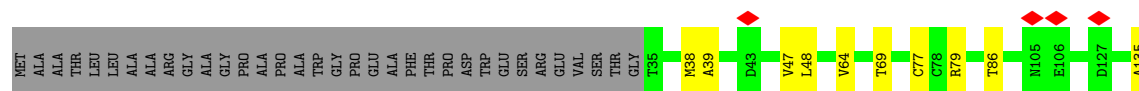
Chain a:  6% 74% 7% 19%

MET GLU ALA PHE LEU GLY SER ARG SER GLY LEU TRP ALA GLY GLY PRO PRO ALA PRO PRO GLN PHE TYR ARG ILE PRO SER THR PRO ASP PHE MET ASP PRO ALA SER ALA LEU TYR ARG GLY PRO ILE THR ARG T46 Q47 N48 P49 L57 M88 M95 Y102 K109



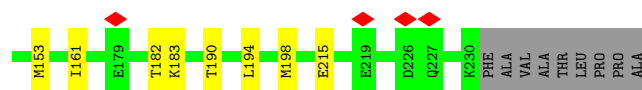
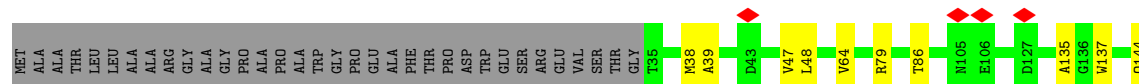
- Molecule 14: Proteasome subunit beta type-6

Chain N: 74% 8% 18%



- Molecule 14: Proteasome subunit beta type-6

Chain b: 74% 8% 18%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 569831                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS GLACIOS                             | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 56.35                                   | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2600                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.052                                   | Depositor |
| Minimum map value                    | -2.057                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.112                                   | Depositor |
| Recommended contour level            | 0.636                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 330.68, 330.68, 330.68                  | wwPDB     |
| Map dimensions                       | 280, 280, 280                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.181, 1.181, 1.181                     | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.22         | 0/1822  | 0.35        | 0/2470         |
| 1   | O     | 0.22         | 0/1822  | 0.35        | 0/2470         |
| 2   | B     | 0.21         | 0/1950  | 0.35        | 0/2626         |
| 2   | P     | 0.21         | 0/1950  | 0.34        | 0/2626         |
| 3   | C     | 0.20         | 0/1893  | 0.35        | 0/2554         |
| 3   | Q     | 0.20         | 0/1893  | 0.36        | 0/2554         |
| 4   | D     | 0.20         | 0/1761  | 0.36        | 0/2376         |
| 4   | R     | 0.21         | 0/1761  | 0.37        | 0/2376         |
| 5   | E     | 0.20         | 0/1871  | 0.35        | 0/2529         |
| 5   | S     | 0.20         | 0/1871  | 0.36        | 0/2529         |
| 6   | F     | 0.21         | 0/1905  | 0.38        | 0/2565         |
| 6   | T     | 0.21         | 0/1905  | 0.39        | 0/2565         |
| 7   | G     | 0.21         | 0/1869  | 0.33        | 0/2524         |
| 7   | U     | 0.20         | 0/1869  | 0.33        | 0/2524         |
| 8   | H     | 0.23         | 0/1677  | 0.37        | 0/2270         |
| 8   | V     | 0.23         | 0/1677  | 0.38        | 0/2270         |
| 9   | I     | 0.25         | 0/1620  | 0.41        | 0/2184         |
| 9   | W     | 0.25         | 0/1620  | 0.39        | 0/2184         |
| 10  | J     | 0.25         | 0/1593  | 0.40        | 0/2156         |
| 10  | X     | 0.27         | 0/1593  | 0.41        | 0/2156         |
| 11  | K     | 0.24         | 0/1584  | 0.38        | 0/2140         |
| 11  | Y     | 0.24         | 0/1584  | 0.38        | 0/2140         |
| 12  | L     | 0.24         | 0/1641  | 0.40        | 0/2206         |
| 12  | Z     | 0.23         | 0/1641  | 0.40        | 0/2206         |
| 13  | M     | 0.29         | 0/1713  | 0.51        | 1/2319 (0.0%)  |
| 13  | a     | 0.26         | 0/1713  | 0.42        | 0/2319         |
| 14  | N     | 0.26         | 0/1493  | 0.44        | 0/2019         |
| 14  | b     | 0.27         | 0/1493  | 0.46        | 0/2019         |
| All | All   | 0.23         | 0/48784 | 0.38        | 1/65876 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:



| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | M     | 50  | MET  | CB-CA-C | -5.90 | 109.21      | 117.23   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1783  | 0        | 1771     | 15      | 0            |
| 1   | O     | 1783  | 0        | 1771     | 14      | 0            |
| 2   | B     | 1922  | 0        | 1937     | 16      | 0            |
| 2   | P     | 1922  | 0        | 1937     | 13      | 0            |
| 3   | C     | 1867  | 0        | 1884     | 18      | 0            |
| 3   | Q     | 1867  | 0        | 1884     | 15      | 0            |
| 4   | D     | 1736  | 0        | 1734     | 16      | 0            |
| 4   | R     | 1736  | 0        | 1734     | 15      | 0            |
| 5   | E     | 1837  | 0        | 1826     | 11      | 0            |
| 5   | S     | 1837  | 0        | 1826     | 11      | 0            |
| 6   | F     | 1870  | 0        | 1857     | 15      | 0            |
| 6   | T     | 1870  | 0        | 1857     | 14      | 0            |
| 7   | G     | 1839  | 0        | 1849     | 8       | 0            |
| 7   | U     | 1839  | 0        | 1849     | 5       | 0            |
| 8   | H     | 1650  | 0        | 1672     | 11      | 0            |
| 8   | V     | 1650  | 0        | 1672     | 15      | 0            |
| 9   | I     | 1591  | 0        | 1609     | 10      | 0            |
| 9   | W     | 1591  | 0        | 1609     | 9       | 0            |
| 10  | J     | 1561  | 0        | 1558     | 17      | 0            |
| 10  | X     | 1561  | 0        | 1558     | 14      | 0            |
| 11  | K     | 1553  | 0        | 1509     | 11      | 0            |
| 11  | Y     | 1553  | 0        | 1509     | 9       | 0            |
| 12  | L     | 1613  | 0        | 1616     | 6       | 0            |
| 12  | Z     | 1613  | 0        | 1616     | 6       | 0            |
| 13  | M     | 1680  | 0        | 1654     | 18      | 0            |
| 13  | a     | 1680  | 0        | 1654     | 12      | 0            |
| 14  | N     | 1468  | 0        | 1432     | 11      | 0            |
| 14  | b     | 1468  | 0        | 1432     | 12      | 0            |
| All | All   | 47940 | 0        | 47816    | 311     | 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 3.

All (311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:9:THR:HG23    | 2:P:20:GLN:HG3    | 1.69                     | 0.75              |
| 13:a:171:ASP:OD1  | 13:a:172:MET:N    | 2.21                     | 0.73              |
| 13:M:83:ASN:OD1   | 13:M:231:ARG:NH2  | 2.22                     | 0.72              |
| 12:L:172:MET:HE1  | 12:L:213:ARG:HB2  | 1.76                     | 0.67              |
| 12:Z:172:MET:HE1  | 12:Z:213:ARG:HB2  | 1.77                     | 0.66              |
| 13:M:88:MET:HE3   | 13:M:90:VAL:HG22  | 1.77                     | 0.65              |
| 14:N:69:THR:OG1   | 14:N:77:CYS:SG    | 2.55                     | 0.65              |
| 4:D:121:LEU:HD12  | 5:E:79:ALA:HB3    | 1.79                     | 0.65              |
| 10:J:27:GLN:NE2   | 10:J:30:ASP:OD1   | 2.30                     | 0.64              |
| 4:R:121:LEU:HD12  | 5:S:79:ALA:HB3    | 1.80                     | 0.63              |
| 13:M:88:MET:SD    | 13:M:109:LYS:HG3  | 2.39                     | 0.62              |
| 14:b:79:ARG:HD2   | 14:b:86:THR:HB    | 1.81                     | 0.62              |
| 2:B:9:THR:HG23    | 2:B:20:GLN:HG3    | 1.81                     | 0.62              |
| 4:R:196:LYS:NZ    | 4:R:240:ASP:OD2   | 2.33                     | 0.61              |
| 9:I:12:MET:HE1    | 9:I:150:CYS:SG    | 2.41                     | 0.60              |
| 13:M:256:ILE:HA   | 13:M:259:MET:HE3  | 1.84                     | 0.60              |
| 13:a:256:ILE:HA   | 13:a:259:MET:HE3  | 1.82                     | 0.60              |
| 8:V:257:GLU:HG2   | 9:W:198:ARG:HG2   | 1.84                     | 0.60              |
| 13:M:238:THR:HG22 | 13:M:239:GLU:H    | 1.66                     | 0.60              |
| 12:Z:44:ALA:HB2   | 12:Z:149:VAL:HG23 | 1.84                     | 0.59              |
| 10:J:43:LEU:HD12  | 10:J:183:ILE:HD11 | 1.83                     | 0.59              |
| 3:Q:99:GLU:OE2    | 11:Y:140:LYS:NZ   | 2.36                     | 0.59              |
| 10:X:27:GLN:NE2   | 10:X:30:ASP:OD1   | 2.35                     | 0.59              |
| 6:T:35:SER:OG     | 6:T:66:ARG:NH1    | 2.35                     | 0.59              |
| 12:L:44:ALA:HB2   | 12:L:149:VAL:HG23 | 1.84                     | 0.59              |
| 3:C:99:GLU:OE2    | 11:K:140:LYS:NZ   | 2.35                     | 0.58              |
| 4:R:91:LYS:O      | 4:R:95:GLU:HG2    | 2.03                     | 0.58              |
| 3:C:209:ALA:HB1   | 3:C:217:LEU:HD11  | 1.85                     | 0.58              |
| 10:X:43:LEU:HD12  | 10:X:183:ILE:HD11 | 1.84                     | 0.58              |
| 6:F:216:TRP:CE3   | 6:F:228:VAL:HG22  | 2.39                     | 0.58              |
| 1:A:50:LYS:NZ     | 1:A:59:GLU:O      | 2.37                     | 0.57              |
| 3:Q:209:ALA:HB1   | 3:Q:217:LEU:HD11  | 1.84                     | 0.57              |
| 8:H:186:ARG:NH2   | 8:H:193:GLU:OE1   | 2.37                     | 0.57              |
| 6:T:216:TRP:CE3   | 6:T:228:VAL:HG22  | 2.39                     | 0.57              |
| 9:W:34:MET:SD     | 9:W:183:MET:HE1   | 2.44                     | 0.57              |
| 9:I:34:MET:SD     | 9:I:183:MET:HE1   | 2.44                     | 0.57              |
| 7:U:193:GLN:HB3   | 7:U:196:GLU:OE1   | 2.05                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:V:206:ILE:HG23 | 8:V:213:GLY:HA2   | 1.87                     | 0.56              |
| 3:C:100:ASP:OD1  | 3:C:101:PRO:HD2   | 2.06                     | 0.56              |
| 13:M:171:ASP:OD1 | 13:M:172:MET:N    | 2.36                     | 0.56              |
| 10:J:27:GLN:O    | 10:X:170:ARG:NH1  | 2.38                     | 0.56              |
| 14:N:79:ARG:HD2  | 14:N:86:THR:HB    | 1.87                     | 0.56              |
| 1:A:119:GLN:HG3  | 2:B:81:SER:HB3    | 1.88                     | 0.56              |
| 9:W:12:MET:HE1   | 9:W:150:CYS:SG    | 2.45                     | 0.56              |
| 8:H:106:LEU:HD11 | 8:H:122:ALA:HB2   | 1.88                     | 0.55              |
| 2:B:197:LEU:O    | 2:B:201:MET:HG2   | 2.07                     | 0.55              |
| 8:H:94:ASP:HB3   | 8:H:137:ILE:HG23  | 1.88                     | 0.55              |
| 3:Q:100:ASP:OD1  | 3:Q:101:PRO:HD2   | 2.06                     | 0.55              |
| 6:T:100:ARG:NH1  | 6:T:106:ASN:OD1   | 2.40                     | 0.55              |
| 14:b:48:LEU:HD21 | 14:b:135:ALA:HB3  | 1.89                     | 0.55              |
| 4:D:91:LYS:O     | 4:D:95:GLU:HG2    | 2.06                     | 0.55              |
| 8:H:206:ILE:HG23 | 8:H:213:GLY:HA2   | 1.87                     | 0.55              |
| 1:A:65:VAL:O     | 1:A:220:ARG:NH1   | 2.39                     | 0.55              |
| 3:Q:148:ASP:OD1  | 3:Q:149:PRO:HD2   | 2.06                     | 0.55              |
| 13:M:152:TRP:HA  | 13:M:172:MET:HE2  | 1.88                     | 0.55              |
| 5:E:226:ASP:O    | 5:E:229:VAL:HG22  | 2.06                     | 0.55              |
| 2:P:34:CYS:SG    | 2:P:75:SER:OG     | 2.65                     | 0.55              |
| 8:V:106:LEU:HD11 | 8:V:122:ALA:HB2   | 1.89                     | 0.54              |
| 10:J:5:ILE:HD11  | 10:J:143:LEU:HD11 | 1.89                     | 0.54              |
| 2:P:154:GLY:O    | 3:Q:81:ARG:NH2    | 2.41                     | 0.54              |
| 4:D:230:THR:OG1  | 4:D:233:GLU:OE2   | 2.25                     | 0.54              |
| 2:P:119:GLN:HG3  | 3:Q:78:ALA:HB1    | 1.88                     | 0.54              |
| 14:N:48:LEU:HD21 | 14:N:135:ALA:HB3  | 1.89                     | 0.54              |
| 2:B:119:GLN:HG3  | 3:C:78:ALA:HB1    | 1.88                     | 0.54              |
| 9:I:159:ASP:OD1  | 9:I:162:HIS:ND1   | 2.36                     | 0.54              |
| 11:K:225:ARG:NH1 | 10:X:144:ASP:OD2  | 2.35                     | 0.54              |
| 2:B:8:ARG:HH21   | 3:C:5:ARG:HH22    | 1.54                     | 0.54              |
| 13:M:224:ARG:CZ  | 8:V:178:MET:HE2   | 2.38                     | 0.54              |
| 2:P:197:LEU:O    | 2:P:201:MET:HG2   | 2.07                     | 0.54              |
| 10:X:5:ILE:HD11  | 10:X:143:LEU:HD11 | 1.89                     | 0.54              |
| 6:F:100:ARG:NH1  | 6:F:106:ASN:OD1   | 2.40                     | 0.53              |
| 13:M:95:MET:HE2  | 13:M:237:VAL:HG12 | 1.91                     | 0.53              |
| 2:B:154:GLY:O    | 3:C:81:ARG:NH2    | 2.41                     | 0.53              |
| 10:X:184:ASP:OD1 | 10:X:185:LYS:N    | 2.35                     | 0.53              |
| 1:O:119:GLN:HG3  | 2:P:81:SER:HB2    | 1.90                     | 0.53              |
| 8:H:177:ALA:HB1  | 8:H:201:ALA:HB1   | 1.90                     | 0.53              |
| 1:O:203:MET:HE2  | 1:O:230:LEU:HD21  | 1.91                     | 0.53              |
| 9:I:35:VAL:HG12  | 9:I:36:THR:HG23   | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:135:GLY:HA2   | 3:C:211:MET:HE1   | 1.91                     | 0.52              |
| 9:W:159:ASP:OD1   | 9:W:162:HIS:ND1   | 2.38                     | 0.52              |
| 8:V:177:ALA:HB1   | 8:V:201:ALA:HB1   | 1.90                     | 0.52              |
| 6:T:196:LYS:O     | 6:T:200:ILE:HD12  | 2.10                     | 0.52              |
| 13:a:57:LEU:HD22  | 13:a:218:MET:HE2  | 1.90                     | 0.52              |
| 10:J:184:ASP:OD1  | 10:J:185:LYS:N    | 2.35                     | 0.52              |
| 13:M:88:MET:HE1   | 13:M:112:LEU:HD23 | 1.90                     | 0.52              |
| 3:Q:135:GLY:HA2   | 3:Q:211:MET:HE1   | 1.91                     | 0.52              |
| 9:W:35:VAL:HG12   | 9:W:36:THR:HG23   | 1.91                     | 0.52              |
| 8:V:186:ARG:NH2   | 8:V:193:GLU:OE1   | 2.43                     | 0.52              |
| 10:X:8:GLN:HE21   | 10:X:113:PRO:HG2  | 1.74                     | 0.52              |
| 2:P:51:ASN:HB3    | 2:P:56:LEU:HD13   | 1.92                     | 0.52              |
| 1:O:42:ASN:ND2    | 1:O:183:GLU:OE1   | 2.43                     | 0.52              |
| 5:S:47:VAL:HG12   | 5:S:195:LEU:HD22  | 1.92                     | 0.52              |
| 14:b:38:MET:HG3   | 14:b:161:ILE:HG22 | 1.92                     | 0.51              |
| 11:K:94:ILE:HD11  | 11:K:104:MET:HE2  | 1.91                     | 0.51              |
| 5:S:226:ASP:O     | 5:S:229:VAL:HG22  | 2.09                     | 0.51              |
| 3:C:148:ASP:OD1   | 3:C:149:PRO:HD2   | 2.10                     | 0.51              |
| 6:F:196:LYS:O     | 6:F:200:ILE:HD12  | 2.11                     | 0.51              |
| 3:Q:208:LEU:HD23  | 3:Q:220:LEU:HD12  | 1.92                     | 0.51              |
| 11:Y:141:LEU:O    | 11:Y:145:MET:HG3  | 2.10                     | 0.51              |
| 13:a:88:MET:SD    | 13:a:109:LYS:HG2  | 2.51                     | 0.51              |
| 11:K:141:LEU:O    | 11:K:145:MET:HG3  | 2.11                     | 0.51              |
| 6:F:153:ASP:OD1   | 6:F:154:PRO:HD2   | 2.10                     | 0.51              |
| 1:A:203:MET:HE2   | 1:A:230:LEU:HD21  | 1.93                     | 0.51              |
| 6:F:44:ASP:OD1    | 6:F:44:ASP:N      | 2.43                     | 0.51              |
| 13:a:238:THR:HG22 | 13:a:239:GLU:H    | 1.75                     | 0.51              |
| 1:A:177:ARG:O     | 1:A:177:ARG:HG2   | 2.11                     | 0.51              |
| 8:H:244:ARG:HH21  | 8:H:246:ARG:HH11  | 1.57                     | 0.51              |
| 3:Q:188:ILE:HG23  | 3:Q:208:LEU:HD21  | 1.93                     | 0.51              |
| 3:C:188:ILE:HG23  | 3:C:208:LEU:HD21  | 1.93                     | 0.50              |
| 13:M:211:ARG:O    | 13:M:215:GLU:HG3  | 2.11                     | 0.50              |
| 3:C:208:LEU:HD23  | 3:C:220:LEU:HD12  | 1.93                     | 0.50              |
| 2:B:51:ASN:HB3    | 2:B:56:LEU:HD13   | 1.93                     | 0.50              |
| 5:E:47:VAL:HG12   | 5:E:195:LEU:HD22  | 1.92                     | 0.50              |
| 10:J:8:GLN:HE21   | 10:J:113:PRO:HG2  | 1.76                     | 0.50              |
| 6:T:153:ASP:OD1   | 6:T:154:PRO:HD2   | 2.11                     | 0.50              |
| 4:D:163:VAL:HG11  | 5:E:53:GLN:HE22   | 1.76                     | 0.50              |
| 13:M:256:ILE:HG13 | 14:b:64:VAL:HG11  | 1.94                     | 0.50              |
| 14:N:38:MET:HG3   | 14:N:161:ILE:HG22 | 1.93                     | 0.49              |
| 6:F:71:ASP:OD1    | 6:F:72:ARG:N      | 2.43                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:174:ASP:OD2  | 11:K:178:ASN:HB2  | 2.12                     | 0.49              |
| 11:Y:174:ASP:OD2  | 11:Y:178:ASN:HB2  | 2.12                     | 0.49              |
| 10:J:37:LYS:O     | 10:J:61:GLN:NE2   | 2.45                     | 0.49              |
| 1:O:35:SER:HB2    | 1:O:163:MET:HG2   | 1.95                     | 0.49              |
| 8:V:121:THR:O     | 8:V:125:MET:HG3   | 2.11                     | 0.49              |
| 9:I:155:GLU:HG2   | 9:I:158:MET:HE3   | 1.95                     | 0.49              |
| 4:R:85:ALA:HB2    | 4:R:139:VAL:HG21  | 1.95                     | 0.49              |
| 11:Y:94:ILE:HD11  | 11:Y:104:MET:HE2  | 1.94                     | 0.49              |
| 11:K:186:SER:HB3  | 11:K:195:TYR:CE1  | 2.47                     | 0.48              |
| 8:V:244:ARG:HH21  | 8:V:246:ARG:HH11  | 1.59                     | 0.48              |
| 4:D:85:ALA:HB2    | 4:D:139:VAL:HG21  | 1.95                     | 0.48              |
| 4:R:50:VAL:HG12   | 4:R:216:GLU:HB3   | 1.95                     | 0.48              |
| 10:J:31:ASP:OD1   | 10:J:31:ASP:N     | 2.46                     | 0.48              |
| 10:J:171:PHE:CE2  | 10:J:173:LEU:HB2  | 2.49                     | 0.48              |
| 14:b:182:THR:HG22 | 14:b:183:LYS:H    | 1.79                     | 0.48              |
| 14:N:38:MET:HE1   | 14:N:190:THR:HA   | 1.96                     | 0.47              |
| 9:W:155:GLU:HG2   | 9:W:158:MET:HE3   | 1.95                     | 0.47              |
| 14:b:38:MET:HE1   | 14:b:190:THR:HA   | 1.96                     | 0.47              |
| 4:D:50:VAL:HG12   | 4:D:216:GLU:HB3   | 1.96                     | 0.47              |
| 2:B:48:GLU:HG3    | 2:B:201:MET:HE1   | 1.96                     | 0.47              |
| 10:J:144:ASP:OD2  | 11:Y:225:ARG:NH1  | 2.34                     | 0.47              |
| 8:V:93:ALA:O      | 8:V:97:MET:HG2    | 2.15                     | 0.47              |
| 1:A:86:LEU:HD13   | 1:A:134:LEU:HD11  | 1.96                     | 0.47              |
| 12:Z:73:LYS:HE3   | 12:Z:231:ILE:HD12 | 1.97                     | 0.47              |
| 7:G:141:ILE:HG22  | 7:G:151:VAL:HG22  | 1.97                     | 0.47              |
| 1:O:179:ASN:OD1   | 1:O:180:GLU:N     | 2.48                     | 0.47              |
| 13:a:102:TYR:CD2  | 14:b:153:MET:HE3  | 2.50                     | 0.47              |
| 7:G:46:ASP:OD1    | 7:G:46:ASP:N      | 2.48                     | 0.47              |
| 12:L:73:LYS:HE3   | 12:L:231:ILE:HD12 | 1.96                     | 0.47              |
| 8:H:121:THR:O     | 8:H:125:MET:HG3   | 2.15                     | 0.46              |
| 7:U:141:ILE:HG22  | 7:U:151:VAL:HG22  | 1.97                     | 0.46              |
| 10:X:37:LYS:O     | 10:X:61:GLN:NE2   | 2.46                     | 0.46              |
| 7:G:52:THR:HG22   | 7:G:216:GLU:HB2   | 1.96                     | 0.46              |
| 10:J:170:ARG:NH1  | 10:X:27:GLN:O     | 2.45                     | 0.46              |
| 2:B:41:ASP:OD1    | 2:B:41:ASP:N      | 2.48                     | 0.46              |
| 8:V:196:ASN:O     | 8:V:200:GLU:HG3   | 2.15                     | 0.46              |
| 2:P:116:ASP:OD1   | 3:Q:81:ARG:NH1    | 2.49                     | 0.46              |
| 11:Y:123:ARG:NH1  | 11:Y:126:GLU:OE1  | 2.48                     | 0.46              |
| 1:O:86:LEU:HD13   | 1:O:134:LEU:HD11  | 1.97                     | 0.46              |
| 5:S:26:MET:HE1    | 5:S:148:CYS:HB3   | 1.98                     | 0.46              |
| 10:X:171:PHE:CE2  | 10:X:173:LEU:HB2  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:145:GLU:CD    | 7:G:145:GLU:H     | 2.23                     | 0.46              |
| 8:H:196:ASN:O     | 8:H:200:GLU:HG3   | 2.15                     | 0.46              |
| 10:X:11:ASP:N     | 10:X:11:ASP:OD1   | 2.49                     | 0.46              |
| 2:P:48:GLU:HG3    | 2:P:201:MET:HE1   | 1.98                     | 0.46              |
| 14:N:64:VAL:HG11  | 13:a:256:ILE:HG13 | 1.98                     | 0.46              |
| 1:A:95:GLN:HG3    | 8:H:108:LEU:HG    | 1.98                     | 0.46              |
| 12:L:56:ARG:NE    | 12:L:219:ASP:OD1  | 2.42                     | 0.46              |
| 13:M:70:ASP:HA    | 13:M:232:PHE:HA   | 1.98                     | 0.46              |
| 13:M:57:LEU:HD22  | 13:M:218:MET:HE2  | 1.98                     | 0.45              |
| 1:A:42:ASN:ND2    | 1:A:183:GLU:OE1   | 2.49                     | 0.45              |
| 9:I:203:ARG:NH2   | 11:Y:250:ASN:OD1  | 2.49                     | 0.45              |
| 4:R:51:GLU:OE1    | 4:R:206:MET:HG2   | 2.17                     | 0.45              |
| 8:V:102:ILE:HG23  | 8:V:125:MET:HE3   | 1.99                     | 0.45              |
| 4:R:85:ALA:O      | 4:R:89:ILE:HG12   | 2.16                     | 0.45              |
| 1:A:32:GLY:O      | 1:A:165:LYS:HG3   | 2.15                     | 0.45              |
| 11:K:123:ARG:NH1  | 11:K:126:GLU:OE1  | 2.47                     | 0.45              |
| 5:E:146:GLN:HG3   | 5:E:159:MET:HG2   | 1.97                     | 0.45              |
| 14:b:194:LEU:O    | 14:b:198:MET:HG3  | 2.16                     | 0.45              |
| 13:M:124:ASP:OD1  | 13:M:124:ASP:N    | 2.45                     | 0.45              |
| 2:B:8:ARG:CZ      | 3:C:5:ARG:HH12    | 2.30                     | 0.45              |
| 10:J:26:VAL:HG21  | 11:K:195:TYR:CD2  | 2.52                     | 0.45              |
| 14:N:194:LEU:O    | 14:N:198:MET:HG3  | 2.17                     | 0.45              |
| 3:Q:173:GLU:HA    | 4:R:58:LEU:HD11   | 1.99                     | 0.45              |
| 7:G:59:LYS:HB3    | 7:G:59:LYS:HE3    | 1.76                     | 0.45              |
| 8:V:209:ASP:OD1   | 8:V:210:LEU:N     | 2.50                     | 0.45              |
| 12:Z:56:ARG:NE    | 12:Z:219:ASP:OD2  | 2.32                     | 0.45              |
| 4:D:51:GLU:OE2    | 4:D:206:MET:HG2   | 2.16                     | 0.44              |
| 8:H:93:ALA:O      | 8:H:97:MET:HG2    | 2.17                     | 0.44              |
| 4:D:85:ALA:O      | 4:D:89:ILE:HG12   | 2.17                     | 0.44              |
| 11:K:79:ALA:HB2   | 11:K:90:VAL:HG21  | 1.99                     | 0.44              |
| 1:O:32:GLY:O      | 1:O:165:LYS:HG3   | 2.17                     | 0.44              |
| 3:Q:196:LEU:HA    | 3:Q:199:VAL:HG12  | 2.00                     | 0.44              |
| 4:R:184:VAL:HG11  | 4:R:197:SER:HB3   | 1.99                     | 0.44              |
| 11:Y:79:ALA:HB2   | 11:Y:90:VAL:HG21  | 1.99                     | 0.44              |
| 4:D:184:VAL:HG11  | 4:D:197:SER:HB3   | 1.97                     | 0.44              |
| 1:O:74:LEU:CD2    | 1:O:136:ILE:HG13  | 2.48                     | 0.44              |
| 1:O:95:GLN:HG3    | 8:V:108:LEU:HG    | 1.99                     | 0.44              |
| 6:T:69:ASN:OD1    | 6:T:225:HIS:ND1   | 2.49                     | 0.44              |
| 4:R:70:ILE:HD11   | 4:R:89:ILE:HD12   | 1.99                     | 0.44              |
| 6:F:231:ASP:OD1   | 6:F:232:ILE:N     | 2.50                     | 0.44              |
| 14:b:182:THR:HG22 | 14:b:183:LYS:N    | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:65:VAL:HG22   | 1:A:75:VAL:HG12   | 2.00                     | 0.44              |
| 10:J:11:ASP:N     | 10:J:11:ASP:OD1   | 2.50                     | 0.44              |
| 14:N:182:THR:HG22 | 14:N:183:LYS:N    | 2.32                     | 0.44              |
| 13:a:95:MET:HE2   | 13:a:237:VAL:HG12 | 2.00                     | 0.44              |
| 1:O:185:GLU:O     | 1:O:189:HIS:ND1   | 2.51                     | 0.44              |
| 4:R:160:GLY:O     | 5:S:82:ARG:NH2    | 2.50                     | 0.44              |
| 6:T:189:ASP:O     | 6:T:193:GLU:HG2   | 2.17                     | 0.44              |
| 2:B:174:MET:HE3   | 2:B:174:MET:HB2   | 1.85                     | 0.43              |
| 6:F:69:ASN:OD1    | 6:F:225:HIS:ND1   | 2.47                     | 0.43              |
| 6:F:76:MET:HE3    | 6:F:136:PHE:CD2   | 2.53                     | 0.43              |
| 9:W:125:ASP:OD1   | 9:W:129:CYS:N     | 2.48                     | 0.43              |
| 3:C:196:LEU:HA    | 3:C:199:VAL:HG12  | 2.00                     | 0.43              |
| 4:D:160:GLY:O     | 5:E:82:ARG:NH2    | 2.51                     | 0.43              |
| 14:N:38:MET:CE    | 14:N:190:THR:HA   | 2.48                     | 0.43              |
| 5:S:80:ASP:OD2    | 5:S:126:ARG:NH2   | 2.50                     | 0.43              |
| 10:X:150:THR:HG22 | 10:X:150:THR:O    | 2.19                     | 0.43              |
| 13:a:238:THR:HG22 | 13:a:239:GLU:N    | 2.31                     | 0.43              |
| 1:A:74:LEU:CD2    | 1:A:136:ILE:HG13  | 2.48                     | 0.43              |
| 2:P:174:MET:HE3   | 2:P:174:MET:HB2   | 1.85                     | 0.43              |
| 13:a:211:ARG:O    | 13:a:215:GLU:OE1  | 2.36                     | 0.43              |
| 2:B:8:ARG:HH21    | 3:C:5:ARG:NH2     | 2.17                     | 0.43              |
| 10:J:150:THR:HG22 | 10:J:150:THR:O    | 2.19                     | 0.43              |
| 5:E:192:LEU:HD12  | 5:E:205:LEU:HD13  | 2.01                     | 0.43              |
| 10:J:160:LEU:O    | 10:J:164:LEU:HG   | 2.19                     | 0.43              |
| 3:Q:185:ASP:OD1   | 3:Q:228:TYR:OH    | 2.34                     | 0.43              |
| 4:R:231:LYS:O     | 4:R:234:LEU:N     | 2.51                     | 0.43              |
| 10:X:160:LEU:O    | 10:X:164:LEU:HG   | 2.19                     | 0.43              |
| 3:C:121:SER:HB2   | 3:C:124:ARG:HD2   | 2.00                     | 0.42              |
| 1:O:65:VAL:HG22   | 1:O:75:VAL:HG12   | 2.01                     | 0.42              |
| 6:T:230:LYS:O     | 6:T:233:ARG:N     | 2.52                     | 0.42              |
| 6:F:35:SER:HB2    | 6:F:66:ARG:HH12   | 1.84                     | 0.42              |
| 9:I:87:LEU:O      | 9:I:91:VAL:HG23   | 2.19                     | 0.42              |
| 9:W:73:LEU:HD23   | 9:W:73:LEU:HA     | 1.90                     | 0.42              |
| 1:A:35:SER:HB2    | 1:A:163:MET:HG2   | 2.01                     | 0.42              |
| 1:O:203:MET:HE3   | 1:O:208:ILE:HG21  | 2.00                     | 0.42              |
| 3:Q:105:GLU:HA    | 3:Q:108:THR:HG22  | 2.02                     | 0.42              |
| 6:T:109:LEU:HD13  | 6:T:140:SER:HB2   | 2.00                     | 0.42              |
| 12:Z:45:GLY:HA3   | 12:Z:48:PHE:CZ    | 2.55                     | 0.42              |
| 4:D:70:ILE:HD11   | 4:D:89:ILE:HD12   | 2.00                     | 0.42              |
| 10:J:26:VAL:HG21  | 11:K:195:TYR:CE2  | 2.54                     | 0.42              |
| 13:a:161:ALA:O    | 13:a:164:GLU:HG3  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:203:MET:HE3  | 1:A:208:ILE:HG21  | 2.01                     | 0.42              |
| 2:B:34:CYS:SG    | 2:B:75:SER:OG     | 2.66                     | 0.42              |
| 2:P:190:LEU:O    | 2:P:194:ILE:HG12  | 2.20                     | 0.42              |
| 5:S:193:ARG:O    | 5:S:197:GLU:HG2   | 2.20                     | 0.42              |
| 12:L:45:GLY:HA3  | 12:L:48:PHE:CZ    | 2.55                     | 0.42              |
| 6:F:136:PHE:CZ   | 6:F:152:ILE:HD12  | 2.55                     | 0.42              |
| 14:b:39:ALA:HA   | 14:b:47:VAL:O     | 2.20                     | 0.42              |
| 2:B:6:ASP:OD2    | 3:C:3:TYR:OH      | 2.26                     | 0.42              |
| 3:C:105:GLU:HA   | 3:C:108:THR:HG22  | 2.02                     | 0.42              |
| 3:C:107:ILE:HD12 | 3:C:107:ILE:HA    | 1.93                     | 0.42              |
| 4:D:21:LEU:O     | 4:D:25:GLU:HG2    | 2.20                     | 0.42              |
| 5:E:230:SER:OG   | 5:E:231:PRO:HD3   | 2.20                     | 0.42              |
| 5:S:26:MET:SD    | 5:S:149:PRO:HD2   | 2.60                     | 0.42              |
| 9:W:87:LEU:O     | 9:W:91:VAL:HG23   | 2.20                     | 0.42              |
| 13:M:169:TYR:HE2 | 13:M:184:THR:HG22 | 1.84                     | 0.41              |
| 3:Q:107:ILE:HD12 | 3:Q:107:ILE:HA    | 1.93                     | 0.41              |
| 4:R:21:LEU:O     | 4:R:25:GLU:HG2    | 2.20                     | 0.41              |
| 9:I:191:GLU:HG2  | 9:I:192:LYS:H     | 1.85                     | 0.41              |
| 4:D:196:LYS:NZ   | 4:D:240:ASP:OD2   | 2.46                     | 0.41              |
| 4:R:87:THR:O     | 4:R:91:LYS:HG2    | 2.21                     | 0.41              |
| 6:T:136:PHE:CZ   | 6:T:152:ILE:HD12  | 2.55                     | 0.41              |
| 12:Z:164:LYS:HA  | 12:Z:164:LYS:HD3  | 1.90                     | 0.41              |
| 13:a:48:ASN:HA   | 13:a:49:PRO:HD3   | 1.86                     | 0.41              |
| 10:J:46:CYS:SG   | 10:J:53:THR:HG23  | 2.60                     | 0.41              |
| 5:E:193:ARG:O    | 5:E:197:GLU:HG2   | 2.21                     | 0.41              |
| 13:M:167:LEU:HG  | 13:M:182:LEU:HD12 | 2.02                     | 0.41              |
| 14:N:39:ALA:HA   | 14:N:47:VAL:O     | 2.19                     | 0.41              |
| 8:V:98:THR:HG23  | 8:V:129:MET:HE1   | 2.02                     | 0.41              |
| 14:b:38:MET:CE   | 14:b:190:THR:HA   | 2.50                     | 0.41              |
| 14:b:137:TRP:CH2 | 14:b:215:GLU:HG3  | 2.55                     | 0.41              |
| 8:H:98:THR:HG23  | 8:H:129:MET:HE1   | 2.03                     | 0.41              |
| 9:I:73:LEU:HD23  | 9:I:73:LEU:HA     | 1.93                     | 0.41              |
| 9:I:135:ASP:OD1  | 9:I:136:PHE:N     | 2.51                     | 0.41              |
| 14:N:137:TRP:CH2 | 14:N:215:GLU:HG3  | 2.56                     | 0.41              |
| 1:O:65:VAL:O     | 1:O:220:ARG:NH1   | 2.53                     | 0.41              |
| 6:T:216:TRP:CZ3  | 6:T:228:VAL:HG13  | 2.56                     | 0.41              |
| 1:A:173:PHE:O    | 1:A:176:LYS:HG3   | 2.20                     | 0.41              |
| 2:B:217:THR:HG22 | 2:B:218:ARG:H     | 1.86                     | 0.41              |
| 3:C:173:GLU:HA   | 4:D:58:LEU:HD11   | 2.02                     | 0.41              |
| 4:D:186:HIS:O    | 4:D:189:MET:HG3   | 2.21                     | 0.41              |
| 5:E:26:MET:HE1   | 5:E:148:CYS:HB3   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:50:ILE:HD12   | 7:G:79:VAL:CG2    | 2.51                     | 0.41              |
| 12:L:75:THR:HG22  | 12:L:76:ASP:N     | 2.36                     | 0.41              |
| 1:O:74:LEU:HD23   | 1:O:136:ILE:HG13  | 2.03                     | 0.41              |
| 4:R:97:GLN:HG3    | 11:Y:124:ILE:HG13 | 2.02                     | 0.41              |
| 6:T:76:MET:HE3    | 6:T:136:PHE:CD2   | 2.56                     | 0.41              |
| 10:X:46:CYS:SG    | 10:X:53:THR:HG23  | 2.60                     | 0.41              |
| 2:B:198:ASN:HD22  | 2:B:240:HIS:CE1   | 2.39                     | 0.41              |
| 6:F:216:TRP:CZ3   | 6:F:228:VAL:HG22  | 2.55                     | 0.41              |
| 2:P:41:ASP:OD1    | 2:P:41:ASP:N      | 2.45                     | 0.41              |
| 1:A:74:LEU:HD23   | 1:A:136:ILE:HG13  | 2.02                     | 0.40              |
| 6:F:75:GLY:HA3    | 6:F:225:HIS:CD2   | 2.56                     | 0.40              |
| 6:T:75:GLY:HA3    | 6:T:225:HIS:CD2   | 2.56                     | 0.40              |
| 5:E:172:LEU:O     | 5:E:176:MET:HG3   | 2.22                     | 0.40              |
| 6:F:189:ASP:O     | 6:F:193:GLU:HG2   | 2.21                     | 0.40              |
| 5:S:220:GLU:O     | 5:S:222:THR:HG23  | 2.21                     | 0.40              |
| 7:U:50:ILE:HD12   | 7:U:79:VAL:CG2    | 2.52                     | 0.40              |
| 7:U:155:ASP:HB2   | 7:U:156:PRO:HD2   | 2.03                     | 0.40              |
| 8:V:98:THR:HG23   | 8:V:129:MET:CE    | 2.52                     | 0.40              |
| 2:P:198:ASN:HD22  | 2:P:240:HIS:CE1   | 2.39                     | 0.40              |
| 5:S:172:LEU:O     | 5:S:176:MET:HG3   | 2.21                     | 0.40              |
| 13:M:238:THR:HG22 | 13:M:239:GLU:OE1  | 2.21                     | 0.40              |
| 4:D:97:GLN:HG3    | 11:K:124:ILE:HG13 | 2.03                     | 0.40              |
| 6:F:109:LEU:HD13  | 6:F:140:SER:HB2   | 2.02                     | 0.40              |
| 7:G:50:ILE:HD12   | 7:G:79:VAL:HG23   | 2.03                     | 0.40              |
| 7:G:141:ILE:HD12  | 7:G:220:VAL:HG22  | 2.03                     | 0.40              |
| 5:S:230:SER:OG    | 5:S:231:PRO:HD3   | 2.21                     | 0.40              |
| 6:T:216:TRP:CZ3   | 6:T:228:VAL:HG22  | 2.56                     | 0.40              |
| 7:U:52:THR:HG22   | 7:U:216:GLU:HB2   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 227/234 (97%)   | 223 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 1   | O     | 227/234 (97%)   | 225 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 2   | B     | 241/261 (92%)   | 236 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | P     | 241/261 (92%)   | 237 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 3   | C     | 235/248 (95%)   | 232 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 3   | Q     | 235/248 (95%)   | 232 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 4   | D     | 223/241 (92%)   | 218 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 4   | R     | 223/241 (92%)   | 217 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 5   | E     | 232/263 (88%)   | 226 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 5   | S     | 232/263 (88%)   | 226 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 6   | F     | 237/255 (93%)   | 233 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 6   | T     | 237/255 (93%)   | 233 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 7   | G     | 233/246 (95%)   | 228 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 7   | U     | 233/246 (95%)   | 229 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 8   | H     | 217/277 (78%)   | 213 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 8   | V     | 217/277 (78%)   | 212 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 9   | I     | 202/205 (98%)   | 195 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 9   | W     | 202/205 (98%)   | 193 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 10  | J     | 194/201 (96%)   | 188 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 10  | X     | 194/201 (96%)   | 189 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 11  | K     | 199/263 (76%)   | 192 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 11  | Y     | 199/263 (76%)   | 191 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 12  | L     | 204/241 (85%)   | 195 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 12  | Z     | 204/241 (85%)   | 197 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 13  | M     | 213/264 (81%)   | 204 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 13  | a     | 213/264 (81%)   | 205 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 14  | N     | 194/239 (81%)   | 187 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 14  | b     | 194/239 (81%)   | 187 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| All | All   | 6102/6876 (89%) | 5943 (97%) | 159 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 187/191 (98%) | 187 (100%) | 0        | 100         | 100 |
| 1   | O     | 187/191 (98%) | 187 (100%) | 0        | 100         | 100 |
| 2   | B     | 204/221 (92%) | 204 (100%) | 0        | 100         | 100 |
| 2   | P     | 204/221 (92%) | 204 (100%) | 0        | 100         | 100 |
| 3   | C     | 200/211 (95%) | 200 (100%) | 0        | 100         | 100 |
| 3   | Q     | 200/211 (95%) | 200 (100%) | 0        | 100         | 100 |
| 4   | D     | 191/203 (94%) | 191 (100%) | 0        | 100         | 100 |
| 4   | R     | 191/203 (94%) | 191 (100%) | 0        | 100         | 100 |
| 5   | E     | 200/224 (89%) | 200 (100%) | 0        | 100         | 100 |
| 5   | S     | 200/224 (89%) | 200 (100%) | 0        | 100         | 100 |
| 6   | F     | 196/212 (92%) | 196 (100%) | 0        | 100         | 100 |
| 6   | T     | 196/212 (92%) | 196 (100%) | 0        | 100         | 100 |
| 7   | G     | 201/210 (96%) | 201 (100%) | 0        | 100         | 100 |
| 7   | U     | 201/210 (96%) | 201 (100%) | 0        | 100         | 100 |
| 8   | H     | 180/228 (79%) | 180 (100%) | 0        | 100         | 100 |
| 8   | V     | 180/228 (79%) | 180 (100%) | 0        | 100         | 100 |
| 9   | I     | 173/174 (99%) | 173 (100%) | 0        | 100         | 100 |
| 9   | W     | 173/174 (99%) | 173 (100%) | 0        | 100         | 100 |
| 10  | J     | 165/171 (96%) | 165 (100%) | 0        | 100         | 100 |
| 10  | X     | 165/171 (96%) | 165 (100%) | 0        | 100         | 100 |
| 11  | K     | 155/202 (77%) | 155 (100%) | 0        | 100         | 100 |
| 11  | Y     | 155/202 (77%) | 155 (100%) | 0        | 100         | 100 |
| 12  | L     | 173/199 (87%) | 173 (100%) | 0        | 100         | 100 |
| 12  | Z     | 173/199 (87%) | 173 (100%) | 0        | 100         | 100 |
| 13  | M     | 178/215 (83%) | 178 (100%) | 0        | 100         | 100 |
| 13  | a     | 178/215 (83%) | 178 (100%) | 0        | 100         | 100 |

*Continued on next page...*

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 14  | N     | 152/180 (84%)   | 152 (100%)  | 0        | 100         | 100 |
| 14  | b     | 152/180 (84%)   | 151 (99%)   | 1 (1%)   | 76          | 88  |
| All | All   | 5110/5682 (90%) | 5109 (100%) | 1 (0%)   | 100         | 100 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | b     | 144 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | GLN  |
| 1   | A     | 52  | GLN  |
| 1   | A     | 109 | GLN  |
| 1   | A     | 140 | ASN  |
| 2   | B     | 84  | ASN  |
| 2   | B     | 95  | GLN  |
| 2   | B     | 142 | HIS  |
| 2   | B     | 240 | HIS  |
| 4   | D     | 23  | GLN  |
| 4   | D     | 41  | GLN  |
| 4   | D     | 155 | HIS  |
| 5   | E     | 60  | GLN  |
| 5   | E     | 175 | HIS  |
| 6   | F     | 23  | GLN  |
| 6   | F     | 202 | HIS  |
| 7   | G     | 90  | GLN  |
| 8   | H     | 109 | HIS  |
| 9   | I     | 61  | GLN  |
| 9   | I     | 81  | GLN  |
| 9   | I     | 93  | ASN  |
| 10  | J     | 27  | GLN  |
| 10  | J     | 186 | ASN  |
| 12  | L     | 36  | ASN  |
| 12  | L     | 136 | ASN  |
| 12  | L     | 174 | GLN  |
| 12  | L     | 187 | GLN  |
| 13  | M     | 253 | ASN  |
| 14  | N     | 144 | GLN  |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 157 | GLN  |
| 1   | O     | 21  | GLN  |
| 1   | O     | 52  | GLN  |
| 1   | O     | 96  | GLN  |
| 1   | O     | 109 | GLN  |
| 2   | P     | 84  | ASN  |
| 2   | P     | 95  | GLN  |
| 2   | P     | 142 | HIS  |
| 2   | P     | 240 | HIS  |
| 4   | R     | 23  | GLN  |
| 4   | R     | 41  | GLN  |
| 4   | R     | 155 | HIS  |
| 5   | S     | 60  | GLN  |
| 5   | S     | 166 | GLN  |
| 6   | T     | 23  | GLN  |
| 6   | T     | 171 | GLN  |
| 7   | U     | 90  | GLN  |
| 7   | U     | 238 | HIS  |
| 8   | V     | 109 | HIS  |
| 9   | W     | 61  | GLN  |
| 9   | W     | 81  | GLN  |
| 9   | W     | 93  | ASN  |
| 10  | X     | 24  | ASN  |
| 10  | X     | 27  | GLN  |
| 10  | X     | 186 | ASN  |
| 12  | Z     | 36  | ASN  |
| 12  | Z     | 136 | ASN  |
| 12  | Z     | 174 | GLN  |
| 14  | b     | 157 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

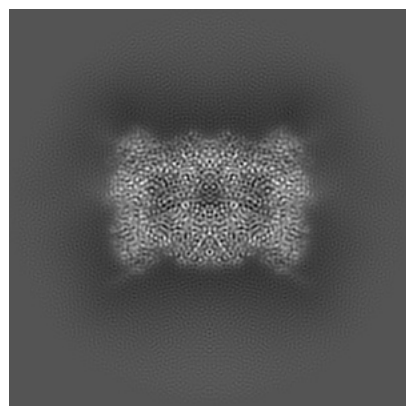
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18760. These allow visual inspection of the internal detail of the map and identification of artifacts.

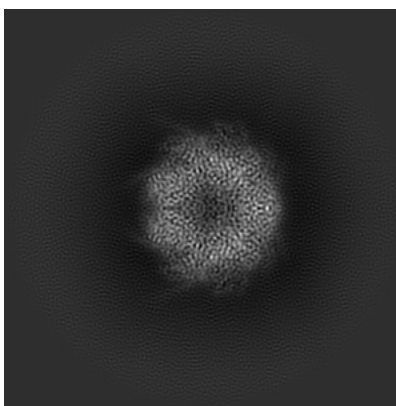
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

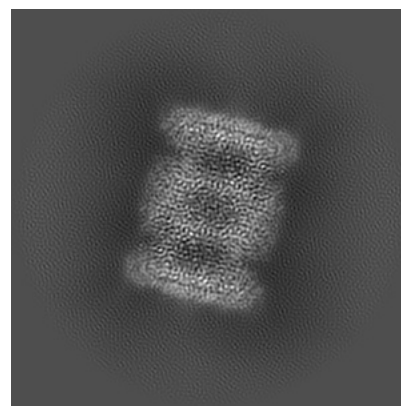
#### 6.1.1 Primary map



X

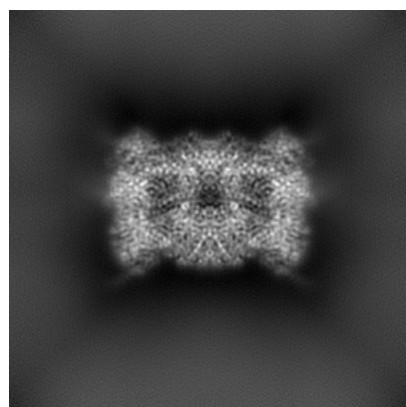


Y

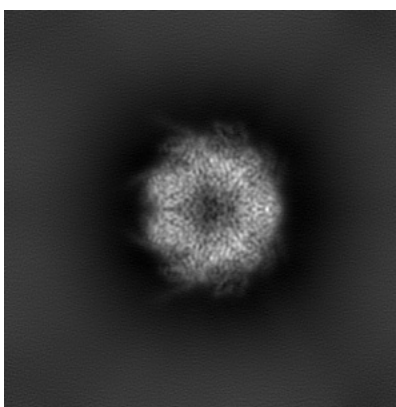


Z

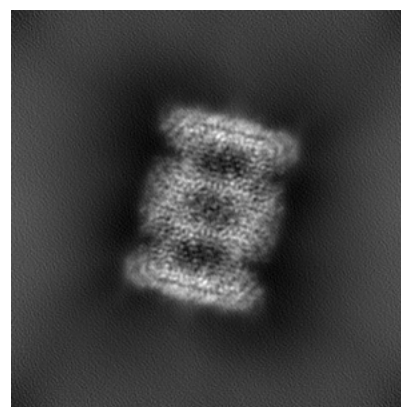
#### 6.1.2 Raw map



X



Y

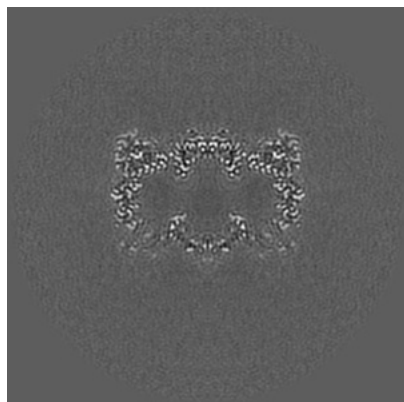


Z

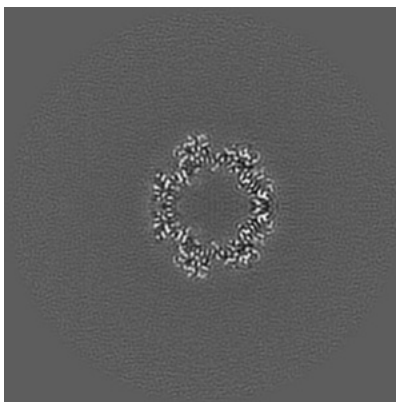
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

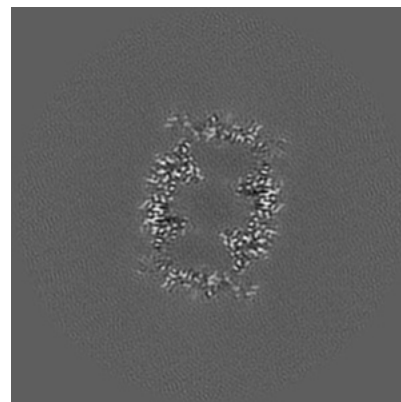
### 6.2.1 Primary map



X Index: 140

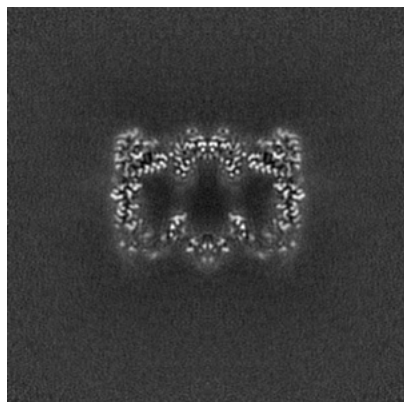


Y Index: 140

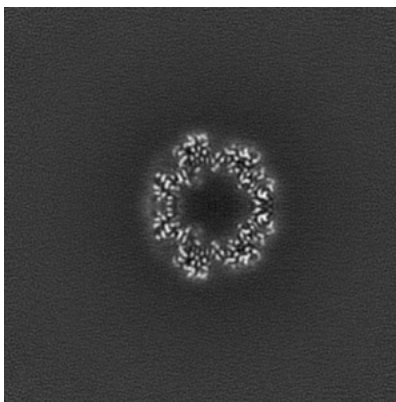


Z Index: 140

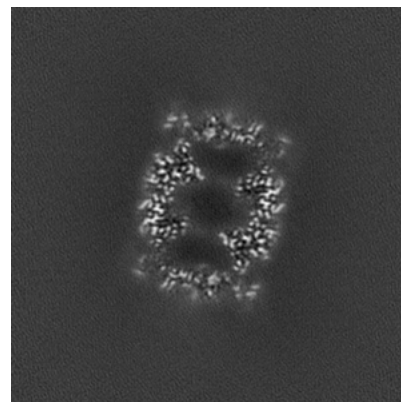
### 6.2.2 Raw map



X Index: 140



Y Index: 140



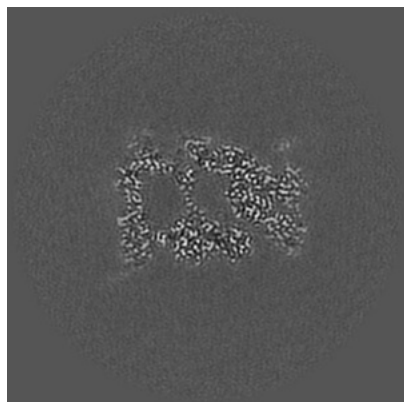
Z Index: 140

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

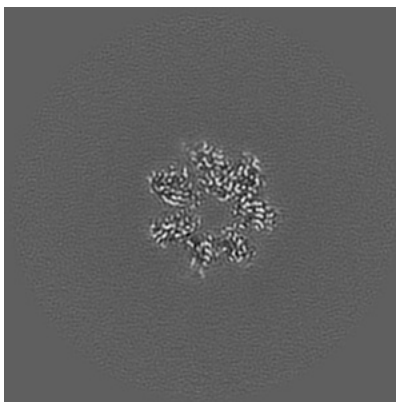


## 6.3 Largest variance slices [i](#)

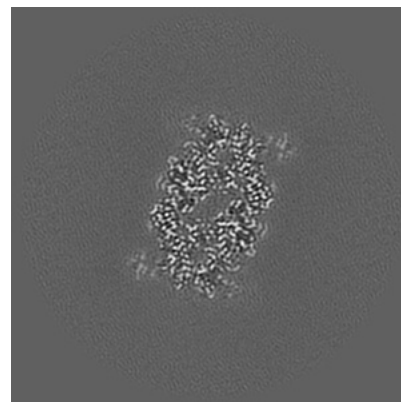
### 6.3.1 Primary map



X Index: 122

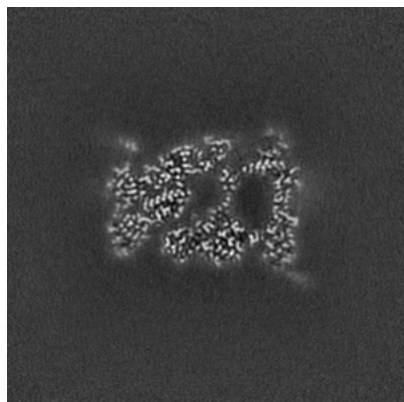


Y Index: 122

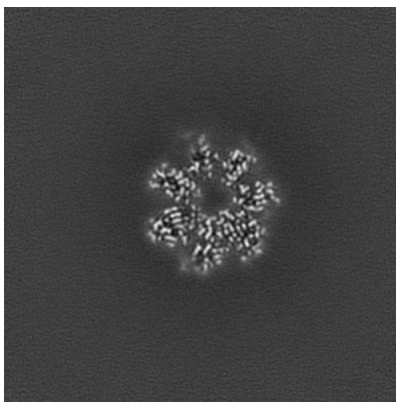


Z Index: 168

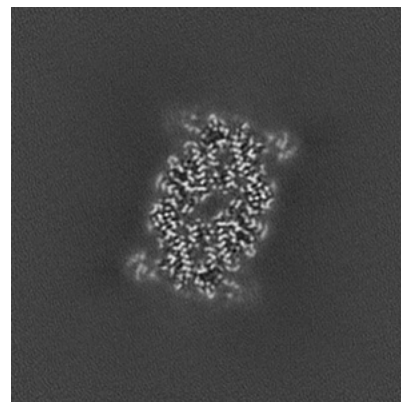
### 6.3.2 Raw map



X Index: 158



Y Index: 159

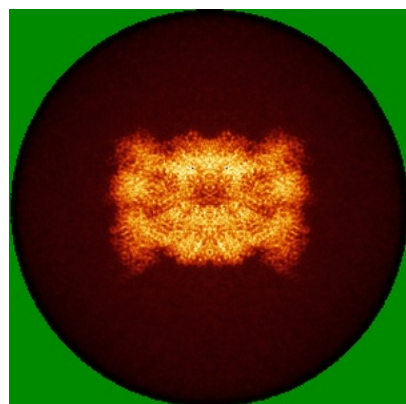


Z Index: 168

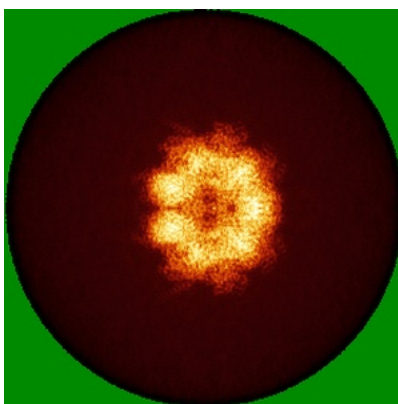
The images above show the largest variance slices of the map in three orthogonal directions.

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

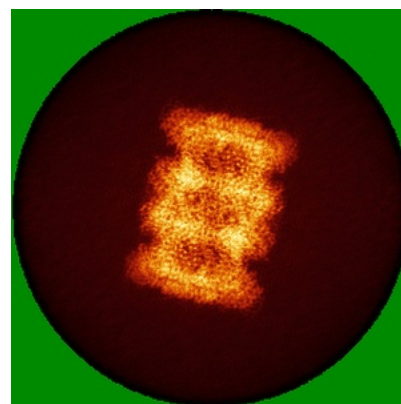
### 6.4.1 Primary map



X

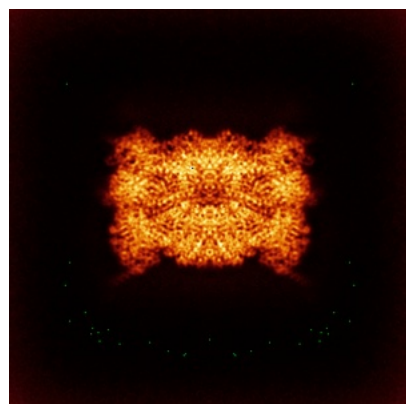


Y

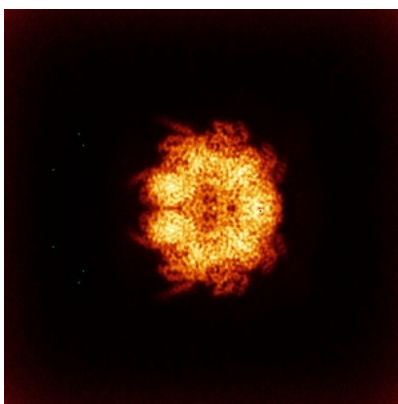


Z

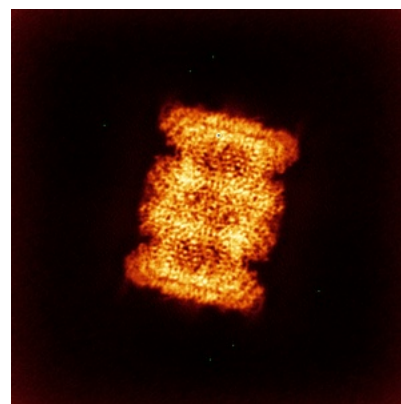
### 6.4.2 Raw map



X



Y

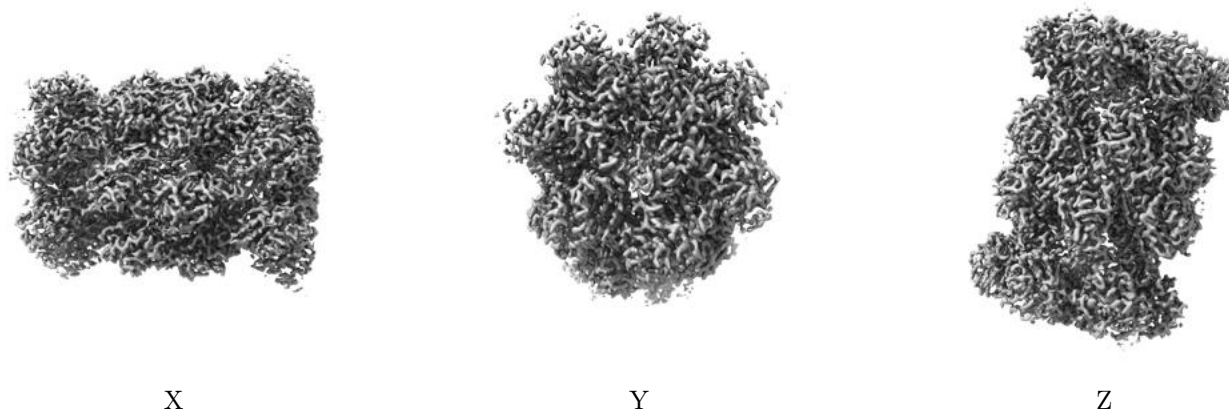


Z

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

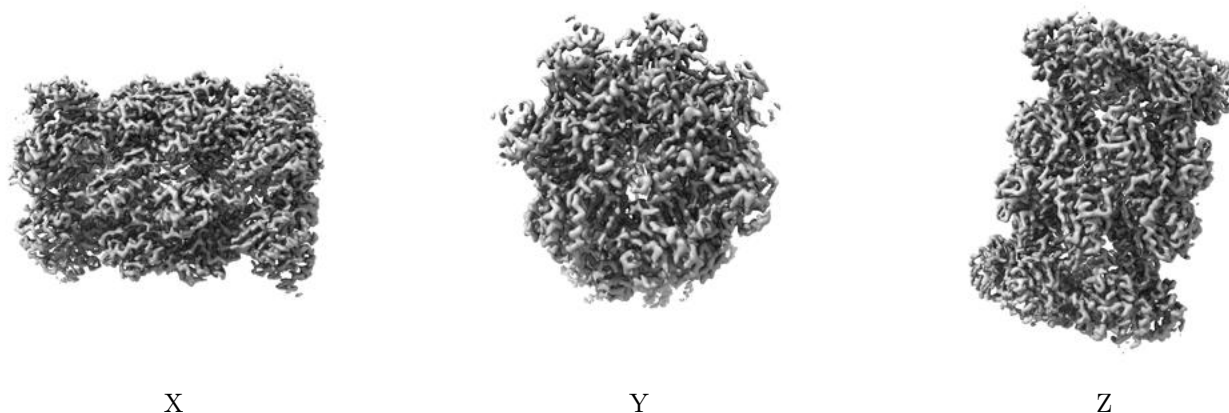
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.636. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

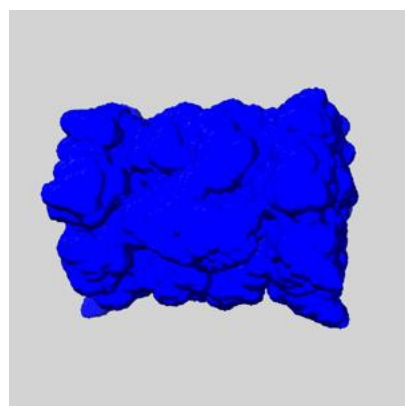
## 6.6 Mask visualisation [i](#)

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

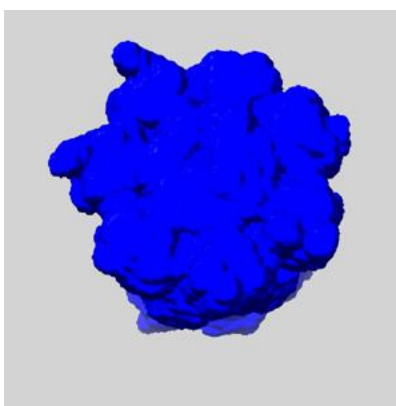
A mask typically either:

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

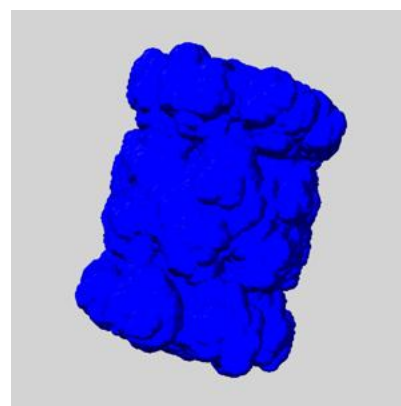
### 6.6.1 emd\_18760\_msk\_1.map [i](#)



X



Y

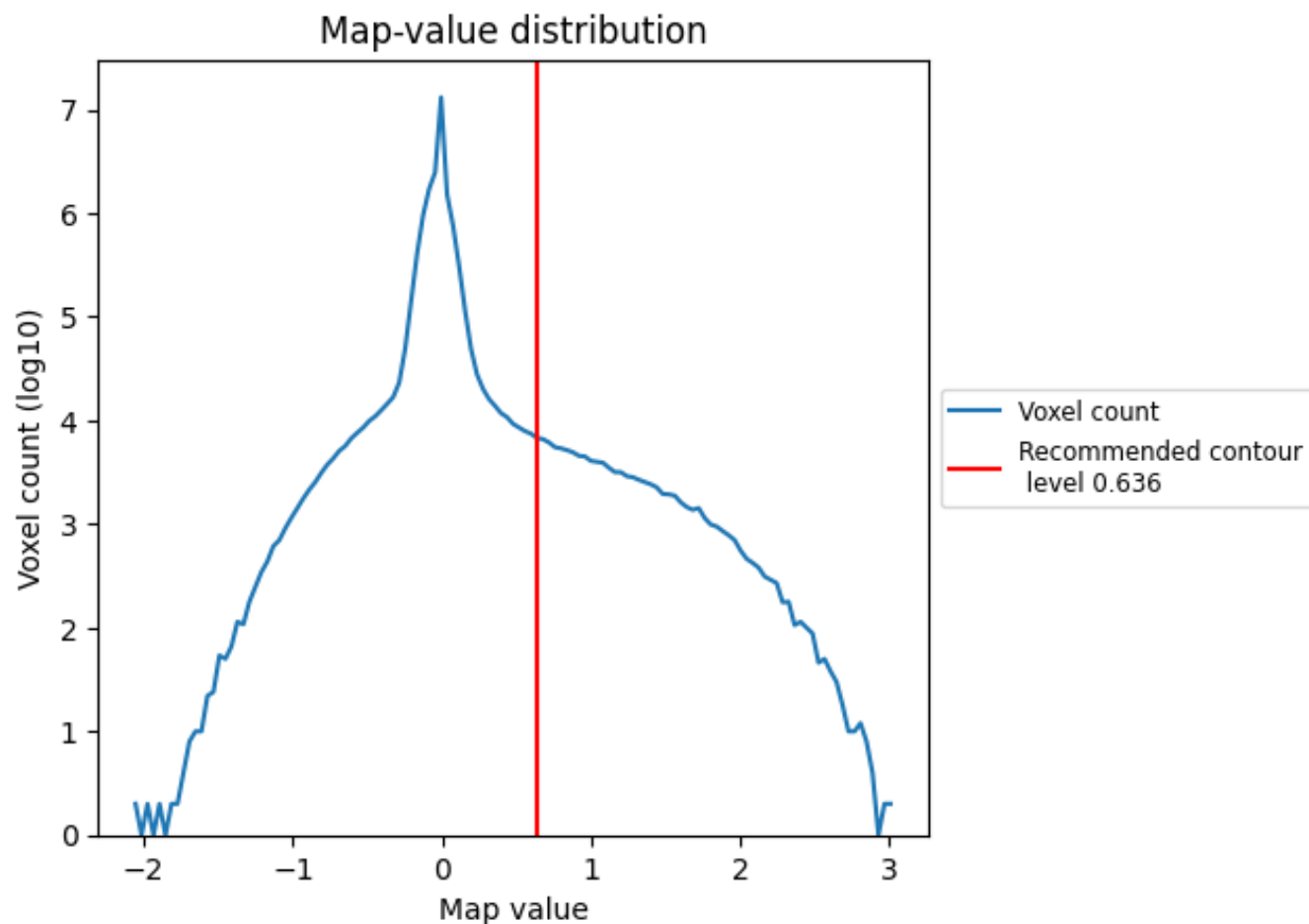


Z

## 7 Map analysis [i](#)

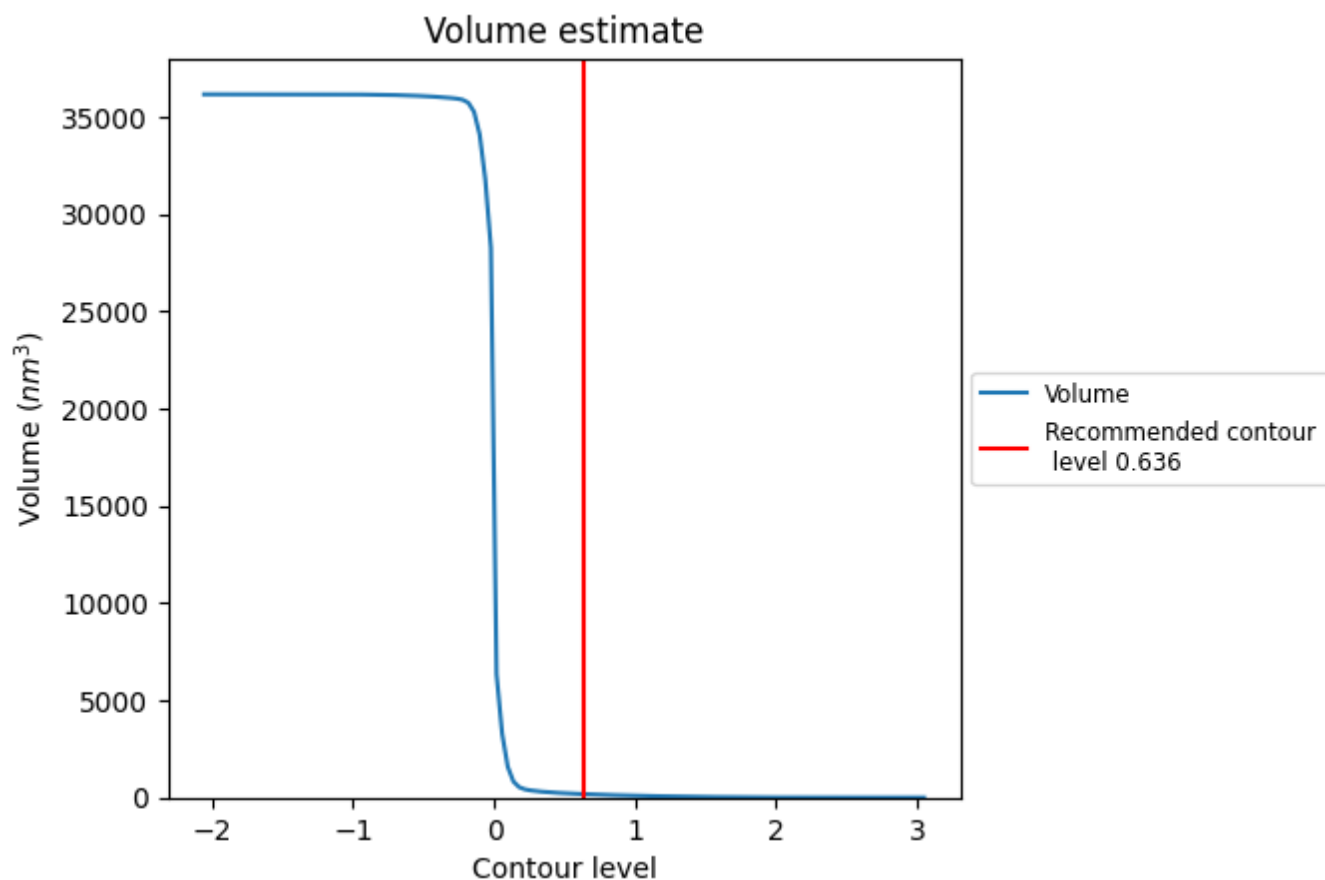
This section contains the results of statistical analysis of the map.

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



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

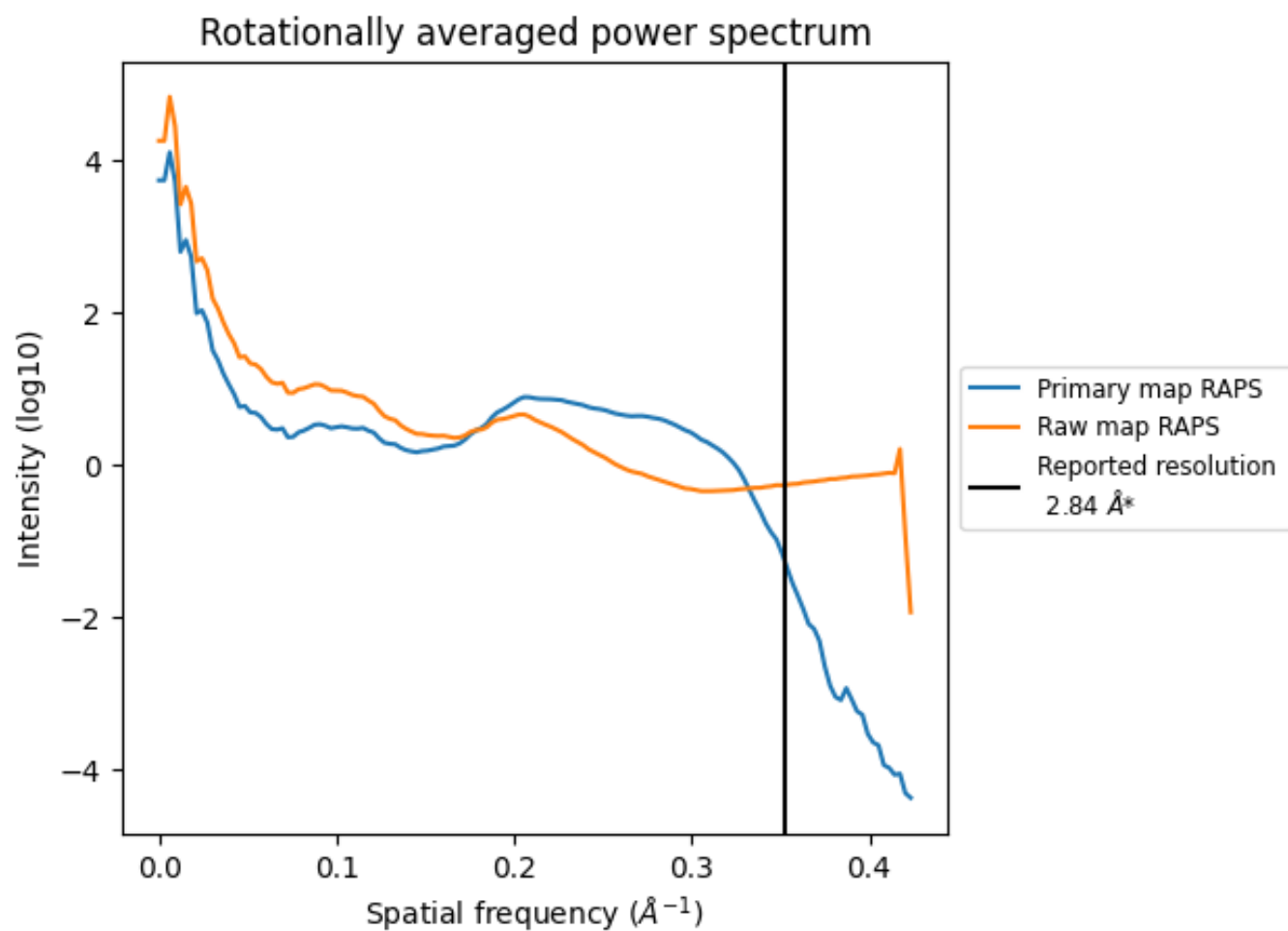
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm<sup>3</sup>; this corresponds to an approximate mass of 161 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

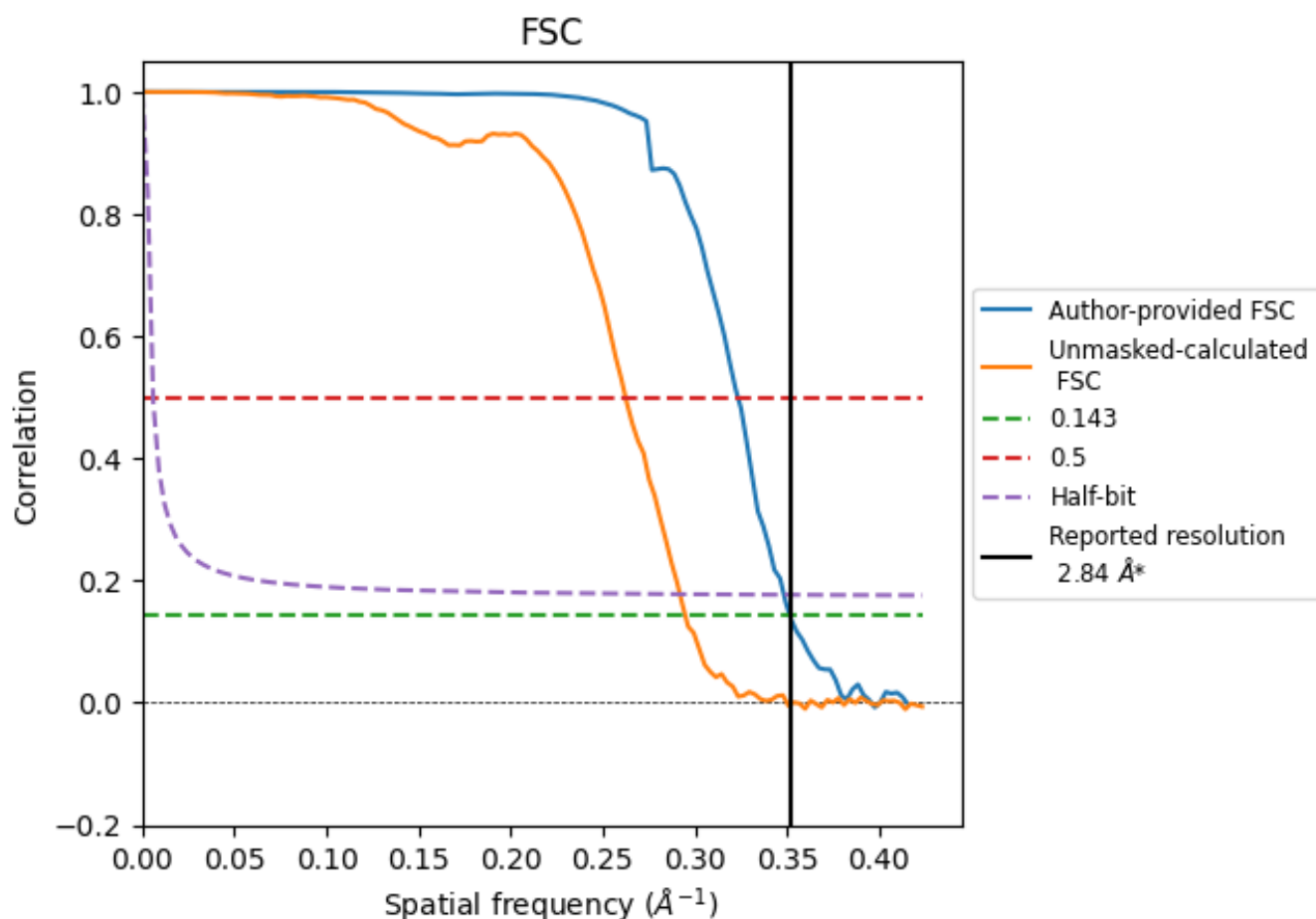


\*Reported resolution corresponds to spatial frequency of 0.352 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.352  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

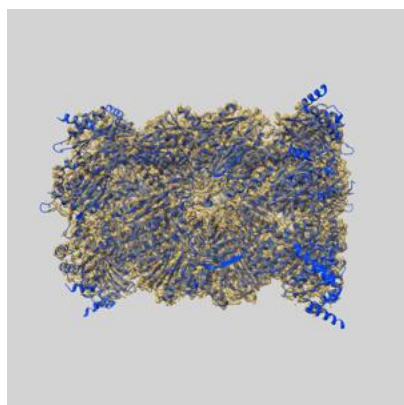
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.84                               | -    | -        |
| Author-provided FSC curve | 2.84                               | 3.09 | 2.87     |
| Unmasked-calculated*      | 3.39                               | 3.81 | 3.43     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.39 differs from the reported value 2.84 by more than 10 %

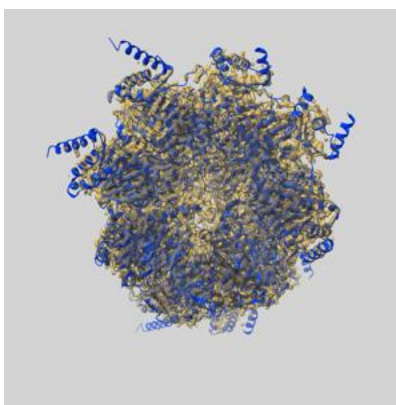
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18760 and PDB model 8QYO. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

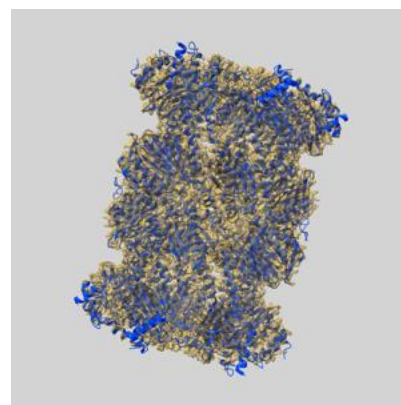
### 9.1 Map-model overlay [i](#)



X



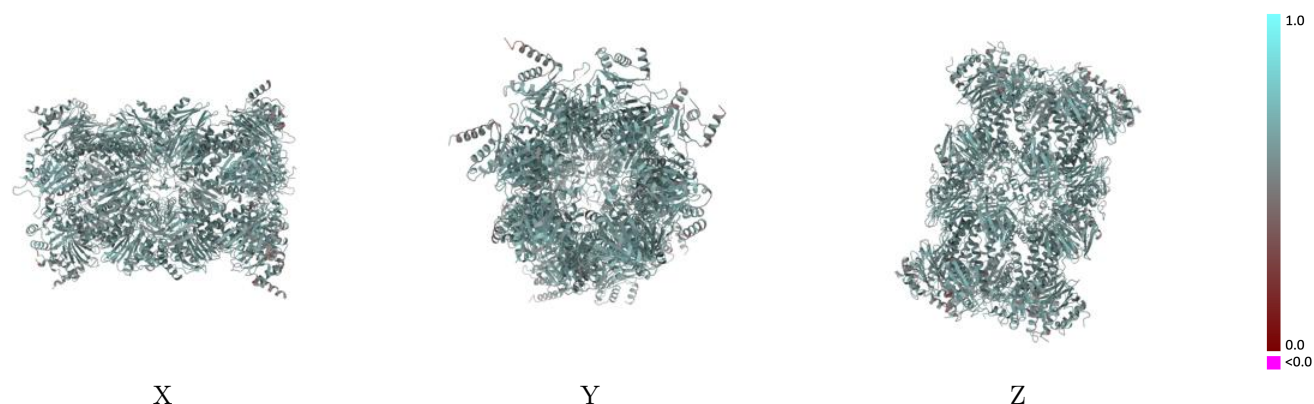
Y



Z

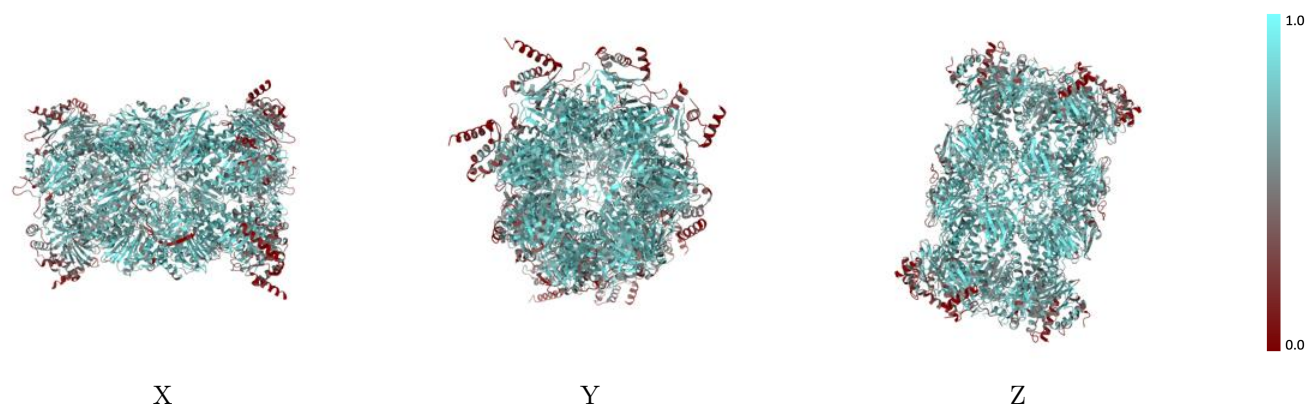
The images above show the 3D surface view of the map at the recommended contour level 0.636 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



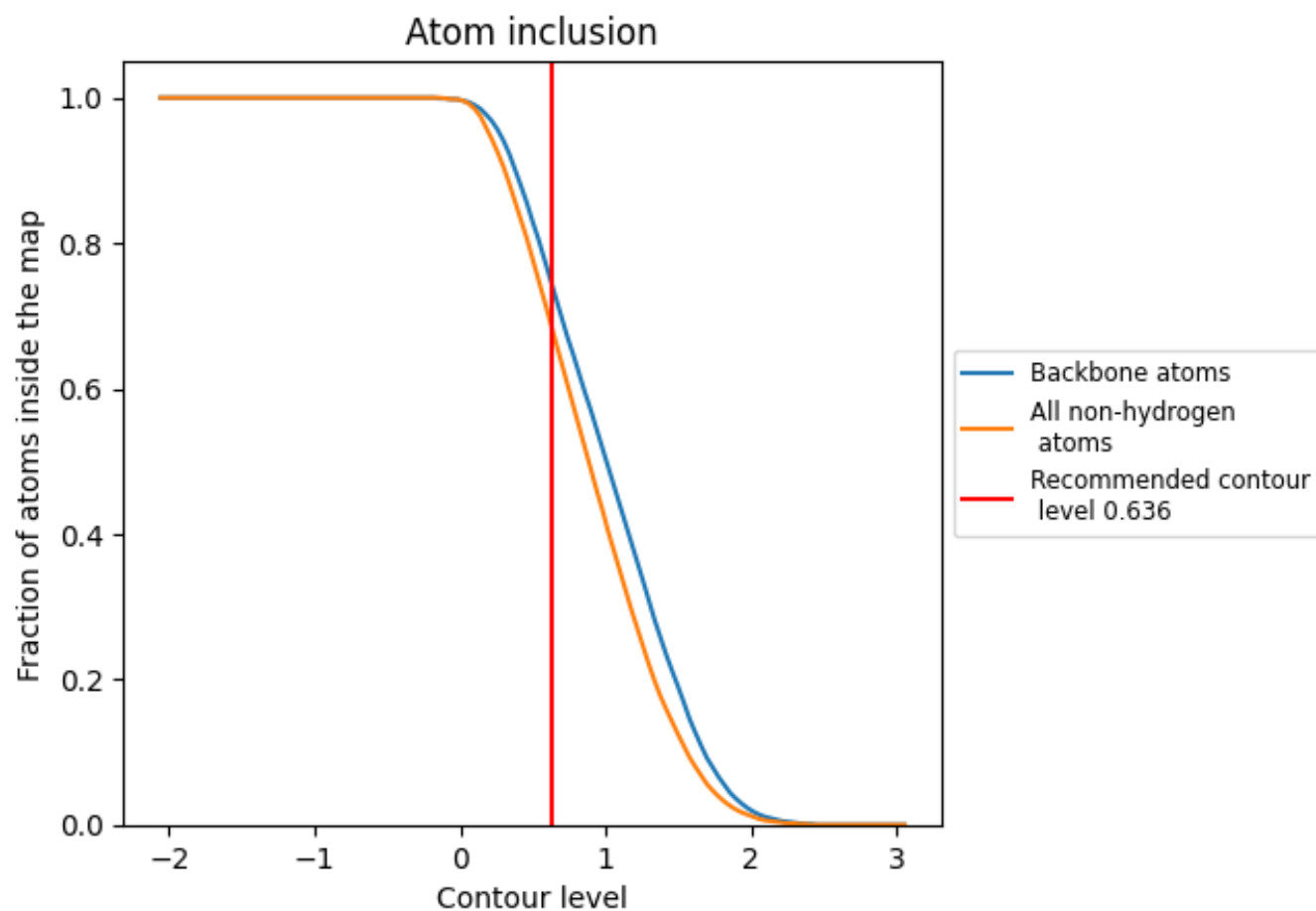
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.636).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.636) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6790   |  0.5960   |
| A     |  0.6300   |  0.5950   |
| B     |  0.5850   |  0.5820   |
| C     |  0.5600   |  0.5810   |
| D     |  0.6140   |  0.5890   |
| E     |  0.6700   |  0.5990   |
| F     |  0.6300   |  0.5870   |
| G     |  0.5900   |  0.5770   |
| H     |  0.7000   |  0.6030   |
| I     |  0.7690   |  0.6090   |
| J     |  0.7840   |  0.6100   |
| K     |  0.7800   |  0.6090   |
| L     |  0.7280   |  0.5960   |
| M     |  0.7700   |  0.6070   |
| N     |  0.7850  |  0.6100  |
| O     |  0.6310 |  0.5940 |
| P     |  0.5840 |  0.5830 |
| Q     |  0.5610 |  0.5790 |
| R     |  0.6150 |  0.5900 |
| S     |  0.6710 |  0.5970 |
| T     |  0.6300 |  0.5860 |
| U     |  0.5880 |  0.5760 |
| V     |  0.7000 |  0.6050 |
| W     |  0.7640 |  0.6080 |
| X     |  0.7820 |  0.6080 |
| Y     |  0.7800 |  0.6120 |
| Z     |  0.7290 |  0.5980 |
| a     |  0.7670 |  0.6030 |
| b     |  0.7880 |  0.6080 |

