



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:06 PM UTC

PDB ID : 7SZ7 / pdb\_00007sz7  
EMDB ID : EMD-25563  
Title : Cryo-EM structure of the extracellular module of the full-length EGFR bound to TGF-alpha. "tips-juxtaposed" conformation  
Authors : Huang, Y.; Ognjenovic, J.; Karandur, D.; Miller, K.; Merk, A.; Subramaniam, S.; Kuriyan, J.  
Deposited on : 2021-11-25  
Resolution : 3.40 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

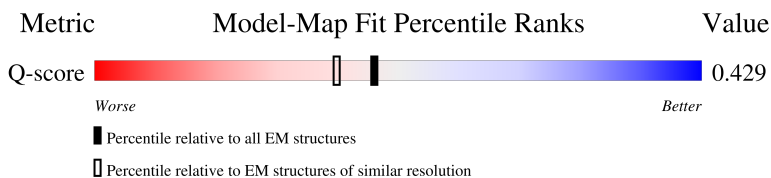
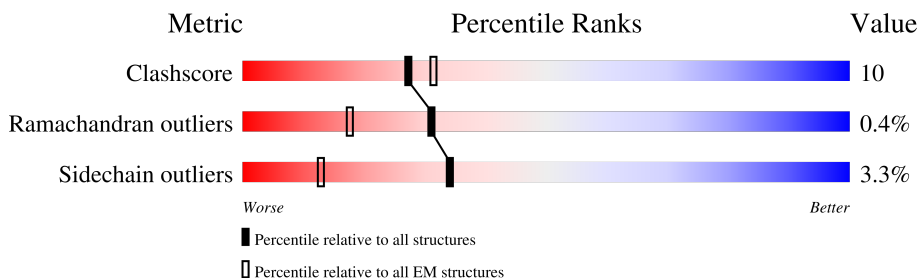
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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                       | 14717 ( 2.90 - 3.90 )                                    |

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     | 1210   |                  |
| 1   | B     | 1210   |                  |
| 2   | C     | 50     |                  |
| 2   | D     | 50     |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10218 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 Epidermal growth factor receptor.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 614      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4723  | 2914 | 842 | 907 | 60 |         |       |
| 1   | B     | 614      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4723  | 2914 | 842 | 907 | 60 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 232     | ASN      | ASP    | conflict | UNP P00533 |
| B     | 232     | ASN      | ASP    | conflict | UNP P00533 |

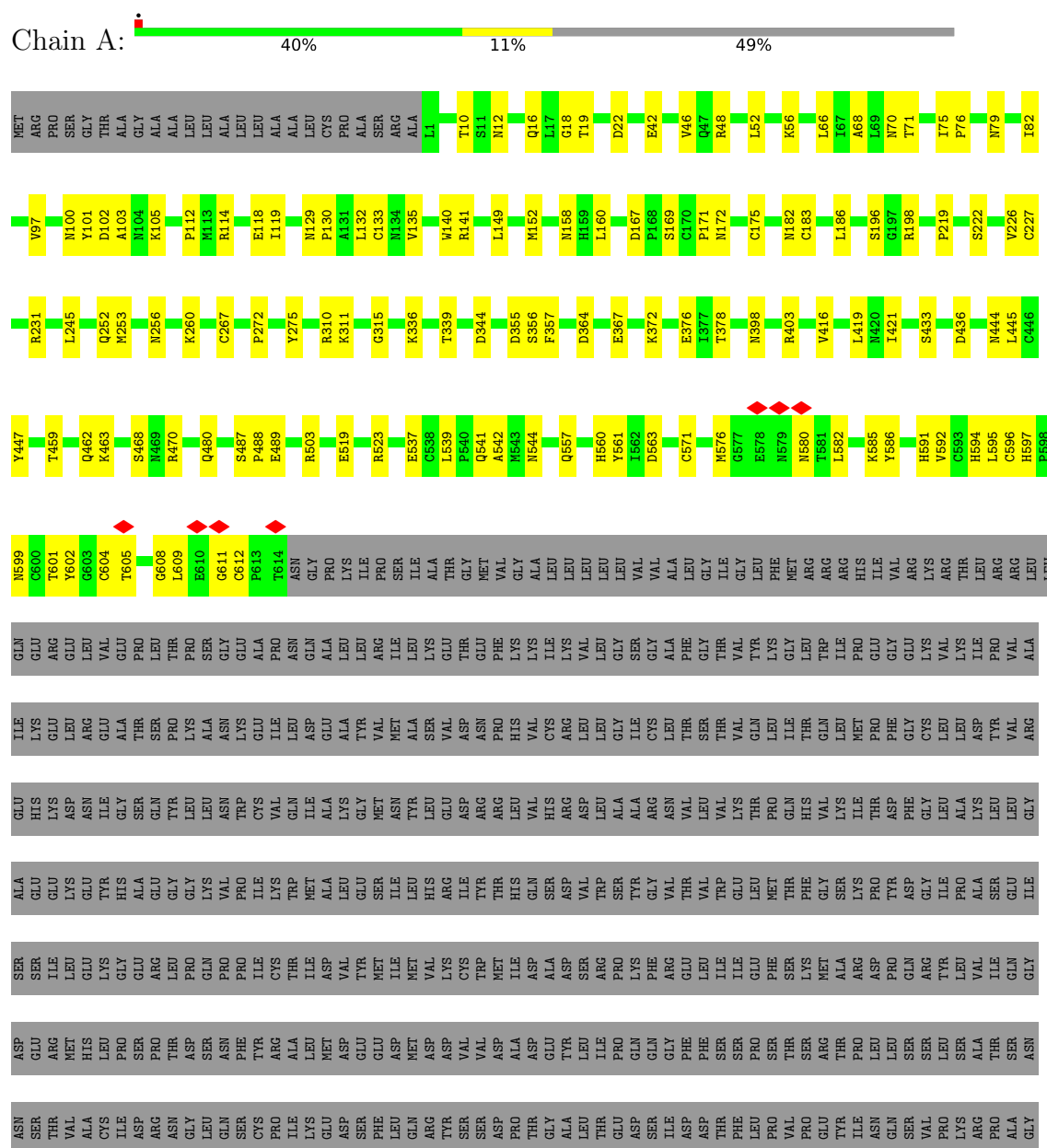
- Molecule 2 is a protein called Transforming growth factor alpha.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | C     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 386   | 239 | 70 | 71 | 6 |         |       |
| 2   | D     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 386   | 239 | 70 | 71 | 6 |         |       |

### 3 Residue-property plots

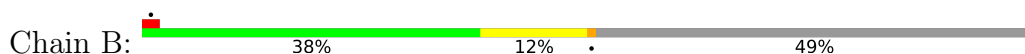
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Epidermal growth factor receptor



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLN | ILE | SER | LEU | ASP | ASN | PRO | ASP | TYR | GLN | GLN | ASP | PHE | PHE | PRO | LYS | GLU | ALA | LYS | PRO | ASN | GLY | ILE | PHE | LYS | GLY | THR | ALA | GLU | ASN | ALA | GLU | TYR | LEU | ARG | VAL | ALA | ALA | PRO | GLN | SER | SER | GLU | PHE | ILE | GLY | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 1: Epidermal growth factor receptor



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |    |    |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| MET | ARG | PRO | SER | GLY | THR | ALA | GLY | ALA | ALA | LEU | LEU | ALA | LEU | LEU | ALA | ALA | LEU | CYS | PRO | ALA | SER | ARG | ALA | L1 | E2 | N12 | Q16 | L17 | L41 | V46 | L52 | V65 | T71 | R74 | A96 | V97 | L98 | D102 | K105 | K109 | E110 | N128 | A131 | L132 | C132 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M134 | D142 | I143 | V144 | S145 | F148 | M152 | M158 | H159 | L160 | G161 | S162 | C163 | Q164 | C170 | C175 | A176 | G177 | A178 | M182 | C183 | L186 | T187 | Q194 | R198 | S203 | D206 | A213 | V226 | C227 | R231 | L243 | Y261 | V268 | Y275 | T278 | D279 | H280 | Z281 | 2952 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |             |      |      |      |      |             |      |      |      |      |      |      |      |      |      |      |             |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------------|------|------|------|------|-------------|------|------|------|------|------|------|------|------|------|------|-------------|------|------|------|------|------|
| R285 | R286 | E293 | M294 | R300 | K303 | G315 | I318 | S326 | F335 | C338 | G343 | D344 | L348 | D364 | P365 | <b>G366</b> | E367 | K372 | F380 | P387 | <b>E388</b> | R389 | R390 | T391 | H394 | E397 | N398 | R405 | Q408 | S413 | L419 | <b>W420</b> | I421 | I422 | S423 | L424 | P427 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------------|------|------|------|------|-------------|------|------|------|------|------|------|------|------|------|------|-------------|------|------|------|------|------|

G435  
 S440  
 G441  
 I442  
 K443  
 I444  
 L445  
 T450  
 F457  
 T464  
 R470  
 G471  
 E472  
 I473  
 S474  
 C475  
 T478  
 G479  
 Q480  
 H483  
 S487  
 P488  
 E489  
 W492  
 P496  
 R497  
 D498  
 C499  
 V500  
 S501  
 C502  
 R503  
 I504  
 V505  
 S506  
 S506  
 V512  
 D513  
 K514  
 C515  
 N516  
 L517  
 E521  
 P522  
 R523  
 E524  
 F525  
 F526

| Category | Item | Value |
|----------|------|-------|
| C500     | C501 | 10    |
|          | C502 | 10    |
|          | C503 | 10    |
|          | C504 | 10    |
|          | C505 | 10    |
|          | C506 | 10    |
|          | C507 | 10    |
|          | C508 | 10    |
|          | C509 | 10    |
|          | C510 | 10    |
| C550     | C551 | 10    |
|          | C552 | 10    |
|          | C553 | 10    |
|          | C554 | 10    |
|          | C555 | 10    |
|          | C556 | 10    |
|          | C557 | 10    |
|          | C558 | 10    |
|          | C559 | 10    |
|          | C560 | 10    |
| C600     | C601 | 10    |
|          | C602 | 10    |
|          | C603 | 10    |
|          | C604 | 10    |
|          | C605 | 10    |
|          | C606 | 10    |
|          | C607 | 10    |
|          | C608 | 10    |
|          | C609 | 10    |
|          | C610 | 10    |

|      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| E610 | G611 | G612 | P613 | T614 | ASN | GLY | GLY | PRO | PRO | LYS | ILE | PRO | SER | ILE | ALA | THR | GLY | GLY | VAL | VAL | GLY | ALA | LEU | LEU | LEU | LEU | LEU | VAL | VAL | ALA | LEU | GLY | ILE | GLY | LEU | PHE | NET | NET | ARG | ARG | ARG | ARG | HIS | ILE | VAL | ARG | LYS | ARG | THR | LEU | ARG | ARG | LEU | LEU | LEU | GLN | GLU | ARG | PRO | LEU | THR |
|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | SER | GLY | GLU | ALA | GLU | PRO | ASN | GLN | ALA | ALA | LEU | LEU | LEU | ARG | ILE | LEU | LEU | GLU | GLU | PHE | LYS | ILE | ILE | ILE | GLY | GLY | GLY | ALA | ALA | PHE | GLY | THR | VAL | TYR | LYS | GLY | LYS | LEU | LEU | GLY | SER | SER | GLY | GLY | VAL | THR | THR | GLU | GLU | GLN | ASN | PRO | GLU | GLU | GLY | SER | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

LYS ASN ALA LYS GLU ILE LEU LEU ASP ASP GLU ALA TYR VAL MET ALA SER VAL ASP ASN PRO HIS VAL VAL CYS ARG LEU LEU GLY ILE LEU CYS LEU THR SER THR VAL GLN VAL LEU ILE THR GLN LEU LEU MET PHE GLY GLY LEU LEU LEU ASP TYR VAL ARG GLU HIS LYS ASP ASN ILE GLY SER GLN TYR

LEU LEU ASN TRP CYS VAL GLN ILE ALA LYS GLY MET ASN TYR LEU LEU GLU ASP ARG ARG LEU VAL HIS ARG ASP LEU ALA ALA ARG VAL LEU VAL LYS THR PRO GLN HIS LYS VAL LYS ILE THR ASP PHE GLY LEU ALA LYS LEU LEU GLY GLU LYS GLU HIS ALA GLU GLY

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | LVS | VAL | PRO | PRO | LYS | TRP | MET | ALA | LEU | GLU | SER | ILE | LEU | HIS | ARG | TYR | THR | HIS | GLN | SER | SER | ASP | VAL | TRP | TRP | SER | TYR | GLY | VAL | THR | THR | VAL | TRP | TRP | GLU | GLU | LEU | LEU | THR | THR | PHE | GLY | SER | GLY | LYS | PRO | TYR | ASP | GLY | ILE | PRO | PRO | ALA | SER | GLU | SER | SER | SER | ILE | LEU | LEU | GLY | GLU | GLU | ARG | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | GLN | PRO | PRO | ILE | CYS | THR | ILE | ASP | VAL | TYR | MET | ILE | MET | VAL | LYS | CYS | CYS | TRP | MET | ILE | ASP | ALA | ALA | SER | ARG | GLU | LEU | ILE | ILE | GLU | GLU | PHEN | SER | LYS | PRO | PRO | ASP | ARG | GLN | PRO | THR | LEU | VAL | ILE | ILE | GLN | GLY | ASP | GLU | GLU | ARG | MET | HIS | LEU | PRO | SER | PRO | PRO | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

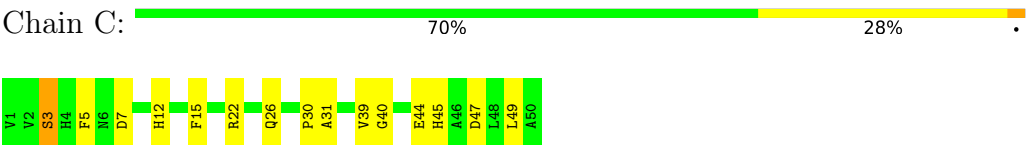
[illegible]

GLY LEU LEU SER CYS PRO ILE LYS GLU ASP PHE SER LEU GLN ARG TYR SER ASP PRO THR GLY ALA LEU THR GLU ASP LYS ILE SER ASP ASP THR PHE LEU LEU PRO VAL PRO PRO TYR ILE GLN VAL VAL PRO LYS ARG PRO ALA GLY SER VAL GLN ASN ASN PRO VAL TYR HIS ASN

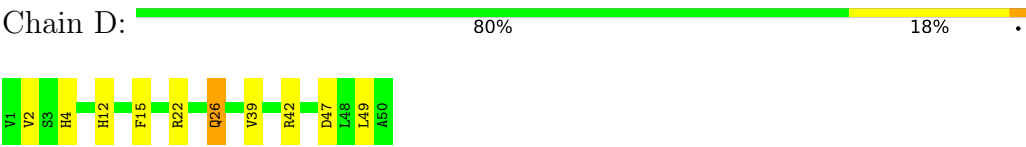
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | LEU | ASN | PRO | ALA | SER | ARG | ASP | PRO | HIS | TYR | GLN | ASP | PRO | PRO | SER | THR | ALA | VAL | GLY | ASN | PRO | GLU | TYR | LEU | ASN | THR | THR | VAL | GLN | PRO | THR | THR | CYS | VAL | VAL | ASN | SER | THR | THR | PHE | ASP | PRO | SER | PRO | ALA | HIS | TRP | ALA | ALA | GLN | GLY | LYS | SER | HIS | GLN | ILE | SER | LEU | ASN | ASP | PRO | ASP | TYR | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

GLN ASP PHE PHE PRO LYS GLU ALA LYS PRO ASN GLY ILE PHE LYS GLY SER THR ALA GLU ASN ALA ALA GLU TYR LEU ARG VAL ALA ALA PRO GLN SER SER GLU PHE ILE GLY ALA

● Molecule 2: Transforming growth factor alpha



● Molecule 2: Transforming growth factor alpha



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 126471                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 1.395                                   | Depositor |
| Minimum map value                    | -0.513                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.027                                   | Depositor |
| Recommended contour level            | 0.2                                     | Depositor |
| Map size (Å)                         | 431.75998, 431.75998, 431.75998         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.0794, 1.0794, 1.0794                  | 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     | 0.24         | 0/4815      | 0.44        | 1/6514 (0.0%)  |
| 1   | B     | 0.34         | 0/4815      | 0.57        | 2/6514 (0.0%)  |
| 2   | C     | 0.39         | 0/397       | 0.64        | 1/538 (0.2%)   |
| 2   | D     | 0.44         | 0/397       | 0.61        | 1/538 (0.2%)   |
| All | All   | 0.31         | 0/10424     | 0.52        | 5/14104 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 169 | SER  | N-CA-C | -6.19 | 105.00      | 113.30   |
| 2   | C     | 3   | SER  | CA-C-O | -6.04 | 114.15      | 120.55   |
| 2   | D     | 4   | HIS  | N-CA-C | -5.67 | 105.11      | 113.61   |
| 1   | B     | 128 | ASN  | CA-C-O | -5.48 | 115.48      | 121.84   |
| 1   | B     | 450 | THR  | N-CA-C | -5.01 | 108.20      | 114.56   |

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     | 4723  | 0        | 4556     | 87      | 0            |
| 1   | B     | 4723  | 0        | 4556     | 101     | 0            |
| 2   | C     | 386   | 0        | 345      | 11      | 0            |
| 2   | D     | 386   | 0        | 345      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 10218 | 0        | 9802     | 196     | 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 10.

All (196) 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:A:602:TYR:HE1  | 1:A:612:CYS:SG   | 1.36                     | 1.45              |
| 1:B:505:VAL:O    | 1:B:512:VAL:CG2  | 1.71                     | 1.36              |
| 1:A:602:TYR:CE1  | 1:A:612:CYS:SG   | 2.24                     | 1.30              |
| 1:B:505:VAL:O    | 1:B:512:VAL:HG23 | 1.22                     | 1.16              |
| 1:B:505:VAL:HG11 | 1:B:531:CYS:SG   | 1.97                     | 1.04              |
| 1:B:505:VAL:O    | 1:B:512:VAL:HG22 | 1.63                     | 0.99              |
| 1:B:521:GLU:HB3  | 1:B:522:PRO:HD3  | 1.57                     | 0.86              |
| 1:B:535:HIS:HD2  | 1:B:537:GLU:HB2  | 1.44                     | 0.82              |
| 1:A:447:TYR:OH   | 1:A:480:GLN:O    | 2.00                     | 0.80              |
| 1:B:364:ASP:HB3  | 1:B:367:GLU:HG3  | 1.69                     | 0.73              |
| 1:B:505:VAL:HG21 | 1:B:515:CYS:HB2  | 1.69                     | 0.72              |
| 1:B:523:ARG:NH1  | 1:B:540:PRO:HB3  | 2.05                     | 0.72              |
| 1:B:397:GLU:OE1  | 1:B:427:ARG:NH1  | 2.23                     | 0.71              |
| 1:B:505:VAL:CG1  | 1:B:531:CYS:SG   | 2.79                     | 0.71              |
| 1:A:576:MET:HE1  | 1:A:580:ASN:HA   | 1.73                     | 0.70              |
| 1:A:252:GLN:NE2  | 1:B:286:ALA:O    | 2.24                     | 0.69              |
| 1:A:444:ASN:HA   | 1:A:470:ARG:HB2  | 1.75                     | 0.68              |
| 1:B:227:CYS:SG   | 1:B:231:ARG:NH1  | 2.66                     | 0.68              |
| 1:B:285:ARG:O    | 1:B:405:ARG:NH1  | 2.26                     | 0.68              |
| 1:A:523:ARG:HH12 | 1:A:541:GLN:H    | 1.39                     | 0.68              |
| 1:B:142:ASP:O    | 1:B:198:ARG:NH2  | 2.28                     | 0.67              |
| 1:B:187:THR:OG1  | 1:B:198:ARG:NH1  | 2.27                     | 0.67              |
| 1:B:472:GLU:OE2  | 1:B:473:ASN:ND2  | 2.27                     | 0.67              |
| 1:B:444:ASN:HA   | 1:B:470:ARG:HE   | 1.61                     | 0.65              |
| 1:B:535:HIS:CD2  | 1:B:537:GLU:HB2  | 2.29                     | 0.65              |
| 1:A:82:ILE:HG21  | 1:A:226:VAL:HG11 | 1.79                     | 0.64              |
| 1:B:523:ARG:HD2  | 1:B:540:PRO:HA   | 1.79                     | 0.64              |
| 1:A:561:TYR:HA   | 1:A:591:HIS:HB3  | 1.80                     | 0.63              |
| 1:A:571:CYS:HB2  | 1:A:585:LYS:HD3  | 1.79                     | 0.62              |
| 1:B:293:GLU:OE2  | 1:B:300:ARG:NE   | 2.32                     | 0.61              |
| 1:B:12:ASN:HD22  | 1:B:17:LEU:HD21  | 1.66                     | 0.61              |
| 1:A:602:TYR:HD1  | 1:A:602:TYR:O    | 1.83                     | 0.61              |
| 1:A:114:ARG:NH1  | 1:A:182:ASN:OD1  | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:71:THR:HG21  | 1:B:102:ASP:HB2  | 1.80                     | 0.61              |
| 1:B:16:GLN:OE1   | 2:D:22:ARG:NH2   | 2.33                     | 0.60              |
| 1:A:105:LYS:HB3  | 1:A:160:LEU:HD21 | 1.81                     | 0.60              |
| 1:A:364:ASP:HB3  | 1:A:367:GLU:HG3  | 1.83                     | 0.60              |
| 1:A:227:CYS:SG   | 1:A:231:ARG:NH1  | 2.75                     | 0.60              |
| 1:A:141:ARG:HB3  | 1:A:149:LEU:HD21 | 1.85                     | 0.59              |
| 1:B:475:CYS:HB2  | 1:B:480:GLN:HB2  | 1.84                     | 0.58              |
| 1:A:523:ARG:NH1  | 1:A:541:GLN:O    | 2.38                     | 0.57              |
| 1:A:118:GLU:OE1  | 1:A:198:ARG:NH1  | 2.37                     | 0.57              |
| 1:A:488:PRO:HD3  | 1:A:503:ARG:HH11 | 1.70                     | 0.57              |
| 1:B:552:PRO:HB2  | 1:B:567:CYS:H    | 1.69                     | 0.57              |
| 1:A:101:TYR:OH   | 2:C:26:GLN:NE2   | 2.37                     | 0.57              |
| 1:B:525:PHE:O    | 1:B:531:CYS:SG   | 2.63                     | 0.56              |
| 1:B:600:CYS:HB3  | 1:B:603:GLY:O    | 2.06                     | 0.56              |
| 1:B:372:LYS:O    | 1:B:398:ASN:ND2  | 2.32                     | 0.55              |
| 1:B:133:CYS:SG   | 1:B:158:ASN:ND2  | 2.80                     | 0.55              |
| 1:B:502:CYS:SG   | 1:B:506:SER:HB3  | 2.46                     | 0.55              |
| 1:A:46:VAL:HG11  | 1:A:52:LEU:HD11  | 1.90                     | 0.54              |
| 1:B:387:PRO:O    | 1:B:389:ASN:N    | 2.37                     | 0.54              |
| 1:B:543:MET:HA   | 1:B:543:MET:HE2  | 1.90                     | 0.54              |
| 1:A:10:THR:OG1   | 1:A:42:GLU:OE1   | 2.25                     | 0.54              |
| 1:A:48:ARG:HD3   | 1:A:71:THR:HG22  | 1.89                     | 0.54              |
| 1:B:134:ASN:HB2  | 1:B:177:GLY:HA2  | 1.90                     | 0.54              |
| 1:A:19:THR:OG1   | 1:A:22:ASP:OD1   | 2.26                     | 0.54              |
| 1:B:1:LEU:HG     | 1:B:2:GLU:H      | 1.73                     | 0.53              |
| 2:C:47:ASP:N     | 2:C:47:ASP:OD1   | 2.41                     | 0.53              |
| 1:B:563:ASP:HA   | 1:B:593:CYS:HB2  | 1.91                     | 0.53              |
| 1:B:604:CYS:HB3  | 1:B:612:CYS:HB3  | 1.91                     | 0.53              |
| 1:A:16:GLN:NE2   | 1:A:18:GLY:O     | 2.42                     | 0.52              |
| 1:A:421:ILE:HG13 | 1:A:445:LEU:HD12 | 1.91                     | 0.52              |
| 1:B:134:ASN:HD22 | 1:B:177:GLY:HA2  | 1.73                     | 0.52              |
| 1:A:355:ASP:OD1  | 1:A:356:SER:N    | 2.42                     | 0.52              |
| 1:A:378:THR:HA   | 1:A:403:ARG:HB2  | 1.90                     | 0.52              |
| 1:A:537:GLU:OE1  | 1:A:560:HIS:ND1  | 2.42                     | 0.52              |
| 1:B:421:ILE:HG13 | 1:B:445:LEU:HD12 | 1.91                     | 0.52              |
| 1:B:457:PHE:HZ   | 1:B:464:THR:HG23 | 1.75                     | 0.52              |
| 1:A:372:LYS:O    | 1:A:398:ASN:ND2  | 2.31                     | 0.52              |
| 1:A:68:ALA:O     | 1:A:70:ASN:N     | 2.42                     | 0.51              |
| 1:A:599:ASN:HB2  | 1:A:609:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:310:ARG:NH1  | 1:A:311:LYS:O    | 2.43                     | 0.51              |
| 1:B:391:THR:HB   | 1:B:422:THR:HB   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:TRP:HB3  | 1:A:152:MET:HE1  | 1.93                     | 0.51              |
| 1:B:609:LEU:C    | 1:B:611:GLY:H    | 2.19                     | 0.50              |
| 1:A:601:THR:HG22 | 1:A:601:THR:O    | 2.10                     | 0.50              |
| 2:D:12:HIS:O     | 2:D:15:PHE:HB3   | 2.11                     | 0.50              |
| 1:B:545:ILE:HG13 | 1:B:556:ILE:HD11 | 1.94                     | 0.50              |
| 1:A:523:ARG:HH12 | 1:A:541:GLN:N    | 2.09                     | 0.49              |
| 1:B:585:LYS:HG2  | 1:B:595:LEU:HA   | 1.94                     | 0.49              |
| 1:A:260:LYS:HB2  | 1:A:267:CYS:HB3  | 1.95                     | 0.49              |
| 1:B:294:MET:SD   | 1:B:303:LYS:NZ   | 2.77                     | 0.49              |
| 1:A:253:MET:HE3  | 1:B:280:HIS:NE2  | 2.28                     | 0.49              |
| 1:B:604:CYS:CB   | 1:B:612:CYS:HB3  | 2.42                     | 0.49              |
| 1:A:175:CYS:HA   | 1:A:183:CYS:HA   | 1.95                     | 0.49              |
| 1:B:164:GLN:H    | 1:B:164:GLN:CD   | 2.20                     | 0.49              |
| 2:D:15:PHE:O     | 2:D:42:ARG:NE    | 2.32                     | 0.48              |
| 1:B:109:LYS:HA   | 1:B:131:ALA:O    | 2.13                     | 0.48              |
| 1:A:459:THR:HB   | 1:A:462:GLN:HE21 | 1.79                     | 0.48              |
| 1:B:279:ASP:N    | 1:B:279:ASP:OD1  | 2.44                     | 0.48              |
| 1:B:380:PHE:HB2  | 1:B:413:SER:O    | 2.13                     | 0.48              |
| 1:A:541:GLN:HG3  | 1:A:544:ASN:H    | 1.78                     | 0.48              |
| 2:C:3:SER:C      | 2:C:5:PHE:H      | 2.22                     | 0.48              |
| 1:A:541:GLN:OE1  | 1:A:542:ALA:N    | 2.47                     | 0.48              |
| 1:B:597:HIS:HB2  | 1:B:608:GLY:HA2  | 1.96                     | 0.47              |
| 1:A:468:SER:O    | 1:A:468:SER:OG   | 2.30                     | 0.47              |
| 1:B:315:GLY:HA3  | 1:B:344:ASP:H    | 1.80                     | 0.47              |
| 1:B:413:SER:HB2  | 1:B:435:GLY:HA3  | 1.95                     | 0.47              |
| 1:B:525:PHE:O    | 1:B:531:CYS:HA   | 2.14                     | 0.47              |
| 1:B:515:CYS:SG   | 1:B:524:GLU:HB2  | 2.54                     | 0.47              |
| 2:C:12:HIS:O     | 2:C:15:PHE:HB3   | 2.14                     | 0.47              |
| 1:A:42:GLU:HG3   | 1:A:66:LEU:HB3   | 1.97                     | 0.47              |
| 1:B:145:SER:HB2  | 1:B:148:PHE:HD2  | 1.79                     | 0.47              |
| 1:B:365:PRO:HB3  | 1:B:387:PRO:HB3  | 1.97                     | 0.47              |
| 2:C:7:ASP:N      | 2:C:7:ASP:OD1    | 2.46                     | 0.46              |
| 1:B:175:CYS:HA   | 1:B:183:CYS:HA   | 1.97                     | 0.46              |
| 1:A:605:THR:H    | 1:A:611:GLY:HA3  | 1.79                     | 0.46              |
| 1:B:483:HIS:ND1  | 1:B:496:PRO:HG3  | 2.30                     | 0.46              |
| 1:A:272:PRO:HG2  | 1:A:275:TYR:CD1  | 2.50                     | 0.46              |
| 1:B:170:CYS:HB2  | 1:B:183:CYS:HB3  | 1.88                     | 0.46              |
| 1:B:515:CYS:C    | 1:B:517:LEU:H    | 2.24                     | 0.46              |
| 2:D:47:ASP:OD1   | 2:D:47:ASP:N     | 2.47                     | 0.46              |
| 1:B:46:VAL:HG11  | 1:B:52:LEU:HD11  | 1.98                     | 0.46              |
| 1:B:164:GLN:HE21 | 1:B:178:ALA:HB2  | 1.81                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:526:VAL:HG22 | 1:B:531:CYS:SG   | 2.56                     | 0.45              |
| 1:B:602:TYR:CD1  | 1:B:602:TYR:N    | 2.84                     | 0.45              |
| 1:A:416:VAL:HG13 | 1:A:419:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:355:ASP:OD1  | 1:A:357:PHE:N    | 2.41                     | 0.45              |
| 1:A:133:CYS:HB3  | 1:A:158:ASN:ND2  | 2.31                     | 0.45              |
| 1:A:586:TYR:N    | 1:A:594:HIS:O    | 2.49                     | 0.45              |
| 1:B:502:CYS:HB3  | 1:B:506:SER:HB3  | 1.98                     | 0.45              |
| 1:A:585:LYS:HA   | 1:A:595:LEU:HA   | 1.99                     | 0.45              |
| 1:A:101:TYR:CD1  | 1:A:130:PRO:HD2  | 2.52                     | 0.45              |
| 1:B:419:LEU:HB2  | 1:B:442:ASN:OD1  | 2.16                     | 0.45              |
| 1:A:102:ASP:OD1  | 1:A:102:ASP:N    | 2.49                     | 0.45              |
| 2:D:39:VAL:HG13  | 2:D:47:ASP:HB3   | 1.99                     | 0.45              |
| 1:A:75:ILE:O     | 1:A:112:PRO:HD2  | 2.17                     | 0.44              |
| 1:B:505:VAL:HG21 | 1:B:515:CYS:CB   | 2.43                     | 0.44              |
| 1:A:336:LYS:HA   | 1:A:336:LYS:HD2  | 1.82                     | 0.44              |
| 1:B:261:TYR:N    | 1:B:268:VAL:O    | 2.50                     | 0.44              |
| 1:A:56:LYS:HG3   | 1:A:76:PRO:HB2   | 1.99                     | 0.44              |
| 1:A:97:VAL:HG13  | 1:A:100:ASN:HD21 | 1.81                     | 0.44              |
| 1:A:436:ASP:OD2  | 1:A:463:LYS:HG2  | 2.18                     | 0.44              |
| 1:B:96:ALA:HB1   | 1:B:98:LEU:HD23  | 2.00                     | 0.44              |
| 1:A:582:LEU:HD21 | 1:B:584:TRP:CH2  | 2.53                     | 0.43              |
| 1:A:344:ASP:OD1  | 1:A:344:ASP:N    | 2.50                     | 0.43              |
| 1:A:12:ASN:HD21  | 2:C:40:GLY:H     | 1.65                     | 0.43              |
| 1:A:582:LEU:HD21 | 1:B:584:TRP:HH2  | 1.82                     | 0.43              |
| 1:B:74:ARG:HB3   | 1:B:110:GLU:HG3  | 2.00                     | 0.43              |
| 1:B:105:LYS:HB3  | 1:B:160:LEU:HD11 | 2.01                     | 0.43              |
| 1:B:475:CYS:HA   | 1:B:478:THR:HG22 | 2.01                     | 0.43              |
| 1:A:219:PRO:HG2  | 1:B:194:GLN:HG2  | 2.00                     | 0.43              |
| 1:B:213:ALA:HB3  | 1:B:226:VAL:HG23 | 2.01                     | 0.43              |
| 1:A:519:GLU:OE2  | 1:A:519:GLU:N    | 2.48                     | 0.43              |
| 1:A:592:VAL:O    | 1:A:592:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:595:LEU:H    | 1:A:595:LEU:HD12 | 1.83                     | 0.43              |
| 1:A:132:LEU:HD21 | 1:A:135:VAL:HB   | 2.01                     | 0.42              |
| 1:A:167:ASP:OD1  | 1:A:167:ASP:N    | 2.51                     | 0.42              |
| 2:C:39:VAL:HG13  | 2:C:47:ASP:HB3   | 2.01                     | 0.42              |
| 2:C:44:GLU:HB2   | 2:C:45:HIS:CD2   | 2.54                     | 0.42              |
| 1:B:424:LEU:HD13 | 1:B:492:TRP:HZ3  | 1.84                     | 0.42              |
| 1:A:419:LEU:HD23 | 1:A:419:LEU:HA   | 1.81                     | 0.42              |
| 1:B:318:ILE:HD12 | 1:B:343:GLY:HA2  | 2.02                     | 0.42              |
| 1:A:100:ASN:H    | 1:A:129:ASN:HB3  | 1.85                     | 0.42              |
| 1:A:245:LEU:HD11 | 1:A:256:ASN:ND2  | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:403:ARG:O    | 1:A:433:SER:HB3  | 2.19                     | 0.42              |
| 1:B:568:VAL:HG12 | 1:B:570:THR:H    | 1.85                     | 0.42              |
| 1:A:186:LEU:HD12 | 1:A:186:LEU:H    | 1.84                     | 0.42              |
| 1:B:326:SER:HB3  | 1:B:348:LEU:HB2  | 2.02                     | 0.42              |
| 2:C:3:SER:C      | 2:C:5:PHE:N      | 2.78                     | 0.42              |
| 1:B:505:VAL:HG21 | 1:B:515:CYS:N    | 2.34                     | 0.42              |
| 1:A:563:ASP:HB3  | 1:A:585:LYS:HE2  | 2.01                     | 0.42              |
| 2:C:22:ARG:HG2   | 2:C:31:ALA:O     | 2.19                     | 0.42              |
| 1:B:278:THR:HG22 | 1:B:282:SER:H    | 1.85                     | 0.42              |
| 1:B:203:SER:OG   | 1:B:206:ASP:OD2  | 2.38                     | 0.42              |
| 1:B:335:PHE:HA   | 1:B:338:CYS:SG   | 2.60                     | 0.42              |
| 1:A:56:LYS:O     | 1:A:79:ASN:ND2   | 2.52                     | 0.41              |
| 1:A:222:SER:O    | 1:A:222:SER:OG   | 2.37                     | 0.41              |
| 1:A:315:GLY:HA3  | 1:A:344:ASP:H    | 1.85                     | 0.41              |
| 1:B:41:LEU:HB3   | 1:B:65:VAL:HG22  | 2.02                     | 0.41              |
| 1:B:178:ALA:O    | 1:B:182:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:586:TYR:HD2  | 1:A:596:CYS:HA   | 1.86                     | 0.41              |
| 1:B:186:LEU:H    | 1:B:186:LEU:HD12 | 1.85                     | 0.41              |
| 1:B:390:ARG:HG2  | 1:B:394:HIS:CD2  | 2.56                     | 0.41              |
| 1:A:196:SER:O    | 1:A:196:SER:OG   | 2.34                     | 0.41              |
| 1:B:427:ARG:HD3  | 1:B:497:ARG:HD2  | 2.02                     | 0.41              |
| 2:C:12:HIS:ND1   | 2:C:30:PRO:HG2   | 2.35                     | 0.41              |
| 1:B:144:VAL:HG21 | 1:B:152:MET:SD   | 2.60                     | 0.41              |
| 1:A:376:GLU:OE2  | 1:A:403:ARG:NH1  | 2.54                     | 0.41              |
| 1:A:102:ASP:CG   | 1:A:103:ALA:H    | 2.29                     | 0.41              |
| 1:B:160:LEU:HD12 | 1:B:160:LEU:H    | 1.86                     | 0.41              |
| 1:B:440:SER:OG   | 1:B:441:GLY:N    | 2.53                     | 0.41              |
| 1:B:548:THR:OG1  | 1:B:554:ASN:HB3  | 2.21                     | 0.41              |
| 1:B:162:SER:O    | 1:B:162:SER:OG   | 2.28                     | 0.41              |
| 1:B:243:LEU:HD23 | 1:B:243:LEU:HA   | 1.94                     | 0.41              |
| 1:A:118:GLU:HG3  | 1:A:119:ILE:N    | 2.35                     | 0.40              |
| 1:A:539:LEU:HD13 | 1:A:557:GLN:HB2  | 2.02                     | 0.40              |
| 1:B:128:ASN:HD22 | 2:D:26:GLN:HG3   | 1.86                     | 0.40              |
| 1:B:275:TYR:HE1  | 1:B:285:ARG:HG3  | 1.86                     | 0.40              |
| 1:A:487:SER:O    | 1:A:489:GLU:N    | 2.46                     | 0.40              |
| 1:A:171:PRO:O    | 1:A:172:ASN:C    | 2.65                     | 0.40              |
| 1:A:310:ARG:NH2  | 1:A:339:THR:HG23 | 2.36                     | 0.40              |
| 1:B:380:PHE:CE2  | 1:B:408:GLN:HB2  | 2.56                     | 0.40              |
| 1:B:609:LEU:C    | 1:B:611:GLY:N    | 2.80                     | 0.40              |
| 1:A:597:HIS:HB2  | 1:A:608:GLY:HA2  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 612/1210 (51%)  | 553 (90%)  | 58 (10%)  | 1 (0%)   | 43          | 71  |
| 1   | B     | 612/1210 (51%)  | 535 (87%)  | 73 (12%)  | 4 (1%)   | 18          | 47  |
| 2   | C     | 48/50 (96%)     | 41 (85%)   | 7 (15%)   | 0        | 100         | 100 |
| 2   | D     | 48/50 (96%)     | 41 (85%)   | 7 (15%)   | 0        | 100         | 100 |
| All | All   | 1320/2520 (52%) | 1170 (89%) | 145 (11%) | 5 (0%)   | 31          | 59  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 504 | ASN  |
| 1   | B     | 600 | CYS  |
| 1   | B     | 488 | PRO  |
| 1   | B     | 489 | GLU  |
| 1   | A     | 604 | CYS  |

### 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   | B     | 438/1053 (42%) | 426 (97%) | 12 (3%)  | 39          | 60 |
| 2   | C     | 2/43 (5%)      | 1 (50%)   | 1 (50%)  | 0           | 0  |
| 2   | D     | 43/43 (100%)   | 40 (93%)  | 3 (7%)   | 14          | 40 |
| All | All   | 483/1139 (42%) | 467 (97%) | 16 (3%)  | 34          | 57 |

All (16) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 49  | LEU  |
| 1   | B     | 487 | SER  |
| 1   | B     | 499 | CYS  |
| 1   | B     | 500 | VAL  |
| 1   | B     | 502 | CYS  |
| 1   | B     | 504 | ASN  |
| 1   | B     | 505 | VAL  |
| 1   | B     | 514 | LYS  |
| 1   | B     | 539 | LEU  |
| 1   | B     | 562 | ILE  |
| 1   | B     | 570 | THR  |
| 1   | B     | 595 | LEU  |
| 1   | B     | 602 | TYR  |
| 2   | D     | 2   | VAL  |
| 2   | D     | 26  | GLN  |
| 2   | D     | 49  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 158 | ASN  |
| 1   | B     | 194 | GLN  |
| 1   | B     | 210 | ASN  |
| 1   | B     | 211 | GLN  |
| 1   | B     | 252 | GLN  |
| 1   | B     | 366 | GLN  |
| 1   | B     | 394 | HIS  |
| 1   | B     | 473 | ASN  |
| 1   | B     | 535 | HIS  |
| 1   | B     | 557 | GLN  |
| 1   | B     | 594 | HIS  |
| 2   | D     | 18  | HIS  |
| 2   | D     | 26  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

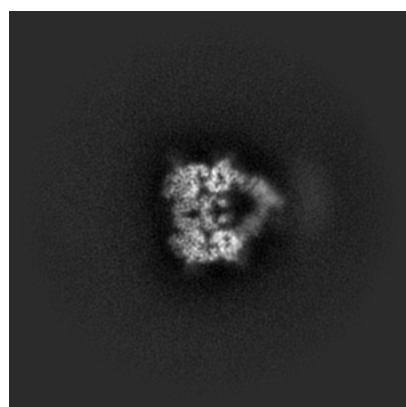
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25563. These allow visual inspection of the internal detail of the map and identification of artifacts.

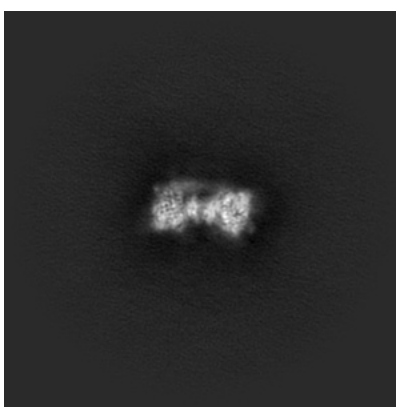
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

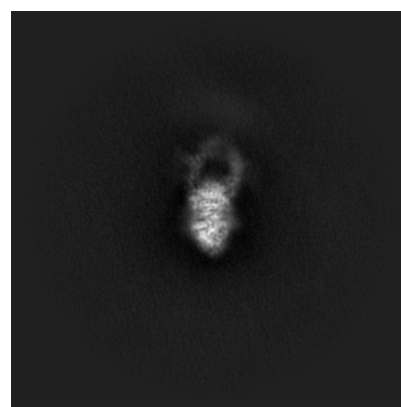
#### 6.1.1 Primary map



X



Y

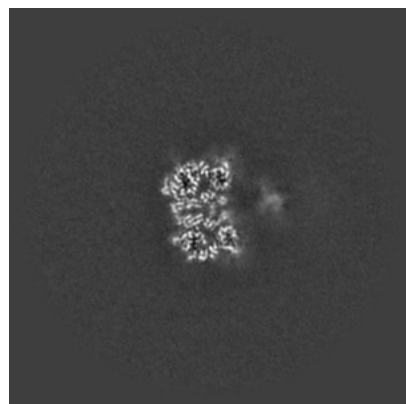


Z

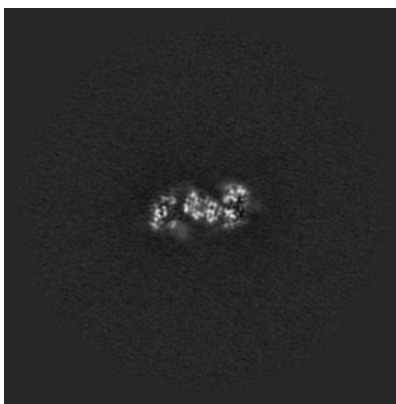
The images above show the map projected in three orthogonal directions.

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

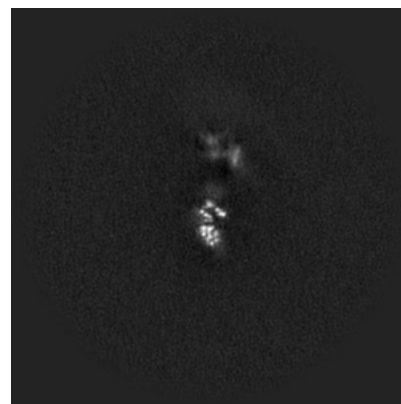
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

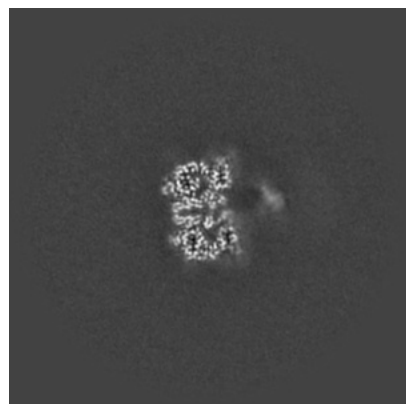


Z Index: 200

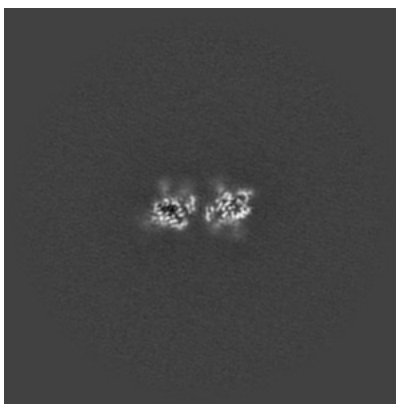
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 198



Y Index: 184

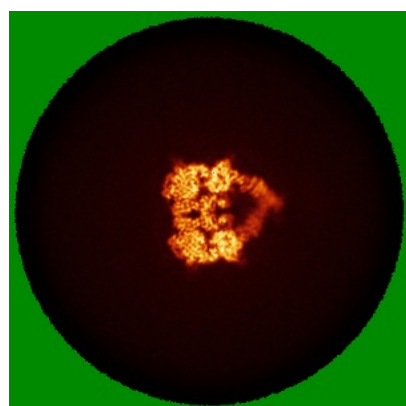


Z Index: 169

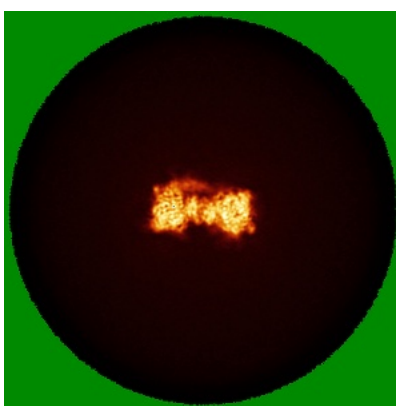
The images above show the largest variance slices of the map in three orthogonal directions.

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

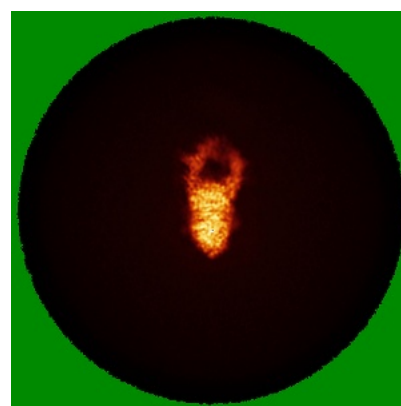
### 6.4.1 Primary map



X



Y

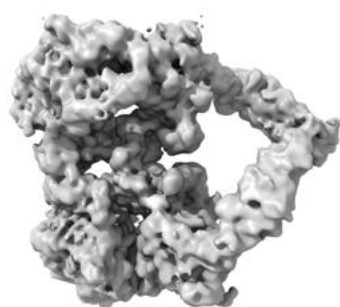


Z

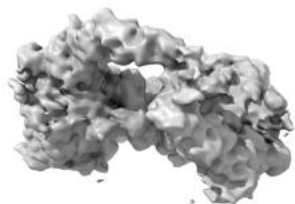
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

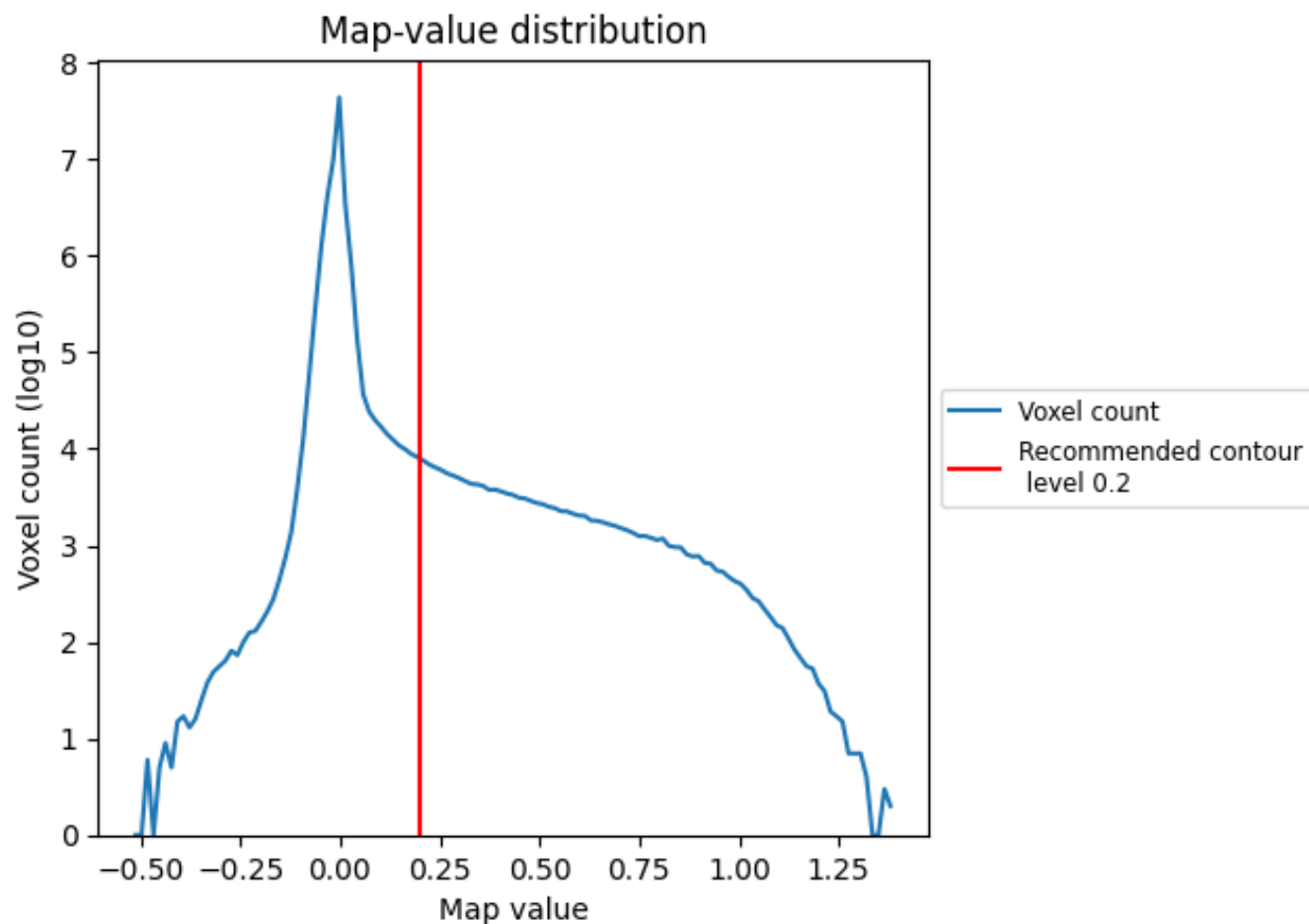
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

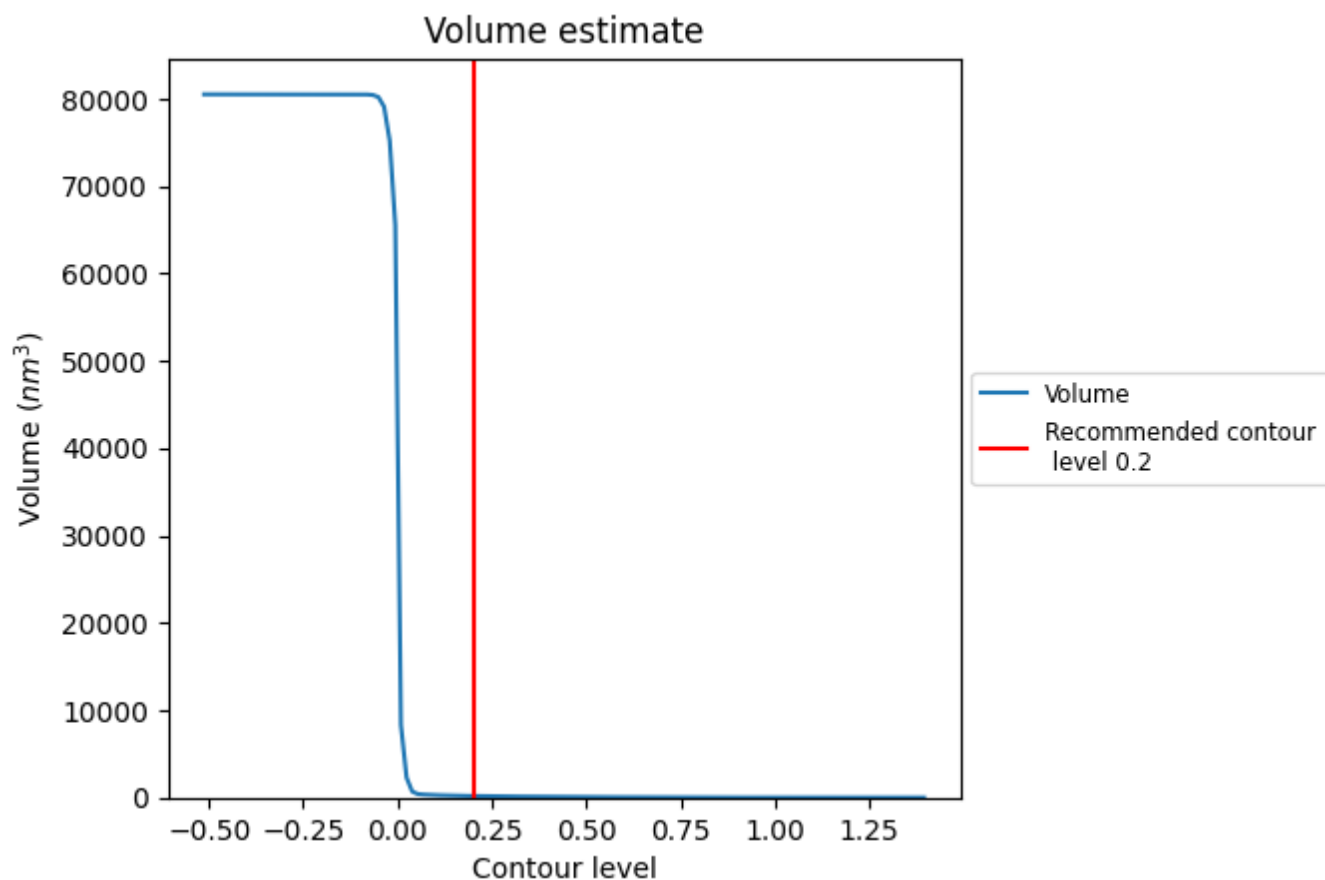
This section contains the results of statistical analysis of the map.

### 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.

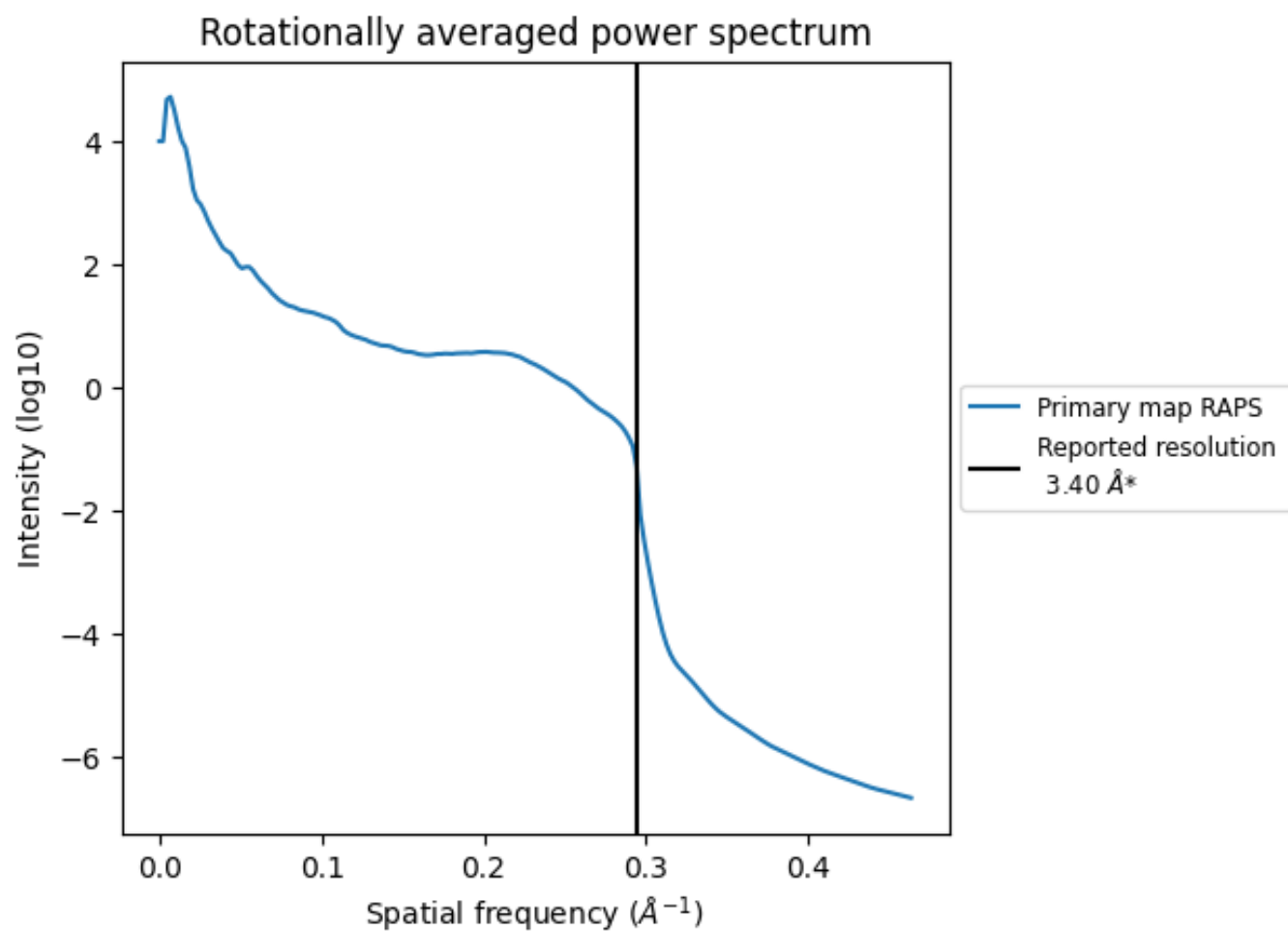
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180  $\text{nm}^3$ ; this corresponds to an approximate mass of 162 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 0.294 Å<sup>-1</sup>

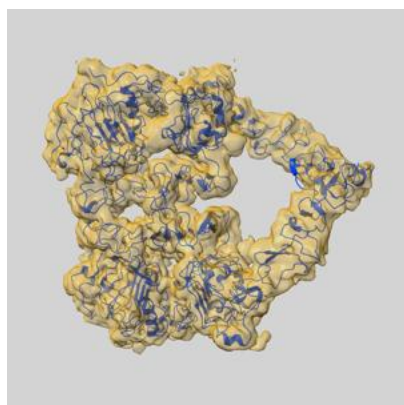
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

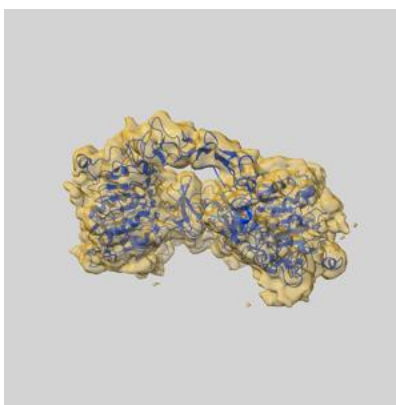
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25563 and PDB model 7SZ7. Per-residue inclusion information can be found in section 3 on page 4.

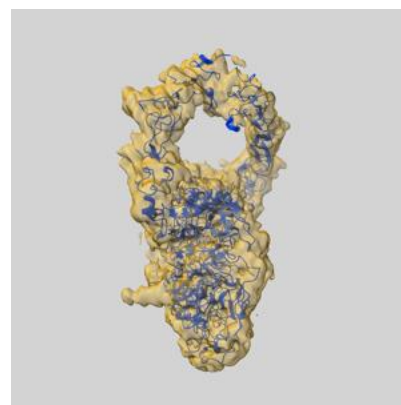
### 9.1 Map-model overlay [i](#)



X



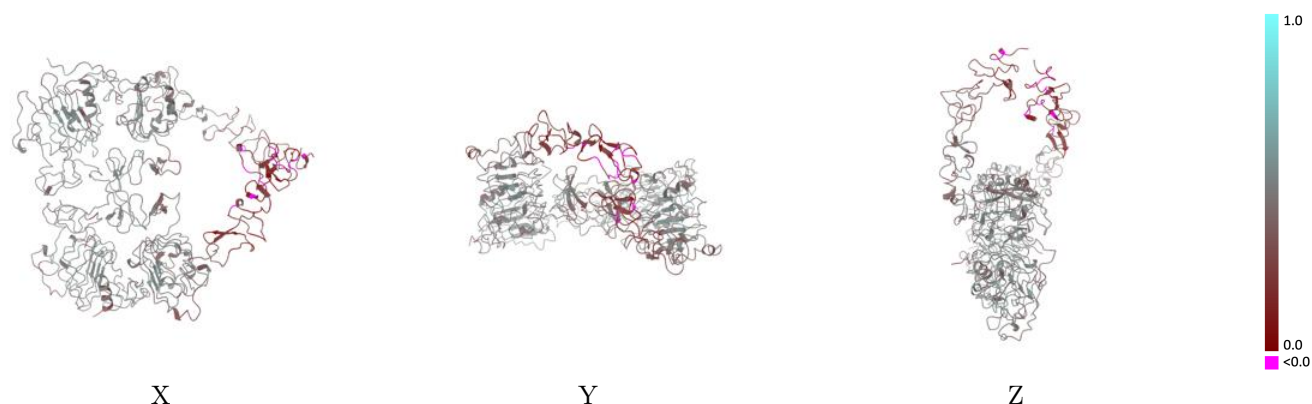
Y



Z

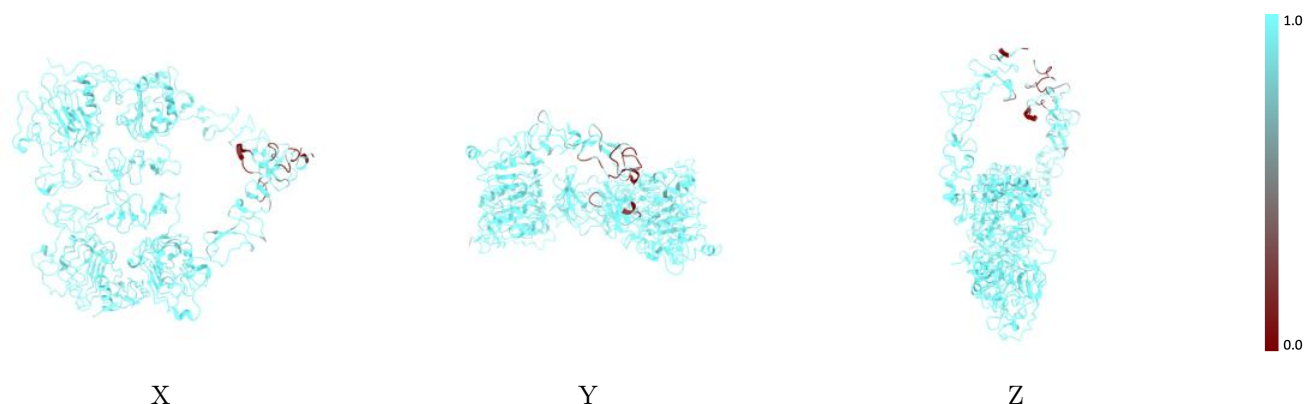
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



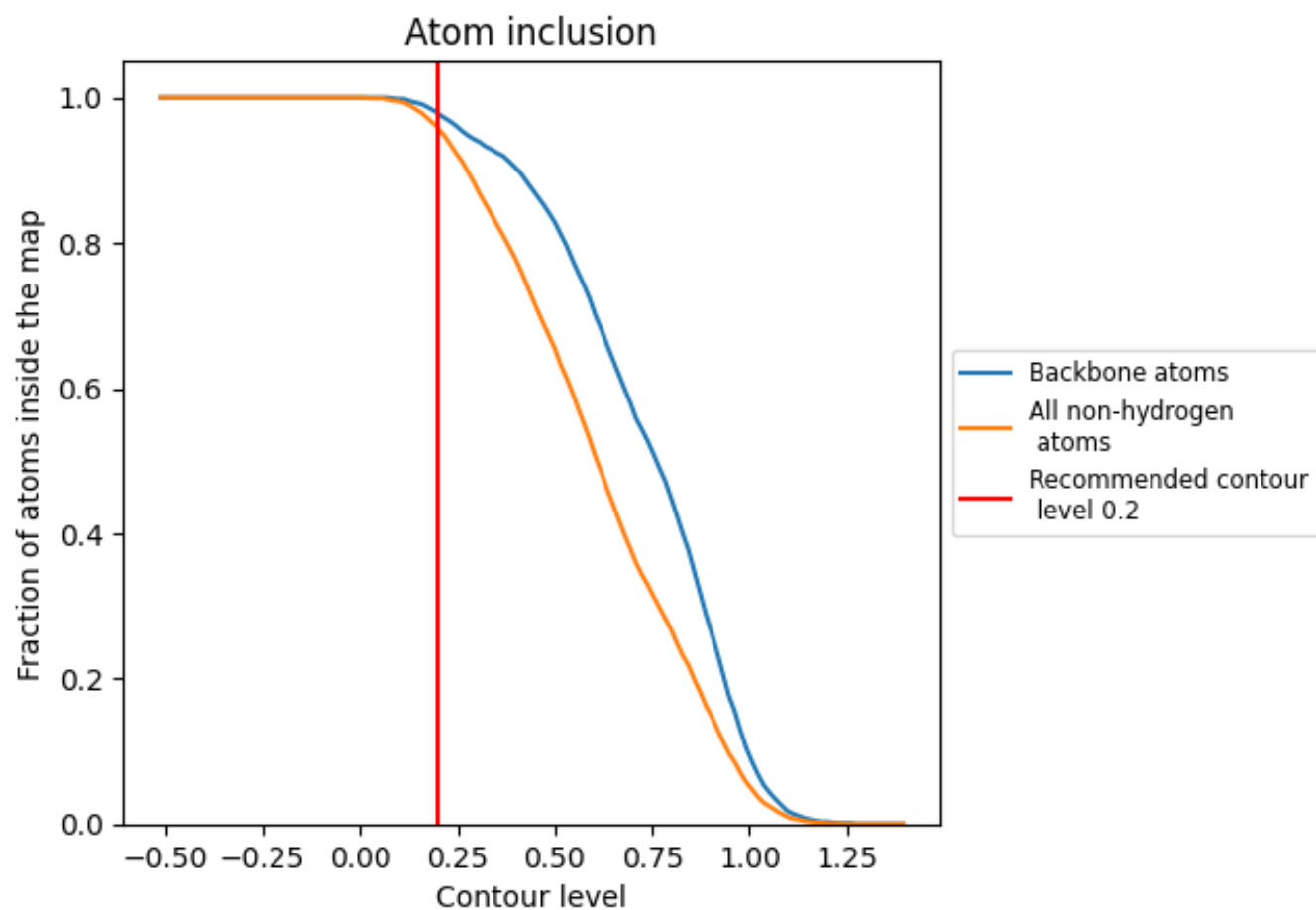
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9590 | <div></div> 0.4290 |
| A     | <div></div> 0.9740 | <div></div> 0.4410 |
| B     | <div></div> 0.9410 | <div></div> 0.4140 |
| C     | <div></div> 0.9790 | <div></div> 0.4620 |
| D     | <div></div> 0.9710 | <div></div> 0.4400 |

