# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:19 am GMT

|  |  |  |
|---|---|---|
| PDB ID | : | 3IYM |
| EMDB ID: | : | EMD-5161 |
| Title | : | Backbone Trace of the Capsid Protein Dimer of a Fungal Partitivirus from Electron Cryomicroscopy and Homology Modeling |
| Authors | : | Tang, J.; Pan, J.; Havens, W.F.; Ochoa, W.F.; Li, H.; Sinkovits, R.S.; Guu, T.S.Y.; Ghabrial, S.A.; Nibert, M.L.; Tao, J.Y.; Baker, T.S. |
| Deposited on | : | 2010-02-05 |
| Resolution | : | 4.70 Å(reported) |

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

# 1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 4.70 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 | Percentile Ranks | Value |
|---|---|---|
| Clashscore | | 40 |
| Ramachandran outliers | | 21.2% |

*Worse*   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
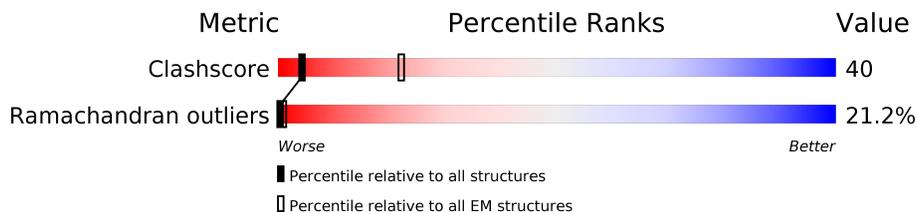
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 125131 | 1336 |
| Ramachandran outliers | 121729 | 1120 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 434 | 53%   32%   6%   9% |
| 1 | B | 434 | 51%   34%   6%   9% |

W O R L D W I D E
**PDB**
PROTEIN DATA BANK
**EMDataBank**
Unified Data Resource for 3DEM

## 2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3168 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 Capsid protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1 | A | 396 | Total | C | N | O | 0 | 0 |
| | | | 1584 | 792 | 396 | 396 | | |
| 1 | B | 396 | Total | C | N | O | 0 | 0 |
| | | | 1584 | 792 | 396 | 396 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|--------------|
| A | 185 | PHE | TYR | ENGINEERED | UNP Q6YDQ6 |
| A | 409 | LEU | ILE | ENGINEERED | UNP Q6YDQ6 |
| B | 185 | PHE | TYR | ENGINEERED | UNP Q6YDQ6 |
| B | 409 | LEU | ILE | ENGINEERED | UNP Q6YDQ6 |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Capsid protein

Chain A:



• Molecule 1: Capsid protein

Chain B:
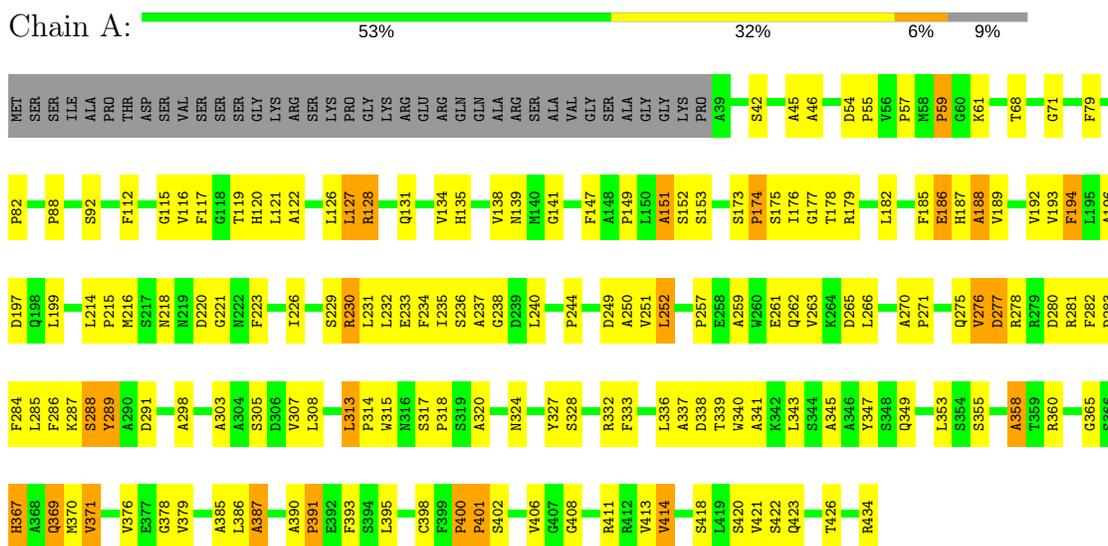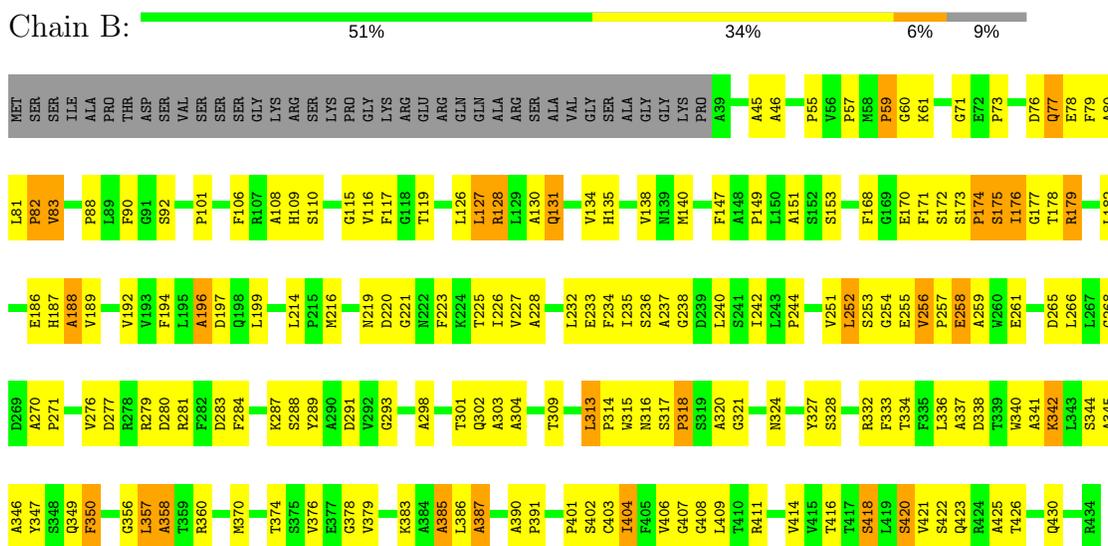
# 4 Experimental information ⓘ

| Property | Value | Source |
|---|---|---|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 14252 | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | TECNAI G2 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 15 | Depositor |
| Minimum defocus (nm) | 1.4 | Depositor |
| Maximum defocus (nm) | 2.2 | Depositor |
| Magnification | 50000 | Depositor |
| Image detector | KODAK SO-163 electron-image FILM | Depositor |

## 5  Model quality ⓘ

### 5.1  Standard geometry ⓘ

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 | $\#|Z|>2$ | RMSZ | $\#|Z|>2$ |
| 1   | A     | 0.34 | 0/1583  | 0.80 | 0/1977  |
| 1   | B     | 0.38 | 0/1583  | 0.87 | 0/1977  |
| All | All   | 0.36 | 0/3166  | 0.84 | 0/3954  |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2  Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1584  | 0        | 428      | 75      | 0            |
| 1   | B     | 1584  | 0        | 428      | 87      | 0            |
| All | All   | 3168  | 0        | 856      | 159     | 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 40.

All (159) 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:B:236:SER:O | 1:B:240:LEU:N | 2.20 | 0.74 |
| 1:B:256:VAL:O | 1:B:258:GLU:N | 2.22 | 0.73 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:328:SER:O | 1:B:332:ARG:N | 2.22 | 0.72 |
| 1:B:385:ALA:O | 1:B:387:ALA:N | 2.21 | 0.71 |
| 1:A:278:ARG:O | 1:A:282:PHE:N | 2.19 | 0.71 |
| 1:A:276:VAL:O | 1:A:278:ARG:N | 2.23 | 0.70 |
| 1:B:420:SER:O | 1:B:422:SER:N | 2.24 | 0.70 |
| 1:A:126:LEU:O | 1:A:128:ARG:N | 2.25 | 0.70 |
| 1:B:284:PHE:O | 1:B:288:SER:N | 2.25 | 0.69 |
| 1:B:301:THR:C | 1:B:303:ALA:H | 1.95 | 0.69 |
| 1:A:236:SER:O | 1:A:240:LEU:N | 2.25 | 0.69 |
| 1:A:420:SER:O | 1:A:422:SER:N | 2.26 | 0.69 |
| 1:B:313:LEU:O | 1:B:315:TRP:N | 2.27 | 0.68 |
| 1:B:115:GLY:O | 1:B:119:THR:N | 2.26 | 0.68 |
| 1:A:337:ALA:O | 1:A:341:ALA:N | 2.27 | 0.68 |
| 1:A:282:PHE:O | 1:A:285:LEU:N | 2.27 | 0.67 |
| 1:A:259:ALA:O | 1:A:263:VAL:N | 2.25 | 0.67 |
| 1:A:115:GLY:O | 1:A:119:THR:N | 2.28 | 0.67 |
| 1:A:338:ASP:O | 1:A:343:LEU:N | 2.28 | 0.67 |
| 1:A:176:ILE:O | 1:A:178:THR:N | 2.28 | 0.67 |
| 1:B:172:SER:O | 1:B:174:PRO:N | 2.28 | 0.67 |
| 1:A:280:ASP:O | 1:A:284:PHE:N | 2.19 | 0.67 |
| 1:A:369:GLN:O | 1:A:371:VAL:N | 2.28 | 0.67 |
| 1:A:313:LEU:O | 1:A:315:TRP:N | 2.28 | 0.66 |
| 1:A:275:GLN:O | 1:A:277:ASP:N | 2.28 | 0.66 |
| 1:A:332:ARG:O | 1:A:336:LEU:N | 2.29 | 0.66 |
| 1:A:281:ARG:O | 1:A:285:LEU:N | 2.28 | 0.65 |
| 1:A:233:GLU:O | 1:A:237:ALA:N | 2.26 | 0.65 |
| 1:B:336:LEU:O | 1:B:340:TRP:N | 2.26 | 0.65 |
| 1:A:328:SER:O | 1:A:332:ARG:N | 2.29 | 0.65 |
| 1:A:376:VAL:O | 1:A:378:GLY:N | 2.30 | 0.65 |
| 1:A:284:PHE:O | 1:A:288:SER:N | 2.29 | 0.64 |
| 1:A:358:ALA:O | 1:A:360:ARG:N | 2.29 | 0.64 |
| 1:A:283:ASP:O | 1:A:287:LYS:N | 2.29 | 0.64 |
| 1:B:233:GLU:O | 1:B:237:ALA:N | 2.27 | 0.64 |
| 1:B:176:ILE:O | 1:B:178:THR:N | 2.30 | 0.64 |
| 1:A:333:PHE:O | 1:A:337:ALA:N | 2.24 | 0.64 |
| 1:B:358:ALA:C | 1:B:360:ARG:H | 2.01 | 0.64 |
| 1:B:126:LEU:O | 1:B:128:ARG:N | 2.32 | 0.63 |
| 1:B:252:LEU:O | 1:B:254:GLY:N | 2.31 | 0.63 |
| 1:B:301:THR:O | 1:B:303:ALA:N | 2.32 | 0.62 |
| 1:B:182:LEU:O | 1:B:186:GLU:N | 2.32 | 0.62 |
| 1:B:402:SER:O | 1:B:404:ILE:N | 2.27 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:320:ALA:O | 1:A:324:ASN:N | 2.34 | 0.61 |
| 1:B:332:ARG:O | 1:B:336:LEU:N | 2.33 | 0.61 |
| 1:B:337:ALA:O | 1:B:341:ALA:N | 2.35 | 0.60 |
| 1:B:59:PRO:C | 1:B:61:LYS:H | 2.04 | 0.60 |
| 1:B:225:THR:O | 1:B:227:VAL:N | 2.34 | 0.60 |
| 1:B:338:ASP:O | 1:B:342:LYS:N | 2.28 | 0.60 |
| 1:B:420:SER:O | 1:B:423:GLN:N | 2.34 | 0.59 |
| 1:B:402:SER:C | 1:B:404:ILE:H | 2.06 | 0.58 |
| 1:B:175:SER:O | 1:B:178:THR:O | 2.22 | 0.57 |
| 1:A:282:PHE:O | 1:A:286:PHE:N | 2.33 | 0.57 |
| 1:A:336:LEU:O | 1:A:340:TRP:N | 2.38 | 0.56 |
| 1:B:108:ALA:O | 1:B:110:SER:N | 2.31 | 0.56 |
| 1:A:422:SER:O | 1:A:426:THR:N | 2.32 | 0.56 |
| 1:B:289:TYR:C | 1:B:291:ASP:H | 2.09 | 0.56 |
| 1:B:345:ALA:C | 1:B:347:TYR:H | 2.09 | 0.56 |
| 1:B:225:THR:O | 1:B:228:ALA:N | 2.29 | 0.56 |
| 1:B:261:GLU:O | 1:B:265:ASP:N | 2.35 | 0.56 |
| 1:A:182:LEU:O | 1:A:186:GLU:N | 2.27 | 0.55 |
| 1:B:376:VAL:O | 1:B:378:GLY:N | 2.34 | 0.55 |
| 1:B:187:HIS:O | 1:B:188:ALA:O | 2.25 | 0.55 |
| 1:B:81:LEU:O | 1:B:82:PRO:O | 2.25 | 0.55 |
| 1:B:426:THR:O | 1:B:430:GLN:N | 2.40 | 0.54 |
| 1:A:187:HIS:O | 1:A:188:ALA:O | 2.25 | 0.54 |
| 1:A:249:ASP:O | 1:A:251:VAL:N | 2.41 | 0.54 |
| 1:B:82:PRO:O | 1:B:83:VAL:O | 2.26 | 0.54 |
| 1:A:358:ALA:C | 1:A:360:ARG:H | 2.10 | 0.54 |
| 1:A:400:PRO:O | 1:A:401:PRO:O | 2.26 | 0.54 |
| 1:B:304:ALA:O | 1:B:309:THR:N | 2.33 | 0.54 |
| 1:A:420:SER:O | 1:A:423:GLN:N | 2.38 | 0.53 |
| 1:B:76:ASP:O | 1:B:78:GLU:N | 2.41 | 0.53 |
| 1:B:313:LEU:O | 1:B:316:ASN:N | 2.41 | 0.53 |
| 1:A:120:HIS:C | 1:A:122:ALA:H | 2.12 | 0.53 |
| 1:A:234:PHE:C | 1:A:236:SER:H | 2.13 | 0.52 |
| 1:B:356:GLY:O | 1:B:357:LEU:O | 2.28 | 0.52 |
| 1:A:54:ASP:O | 1:A:151:ALA:O | 2.28 | 0.52 |
| 1:A:196:ALA:O | 1:A:199:LEU:N | 2.43 | 0.52 |
| 1:B:131:GLN:O | 1:B:135:HIS:N | 2.27 | 0.52 |
| 1:A:385:ALA:O | 1:A:387:ALA:N | 2.42 | 0.51 |
| 1:B:407:GLY:O | 1:B:409:LEU:N | 2.44 | 0.51 |
| 1:A:261:GLU:O | 1:A:265:ASP:N | 2.40 | 0.51 |
| 1:A:193:VAL:O | 1:A:194:PHE:O | 2.28 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:379:VAL:O | 1:B:414:VAL:O | 2.30 | 0.50 |
| 1:B:128:ARG:C | 1:B:130:ALA:H | 2.14 | 0.50 |
| 1:B:134:VAL:O | 1:B:138:VAL:N | 2.35 | 0.50 |
| 1:A:367:HIS:C | 1:A:369:GLN:H | 2.14 | 0.50 |
| 1:A:414:VAL:O | 1:B:379:VAL:O | 2.29 | 0.50 |
| 1:A:174:PRO:C | 1:A:176:ILE:H | 2.15 | 0.50 |
| 1:A:134:VAL:O | 1:A:138:VAL:N | 2.44 | 0.50 |
| 1:B:301:THR:C | 1:B:303:ALA:N | 2.64 | 0.50 |
| 1:B:127:LEU:O | 1:B:128:ARG:O | 2.28 | 0.50 |
| 1:A:218:ASN:C | 1:A:220:ASP:H | 2.13 | 0.50 |
| 1:A:336:LEU:O | 1:A:339:THR:N | 2.42 | 0.50 |
| 1:A:185:PHE:C | 1:A:187:HIS:H | 2.15 | 0.50 |
| 1:B:236:SER:C | 1:B:238:GLY:N | 2.65 | 0.50 |
| 1:B:59:PRO:O | 1:B:61:LYS:N | 2.45 | 0.49 |
| 1:B:280:ASP:O | 1:B:284:PHE:N | 2.26 | 0.49 |
| 1:A:127:LEU:O | 1:A:128:ARG:O | 2.31 | 0.49 |
| 1:A:226:ILE:O | 1:A:231:LEU:O | 2.30 | 0.49 |
| 1:B:131:GLN:H | 1:B:134:VAL:H | 1.59 | 0.49 |
| 1:B:240:LEU:C | 1:B:242:ILE:H | 2.16 | 0.49 |
| 1:B:318:PRO:O | 1:B:321:GLY:N | 2.46 | 0.48 |
| 1:B:333:PHE:O | 1:B:337:ALA:N | 2.25 | 0.48 |
| 1:B:236:SER:C | 1:B:238:GLY:H | 2.16 | 0.48 |
| 1:B:59:PRO:C | 1:B:61:LYS:N | 2.67 | 0.48 |
| 1:A:289:TYR:C | 1:A:291:ASP:H | 2.17 | 0.48 |
| 1:A:259:ALA:O | 1:A:262:GLN:N | 2.47 | 0.48 |
| 1:B:342:LYS:O | 1:B:345:ALA:N | 2.43 | 0.48 |
| 1:B:279:ARG:O | 1:B:283:ASP:N | 2.47 | 0.47 |
| 1:B:416:THR:C | 1:B:418:SER:H | 2.18 | 0.47 |
| 1:B:255:GLU:O | 1:B:256:VAL:O | 2.32 | 0.47 |
| 1:B:225:THR:C | 1:B:227:VAL:H | 2.18 | 0.47 |
| 1:B:219:ASN:O | 1:B:221:GLY:N | 2.48 | 0.46 |
| 1:A:251:VAL:O | 1:A:252:LEU:O | 2.33 | 0.46 |
| 1:A:59:PRO:C | 1:A:61:LYS:H | 2.17 | 0.46 |
| 1:B:334:THR:O | 1:B:338:ASP:N | 2.30 | 0.46 |
| 1:B:277:ASP:O | 1:B:281:ARG:N | 2.49 | 0.45 |
| 1:B:77:GLN:C | 1:B:79:PHE:H | 2.18 | 0.45 |
| 1:B:358:ALA:O | 1:B:360:ARG:N | 2.50 | 0.45 |
| 1:A:214:LEU:O | 1:A:216:MET:N | 2.50 | 0.45 |
| 1:B:179:ARG:O | 1:B:182:LEU:N | 2.50 | 0.45 |
| 1:A:336:LEU:C | 1:A:339:THR:H | 2.19 | 0.44 |
| 1:B:291:ASP:C | 1:B:293:GLY:H | 2.20 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:434:ARG:O | 1:B:350:PHE:N | 2.49 | 0.44 |
| 1:A:194:PHE:C | 1:A:196:ALA:H | 2.20 | 0.44 |
| 1:A:236:SER:C | 1:A:238:GLY:N | 2.70 | 0.44 |
| 1:A:275:GLN:C | 1:A:277:ASP:N | 2.71 | 0.44 |
| 1:A:391:PRO:O | 1:A:395:LEU:N | 2.48 | 0.43 |
| 1:B:251:VAL:O | 1:B:252:LEU:O | 2.36 | 0.43 |
| 1:A:120:HIS:O | 1:A:122:ALA:N | 2.44 | 0.43 |
| 1:A:174:PRO:O | 1:A:176:ILE:N | 2.51 | 0.43 |
| 1:A:278:ARG:O | 1:A:281:ARG:N | 2.52 | 0.43 |
| 1:B:196:ALA:O | 1:B:199:LEU:N | 2.52 | 0.43 |
| 1:B:345:ALA:C | 1:B:347:TYR:N | 2.73 | 0.42 |
| 1:A:229:SER:O | 1:A:230:ARG:O | 2.37 | 0.42 |
| 1:A:236:SER:C | 1:A:238:GLY:H | 2.23 | 0.42 |
| 1:A:333:PHE:C | 1:A:336:LEU:H | 2.24 | 0.42 |
| 1:B:358:ALA:C | 1:B:360:ARG:N | 2.70 | 0.41 |
| 1:A:345:ALA:C | 1:A:347:TYR:H | 2.24 | 0.41 |
| 1:B:236:SER:O | 1:B:238:GLY:N | 2.54 | 0.41 |
| 1:B:283:ASP:O | 1:B:287:LYS:N | 2.54 | 0.41 |
| 1:B:78:GLU:C | 1:B:80:ALA:H | 2.24 | 0.41 |
| 1:B:214:LEU:O | 1:B:216:MET:N | 2.54 | 0.41 |
| 1:B:266:LEU:C | 1:B:268:GLY:N | 2.74 | 0.41 |
| 1:B:402:SER:C | 1:B:404:ILE:N | 2.73 | 0.41 |
| 1:A:135:HIS:O | 1:A:139:ASN:N | 2.53 | 0.41 |
| 1:B:422:SER:O | 1:B:425:ALA:N | 2.54 | 0.41 |
| 1:A:358:ALA:C | 1:A:360:ARG:N | 2.73 | 0.41 |
| 1:A:262:GLN:O | 1:A:266:LEU:N | 2.38 | 0.41 |
| 1:B:320:ALA:O | 1:B:324:ASN:N | 2.48 | 0.41 |
| 1:B:344:SER:C | 1:B:346:ALA:N | 2.74 | 0.41 |
| 1:A:303:ALA:C | 1:A:305:SER:H | 2.25 | 0.40 |
| 1:B:168:PHE:C | 1:B:170:GLU:H | 2.25 | 0.40 |
| 1:B:234:PHE:C | 1:B:236:SER:H | 2.25 | 0.40 |
| 1:A:185:PHE:C | 1:A:187:HIS:N | 2.75 | 0.40 |
| 1:A:262:GLN:O | 1:A:265:ASP:N | 2.54 | 0.40 |
| 1:B:90:PHE:C | 1:B:92:SER:H | 2.24 | 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 | 394/434 (91%) | 226 (57%) | 83 (21%) | 85 (22%) | 0 | 2 |
| 1 | B | 394/434 (91%) | 219 (56%) | 93 (24%) | 82 (21%) | 0 | 2 |
| All | All | 788/868 (91%) | 445 (56%) | 176 (22%) | 167 (21%) | 0 | 2 |

All (167) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 42 | SER |
| 1 | A | 46 | ALA |
| 1 | A | 57 | PRO |
| 1 | A | 82 | PRO |
| 1 | A | 92 | SER |
| 1 | A | 127 | LEU |
| 1 | A | 128 | ARG |
| 1 | A | 131 | GLN |
| 1 | A | 147 | PHE |
| 1 | A | 149 | PRO |
| 1 | A | 152 | SER |
| 1 | A | 174 | PRO |
| 1 | A | 177 | GLY |
| 1 | A | 179 | ARG |
| 1 | A | 188 | ALA |
| 1 | A | 192 | VAL |
| 1 | A | 194 | PHE |
| 1 | A | 223 | PHE |
| 1 | A | 230 | ARG |
| 1 | A | 232 | LEU |
| 1 | A | 244 | PRO |
| 1 | A | 250 | ALA |
| 1 | A | 252 | LEU |
| 1 | A | 257 | PRO |
| 1 | A | 270 | ALA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 271 | PRO |
| 1 | A | 277 | ASP |
| 1 | A | 314 | PRO |
| 1 | A | 318 | PRO |
| 1 | A | 353 | LEU |
| 1 | A | 369 | GLN |
| 1 | A | 370 | MET |
| 1 | A | 390 | ALA |
| 1 | A | 400 | PRO |
| 1 | A | 401 | PRO |
| 1 | A | 402 | SER |
| 1 | A | 406 | VAL |
| 1 | A | 413 | VAL |
| 1 | A | 421 | VAL |
| 1 | B | 46 | ALA |
| 1 | B | 55 | PRO |
| 1 | B | 57 | PRO |
| 1 | B | 77 | GLN |
| 1 | B | 82 | PRO |
| 1 | B | 83 | VAL |
| 1 | B | 127 | LEU |
| 1 | B | 128 | ARG |
| 1 | B | 131 | GLN |
| 1 | B | 147 | PHE |
| 1 | B | 149 | PRO |
| 1 | B | 151 | ALA |
| 1 | B | 173 | SER |
| 1 | B | 174 | PRO |
| 1 | B | 179 | ARG |
| 1 | B | 188 | ALA |
| 1 | B | 192 | VAL |
| 1 | B | 194 | PHE |
| 1 | B | 223 | PHE |
| 1 | B | 226 | ILE |
| 1 | B | 244 | PRO |
| 1 | B | 252 | LEU |
| 1 | B | 253 | SER |
| 1 | B | 257 | PRO |
| 1 | B | 259 | ALA |
| 1 | B | 270 | ALA |
| 1 | B | 271 | PRO |
| 1 | B | 276 | VAL |

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 302 | GLN |
| 1 | B | 314 | PRO |
| 1 | B | 350 | PHE |
| 1 | B | 358 | ALA |
| 1 | B | 370 | MET |
| 1 | B | 385 | ALA |
| 1 | B | 386 | LEU |
| 1 | B | 387 | ALA |
| 1 | B | 390 | ALA |
| 1 | B | 401 | PRO |
| 1 | B | 403 | CYS |
| 1 | B | 421 | VAL |
| 1 | A | 55 | PRO |
| 1 | A | 175 | SER |
| 1 | A | 197 | ASP |
| 1 | A | 221 | GLY |
| 1 | A | 235 | ILE |
| 1 | A | 276 | VAL |
| 1 | A | 289 | TYR |
| 1 | A | 308 | LEU |
| 1 | A | 358 | ALA |
| 1 | A | 371 | VAL |
| 1 | A | 386 | LEU |
| 1 | A | 387 | ALA |
| 1 | A | 398 | CYS |
| 1 | A | 408 | GLY |
| 1 | A | 414 | VAL |
| 1 | B | 109 | HIS |
| 1 | B | 153 | SER |
| 1 | B | 171 | PHE |
| 1 | B | 177 | GLY |
| 1 | B | 220 | ASP |
| 1 | B | 232 | LEU |
| 1 | B | 318 | PRO |
| 1 | B | 357 | LEU |
| 1 | B | 404 | ILE |
| 1 | B | 408 | GLY |
| 1 | B | 418 | SER |
| 1 | A | 68 | THR |
| 1 | A | 112 | PHE |
| 1 | A | 117 | PHE |
| 1 | A | 121 | LEU |

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 151 | ALA |
| 1 | A | 298 | ALA |
| 1 | A | 327 | TYR |
| 1 | A | 349 | GLN |
| 1 | A | 367 | HIS |
| 1 | A | 391 | PRO |
| 1 | A | 411 | ARG |
| 1 | A | 418 | SER |
| 1 | B | 45 | ALA |
| 1 | B | 116 | VAL |
| 1 | B | 117 | PHE |
| 1 | B | 140 | MET |
| 1 | B | 175 | SER |
| 1 | B | 197 | ASP |
| 1 | B | 258 | GLU |
| 1 | B | 374 | THR |
| 1 | B | 411 | ARG |
| 1 | A | 45 | ALA |
| 1 | A | 79 | PHE |
| 1 | A | 153 | SER |
| 1 | A | 288 | SER |
| 1 | A | 313 | LEU |
| 1 | A | 355 | SER |
| 1 | A | 393 | PHE |
| 1 | B | 59 | PRO |
| 1 | B | 60 | GLY |
| 1 | B | 106 | PHE |
| 1 | B | 176 | ILE |
| 1 | B | 189 | VAL |
| 1 | B | 196 | ALA |
| 1 | B | 298 | ALA |
| 1 | B | 342 | LYS |
| 1 | B | 349 | GLN |
| 1 | B | 383 | LYS |
| 1 | B | 391 | PRO |
| 1 | B | 406 | VAL |
| 1 | B | 420 | SER |
| 1 | A | 88 | PRO |
| 1 | A | 189 | VAL |
| 1 | B | 235 | ILE |
| 1 | B | 313 | LEU |
| 1 | B | 327 | TYR |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 186 | GLU |
| 1 | A | 317 | SER |
| 1 | B | 256 | VAL |
| 1 | A | 215 | PRO |
| 1 | A | 59 | PRO |
| 1 | A | 141 | GLY |
| 1 | A | 173 | SER |
| 1 | A | 365 | GLY |
| 1 | B | 88 | PRO |
| 1 | B | 317 | SER |
| 1 | A | 116 | VAL |
| 1 | A | 307 | VAL |
| 1 | B | 71 | GLY |
| 1 | B | 73 | PRO |
| 1 | B | 101 | PRO |
| 1 | A | 71 | GLY |

### 5.3.2 Protein sidechains ⓘ

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.