



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 02:16 AM EST

PDB ID : 6WXG
EMDB ID : EMD-21957
Title : Cryo-EM reconstruction of VP5*/VP8* assembly from rhesus rotavirus particles - Reversed conformation
Authors : Herrmann, T.; Harrison, S.C.; Jenni, S.
Deposited on : 2020-05-10
Resolution : 3.30 Å (reported)
Based on initial models : 4V7Q, 1SLQ

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

We welcome your comments at 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>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

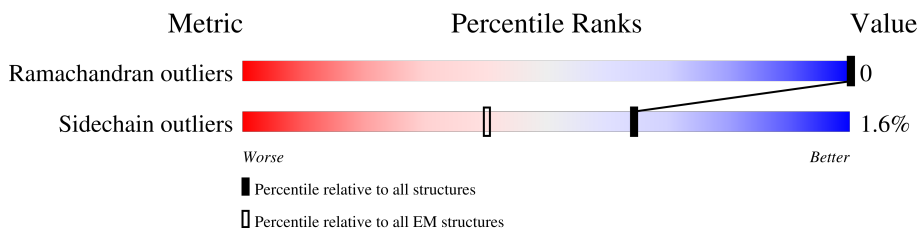
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



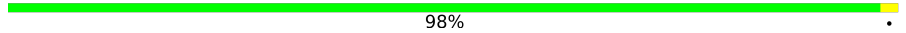
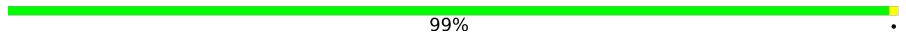
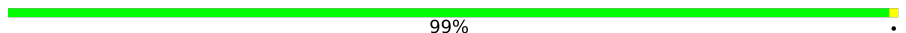
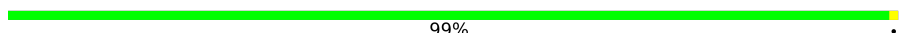

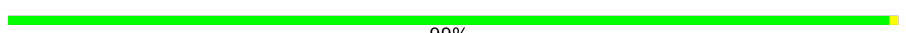



















| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 ≥ 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1 | 776 | 35% 65% |
| 1 | 2 | 776 | 35% 65% |
| 1 | 3 | 776 | 35% 65% |
| 2 | A | 397 | 99% |
| 2 | B | 397 | 98% |
| 2 | C | 397 | 98% |
| 2 | D | 397 | 99% |
| 2 | E | 397 | 99% |
| 2 | F | 397 | 98% |
| 2 | G | 397 | 98% |





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | H | 397 |  98% |
| 2 | I | 397 |  99% |
| 2 | J | 397 |  99% |
| 2 | K | 397 |  99% |
| 2 | L | 397 |  98% |
| 2 | M | 397 |  99% |
| 2 | N | 397 |  99% |
| 2 | O | 397 |  98% |
| 2 | P | 397 |  98% |
| 2 | Q | 397 |  99% |
| 2 | R | 397 |  99% |
| 3 | a | 326 |  79% |
| 3 | b | 326 |  83% |
| 3 | c | 326 |  79% |
| 3 | d | 326 |  80% |
| 3 | e | 326 |  79% |
| 3 | f | 326 |  80% |
| 3 | g | 326 |  82% |
| 3 | h | 326 |  79% |
| 3 | i | 326 |  82% |
| 3 | j | 326 |  81% |
| 3 | k | 326 |  80% |
| 3 | l | 326 |  79% |
| 3 | m | 326 |  82% |
| 3 | n | 326 |  80% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 3 | o | 326 |  79% 19% |
| 3 | p | 326 |  81% 17% |
| 3 | q | 326 |  78% 21% |
| 3 | r | 326 |  82% 17% |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 201212 atoms, of which 99503 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 Outer capsid protein VP4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|------|------|-----|-----|---------|-------|---|
| | | | Total | C | H | N | O | | | S |
| 1 | 1 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4291 | 1382 | 2107 | 368 | 427 | 7 | | |
| 1 | 2 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4291 | 1382 | 2107 | 368 | 427 | 7 | | |
| 1 | 3 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4291 | 1382 | 2107 | 368 | 427 | 7 | | |

- Molecule 2 is a protein called Intermediate capsid protein VP6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|------|------|-----|-----|---------|-------|---|
| | | | Total | C | H | N | O | | | S |
| 2 | A | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | B | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | C | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | D | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | E | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |
| 2 | F | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |
| 2 | G | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |
| 2 | H | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |
| 2 | I | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | J | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | K | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | L | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|------|------|-----|-----|---------|-------|---|
| 2 | M | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |
| 2 | N | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | O | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |
| 2 | P | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |
| 2 | Q | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6276 | 2004 | 3113 | 551 | 593 | 15 | | |
| 2 | R | 397 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6275 | 2004 | 3112 | 551 | 593 | 15 | | |

- Molecule 3 is a protein called Outer capsid glycoprotein VP7.

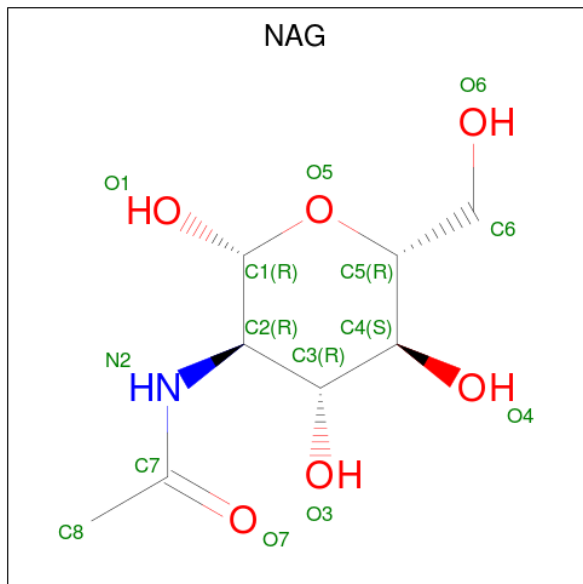
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|------|------|-----|-----|---------|-------|---|
| 3 | a | 259 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4041 | 1298 | 1994 | 324 | 409 | 16 | | |
| 3 | b | 272 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4254 | 1369 | 2099 | 342 | 428 | 16 | | |
| 3 | c | 261 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4074 | 1308 | 2011 | 327 | 412 | 16 | | |
| 3 | d | 265 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4133 | 1328 | 2037 | 333 | 419 | 16 | | |
| 3 | e | 260 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4050 | 1302 | 1998 | 323 | 411 | 16 | | |
| 3 | f | 265 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4133 | 1328 | 2037 | 333 | 419 | 16 | | |
| 3 | g | 272 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4254 | 1369 | 2099 | 342 | 428 | 16 | | |
| 3 | h | 259 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4041 | 1298 | 1994 | 324 | 409 | 16 | | |
| 3 | i | 272 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4254 | 1369 | 2099 | 342 | 428 | 16 | | |
| 3 | j | 272 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4254 | 1369 | 2099 | 342 | 428 | 16 | | |
| 3 | k | 265 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4133 | 1328 | 2037 | 333 | 419 | 16 | | |
| 3 | l | 265 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4133 | 1328 | 2037 | 333 | 419 | 16 | | |
| 3 | m | 272 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4254 | 1369 | 2099 | 342 | 428 | 16 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace | |
|-----|-------|----------|-------|------|------|-----|-----|---------|-------|---|
| | | | Total | C | H | N | O | | | S |
| 3 | n | 265 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4133 | 1328 | 2037 | 333 | 419 | 16 | | |
| 3 | o | 265 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4133 | 1328 | 2037 | 333 | 419 | 16 | | |
| 3 | p | 272 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4254 | 1369 | 2099 | 342 | 428 | 16 | | |
| 3 | q | 259 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4041 | 1298 | 1994 | 324 | 409 | 16 | | |
| 3 | r | 272 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4254 | 1369 | 2099 | 342 | 428 | 16 | | |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| | | | Total | C | H | N | O | |
| 4 | a | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | b | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | c | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | d | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | e | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | f | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf | |
|-----|-------|----------|-------|---|----|---|---------|---|
| 4 | g | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | h | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | i | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | j | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | k | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | l | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | m | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | n | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | o | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | p | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | q | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 4 | r | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 5 | a | 5 | Total | Ca | 0 |
| | | | 5 | 5 | |
| 5 | b | 3 | Total | Ca | 0 |
| | | | 3 | 3 | |
| 5 | c | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 5 | d | 5 | Total | Ca | 0 |
| | | | 5 | 5 | |
| 5 | e | 3 | Total | Ca | 0 |
| | | | 3 | 3 | |
| 5 | f | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 5 | g | 5 | Total | Ca | 0 |
| | | | 5 | 5 | |

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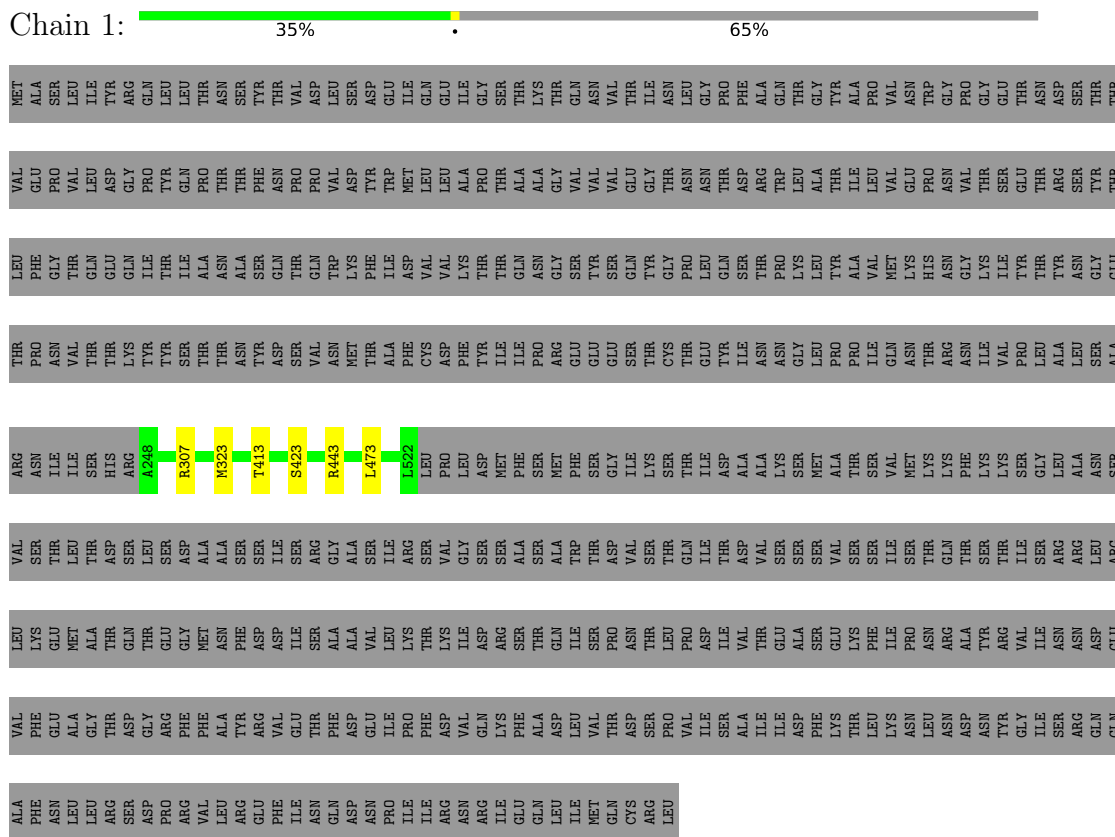
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 5 | h | 3 | Total 3 | Ca 3 | 0 |
| 5 | i | 1 | Total 1 | Ca 1 | 0 |
| 5 | j | 5 | Total 5 | Ca 5 | 0 |
| 5 | k | 3 | Total 3 | Ca 3 | 0 |
| 5 | l | 1 | Total 1 | Ca 1 | 0 |
| 5 | m | 5 | Total 5 | Ca 5 | 0 |
| 5 | n | 3 | Total 3 | Ca 3 | 0 |
| 5 | o | 1 | Total 1 | Ca 1 | 0 |
| 5 | p | 5 | Total 5 | Ca 5 | 0 |
| 5 | q | 3 | Total 3 | Ca 3 | 0 |
| 5 | r | 1 | Total 1 | Ca 1 | 0 |

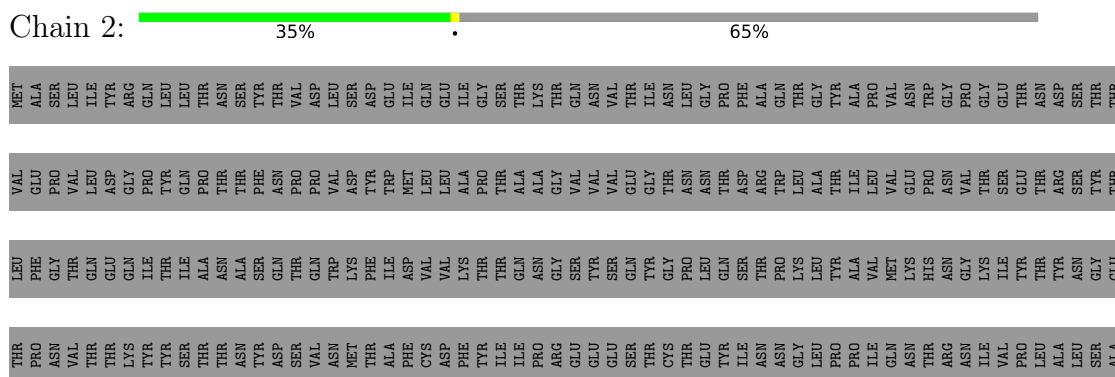
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Outer capsid protein VP4



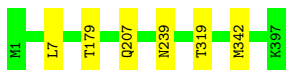
- Molecule 1: Outer capsid protein VP4





- Molecule 2: Intermediate capsid protein VP6

Chain C: 98%



- Molecule 2: Intermediate capsid protein VP6

Chain D: 99%



- Molecule 2: Intermediate capsid protein VP6

Chain E: 99%



- Molecule 2: Intermediate capsid protein VP6

Chain F: 98%



- Molecule 2: Intermediate capsid protein VP6

Chain G: 98%



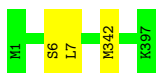
- Molecule 2: Intermediate capsid protein VP6

Chain H: 98%



- Molecule 2: Intermediate capsid protein VP6

Chain I: 99%



- Molecule 2: Intermediate capsid protein VP6

Chain J: 99%



- Molecule 2: Intermediate capsid protein VP6

Chain K: 99%



- Molecule 2: Intermediate capsid protein VP6

Chain L: 98%



- Molecule 2: Intermediate capsid protein VP6

Chain M: 99%



- Molecule 2: Intermediate capsid protein VP6

Chain N: 99%



- Molecule 2: Intermediate capsid protein VP6

Chain O: 98%



- Molecule 2: Intermediate capsid protein VP6

Chain P: 98%



- Molecule 2: Intermediate capsid protein VP6

Chain Q: 99%



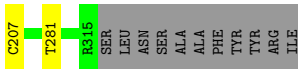
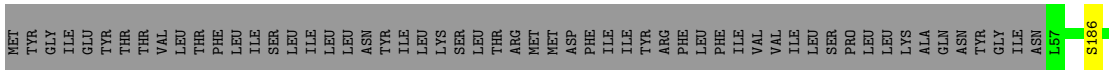
- Molecule 2: Intermediate capsid protein VP6

Chain R: 99%



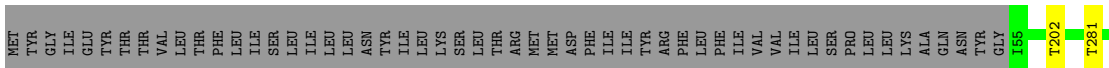
- Molecule 3: Outer capsid glycoprotein VP7

Chain a: 79%



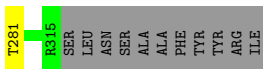
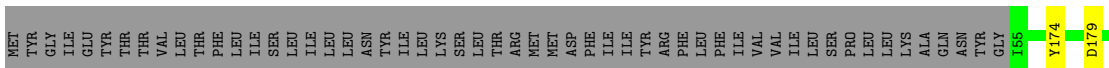
- Molecule 3: Outer capsid glycoprotein VP7

Chain b: 83%

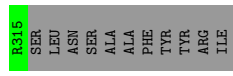
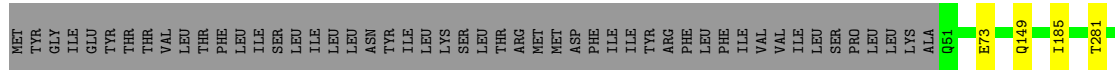
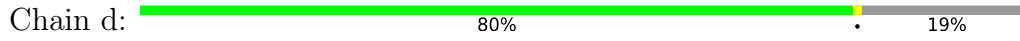


- Molecule 3: Outer capsid glycoprotein VP7

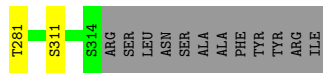
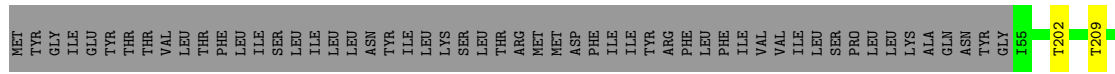
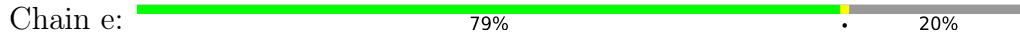
Chain c: 79%



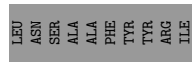
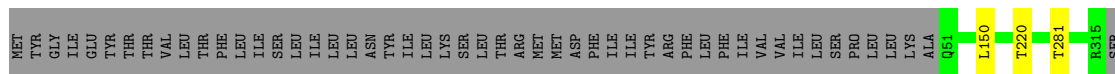
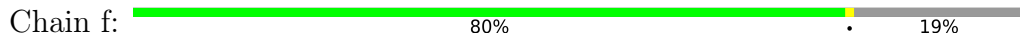
- Molecule 3: Outer capsid glycoprotein VP7



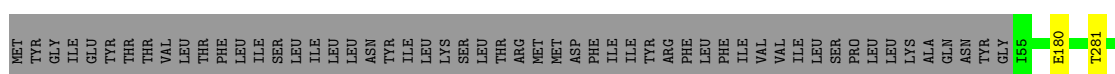
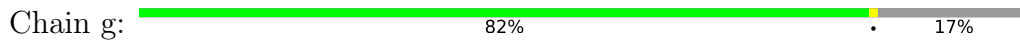
● Molecule 3: Outer capsid glycoprotein VP7



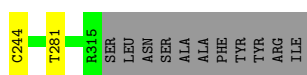
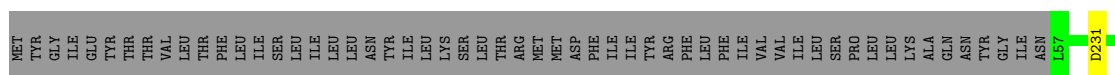
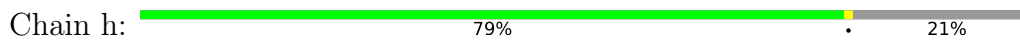
● Molecule 3: Outer capsid glycoprotein VP7




● Molecule 3: Outer capsid glycoprotein VP7

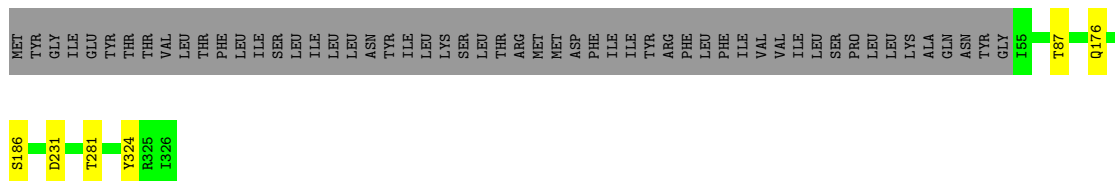


● Molecule 3: Outer capsid glycoprotein VP7




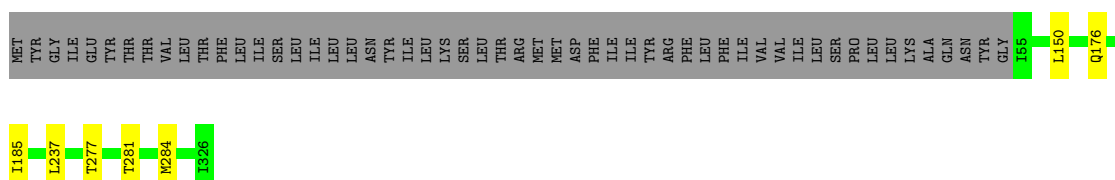
● Molecule 3: Outer capsid glycoprotein VP7

Chain i:  82% . 17%




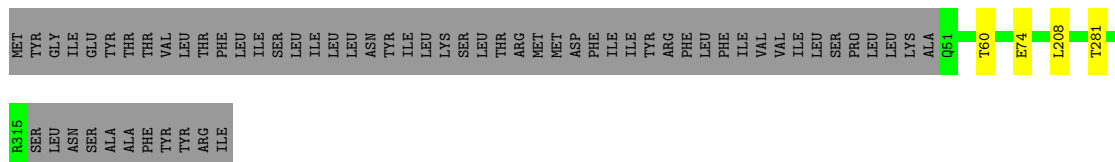
• Molecule 3: Outer capsid glycoprotein VP7

Chain j:  81% . 17%




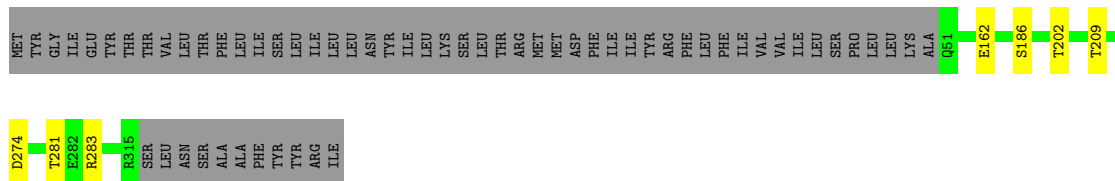
• Molecule 3: Outer capsid glycoprotein VP7

Chain k:  80% . 19%




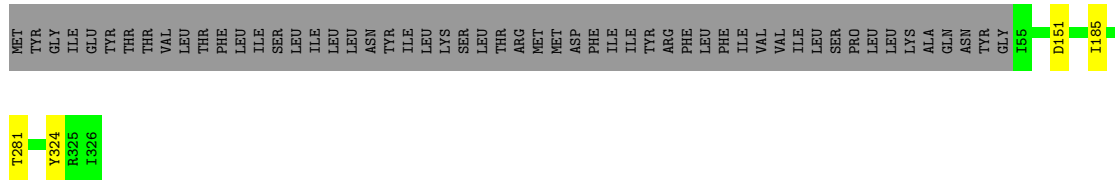
• Molecule 3: Outer capsid glycoprotein VP7

Chain l:  79% . 19%




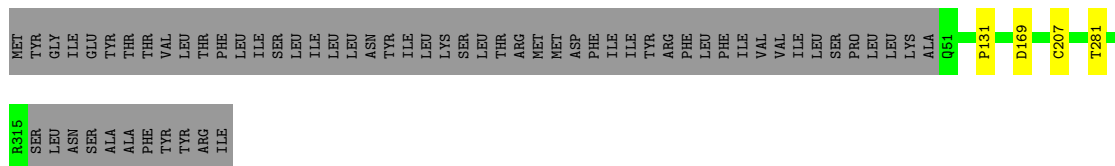
• Molecule 3: Outer capsid glycoprotein VP7

Chain m:  82% . 17%




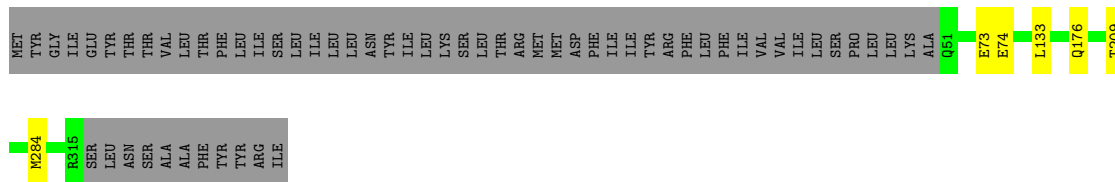
• Molecule 3: Outer capsid glycoprotein VP7

Chain n:  80% 19%




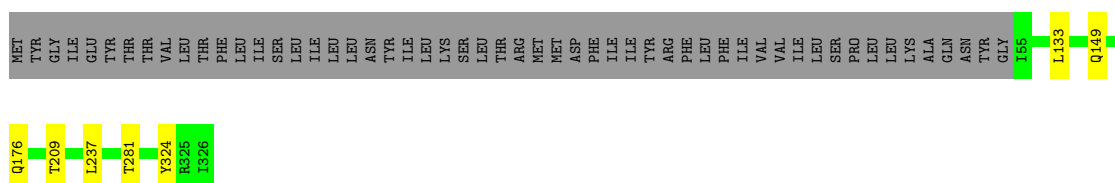
● Molecule 3: Outer capsid glycoprotein VP7

Chain o:  79% 19%




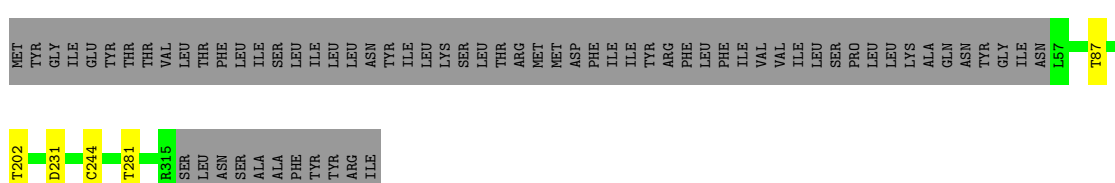
● Molecule 3: Outer capsid glycoprotein VP7

Chain p:  81% 17%




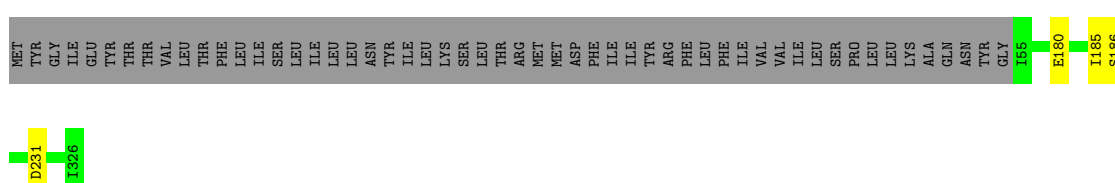
● Molecule 3: Outer capsid glycoprotein VP7

Chain q:  78% 21%



● Molecule 3: Outer capsid glycoprotein VP7

Chain r:  82% 17%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 252548 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 33 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | 40605 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 1 | 0.27 | 0/2232 | 0.57 | 0/3032 |
| 1 | 2 | 0.27 | 0/2232 | 0.57 | 0/3032 |
| 1 | 3 | 0.27 | 0/2232 | 0.56 | 0/3032 |
| 2 | A | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | B | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | C | 0.27 | 0/3233 | 0.59 | 0/4397 |
| 2 | D | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | E | 0.28 | 0/3233 | 0.59 | 1/4397 (0.0%) |
| 2 | F | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | G | 0.28 | 0/3233 | 0.60 | 1/4397 (0.0%) |
| 2 | H | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | I | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | J | 0.28 | 0/3233 | 0.58 | 0/4397 |
| 2 | K | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | L | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | M | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | N | 0.27 | 0/3233 | 0.58 | 0/4397 |
| 2 | O | 0.28 | 0/3233 | 0.59 | 1/4397 (0.0%) |
| 2 | P | 0.28 | 0/3233 | 0.59 | 0/4397 |
| 2 | Q | 0.28 | 0/3233 | 0.60 | 0/4397 |
| 2 | R | 0.27 | 0/3233 | 0.58 | 0/4397 |
| 3 | a | 0.27 | 0/2089 | 0.55 | 0/2854 |
| 3 | b | 0.26 | 0/2200 | 0.54 | 0/3005 |
| 3 | c | 0.27 | 0/2105 | 0.54 | 0/2876 |
| 3 | d | 0.27 | 0/2139 | 0.54 | 0/2922 |
| 3 | e | 0.27 | 0/2094 | 0.54 | 0/2862 |
| 3 | f | 0.27 | 0/2139 | 0.54 | 0/2922 |
| 3 | g | 0.27 | 0/2200 | 0.55 | 0/3005 |
| 3 | h | 0.26 | 0/2089 | 0.54 | 0/2854 |
| 3 | i | 0.28 | 0/2200 | 0.55 | 0/3005 |
| 3 | j | 0.27 | 0/2200 | 0.54 | 0/3005 |
| 3 | k | 0.27 | 0/2139 | 0.55 | 0/2922 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 3 | l | 0.27 | 0/2139 | 0.55 | 0/2922 |
| 3 | m | 0.27 | 0/2200 | 0.55 | 0/3005 |
| 3 | n | 0.26 | 0/2139 | 0.55 | 0/2922 |
| 3 | o | 0.27 | 0/2139 | 0.54 | 0/2922 |
| 3 | p | 0.27 | 0/2200 | 0.55 | 0/3005 |
| 3 | q | 0.26 | 0/2089 | 0.54 | 0/2854 |
| 3 | r | 0.27 | 0/2200 | 0.55 | 0/3005 |
| All | All | 0.27 | 0/103590 | 0.57 | 3/141109 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | e | 0 | 1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | E | 168 | ARG | NE-CZ-NH1 | 5.33 | 122.97 | 120.30 |
| 2 | G | 168 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 2 | O | 168 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 3 | e | 311 | SER | Peptide |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 | 1 | 273/776 (35%) | 273 (100%) | 0 | 0 | 100 | 100 |
| 1 | 2 | 273/776 (35%) | 273 (100%) | 0 | 0 | 100 | 100 |
| 1 | 3 | 273/776 (35%) | 273 (100%) | 0 | 0 | 100 | 100 |
| 2 | A | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | B | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | C | 395/397 (100%) | 393 (100%) | 2 (0%) | 0 | 100 | 100 |
| 2 | D | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | E | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | F | 395/397 (100%) | 391 (99%) | 4 (1%) | 0 | 100 | 100 |
| 2 | G | 395/397 (100%) | 393 (100%) | 2 (0%) | 0 | 100 | 100 |
| 2 | H | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | I | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | J | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | K | 395/397 (100%) | 391 (99%) | 4 (1%) | 0 | 100 | 100 |
| 2 | L | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | M | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | N | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | O | 395/397 (100%) | 393 (100%) | 2 (0%) | 0 | 100 | 100 |
| 2 | P | 395/397 (100%) | 392 (99%) | 3 (1%) | 0 | 100 | 100 |
| 2 | Q | 395/397 (100%) | 393 (100%) | 2 (0%) | 0 | 100 | 100 |
| 2 | R | 395/397 (100%) | 393 (100%) | 2 (0%) | 0 | 100 | 100 |
| 3 | a | 257/326 (79%) | 257 (100%) | 0 | 0 | 100 | 100 |
| 3 | b | 270/326 (83%) | 269 (100%) | 1 (0%) | 0 | 100 | 100 |
| 3 | c | 259/326 (79%) | 258 (100%) | 1 (0%) | 0 | 100 | 100 |
| 3 | d | 263/326 (81%) | 263 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|---------|----------|-------------|-----|
| 3 | e | 258/326 (79%) | 257 (100%) | 1 (0%) | 0 | 100 | 100 |
| 3 | f | 263/326 (81%) | 263 (100%) | 0 | 0 | 100 | 100 |
| 3 | g | 270/326 (83%) | 269 (100%) | 1 (0%) | 0 | 100 | 100 |
| 3 | h | 257/326 (79%) | 257 (100%) | 0 | 0 | 100 | 100 |
| 3 | i | 270/326 (83%) | 270 (100%) | 0 | 0 | 100 | 100 |
| 3 | j | 270/326 (83%) | 268 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | k | 263/326 (81%) | 263 (100%) | 0 | 0 | 100 | 100 |
| 3 | l | 263/326 (81%) | 263 (100%) | 0 | 0 | 100 | 100 |
| 3 | m | 270/326 (83%) | 269 (100%) | 1 (0%) | 0 | 100 | 100 |
| 3 | n | 263/326 (81%) | 263 (100%) | 0 | 0 | 100 | 100 |
| 3 | o | 263/326 (81%) | 263 (100%) | 0 | 0 | 100 | 100 |
| 3 | p | 270/326 (83%) | 270 (100%) | 0 | 0 | 100 | 100 |
| 3 | q | 257/326 (79%) | 257 (100%) | 0 | 0 | 100 | 100 |
| 3 | r | 270/326 (83%) | 269 (100%) | 1 (0%) | 0 | 100 | 100 |
| All | All | 12685/15342 (83%) | 12626 (100%) | 59 (0%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | 1 | 241/688 (35%) | 235 (98%) | 6 (2%) | 47 | 72 |
| 1 | 2 | 241/688 (35%) | 235 (98%) | 6 (2%) | 47 | 72 |
| 1 | 3 | 241/688 (35%) | 235 (98%) | 6 (2%) | 47 | 72 |
| 2 | A | 350/350 (100%) | 347 (99%) | 3 (1%) | 78 | 87 |
| 2 | B | 350/350 (100%) | 344 (98%) | 6 (2%) | 60 | 78 |
| 2 | C | 350/350 (100%) | 344 (98%) | 6 (2%) | 60 | 78 |
| 2 | D | 350/350 (100%) | 345 (99%) | 5 (1%) | 67 | 82 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | E | 350/350 (100%) | 346 (99%) | 4 (1%) | 73 | 85 |
| 2 | F | 350/350 (100%) | 343 (98%) | 7 (2%) | 55 | 76 |
| 2 | G | 350/350 (100%) | 345 (99%) | 5 (1%) | 67 | 82 |
| 2 | H | 350/350 (100%) | 343 (98%) | 7 (2%) | 55 | 76 |
| 2 | I | 350/350 (100%) | 347 (99%) | 3 (1%) | 78 | 87 |
| 2 | J | 350/350 (100%) | 346 (99%) | 4 (1%) | 73 | 85 |
| 2 | K | 350/350 (100%) | 348 (99%) | 2 (1%) | 86 | 91 |
| 2 | L | 350/350 (100%) | 343 (98%) | 7 (2%) | 55 | 76 |
| 2 | M | 350/350 (100%) | 347 (99%) | 3 (1%) | 78 | 87 |
| 2 | N | 350/350 (100%) | 347 (99%) | 3 (1%) | 78 | 87 |
| 2 | O | 350/350 (100%) | 343 (98%) | 7 (2%) | 55 | 76 |
| 2 | P | 350/350 (100%) | 344 (98%) | 6 (2%) | 60 | 78 |
| 2 | Q | 350/350 (100%) | 347 (99%) | 3 (1%) | 78 | 87 |
| 2 | R | 350/350 (100%) | 347 (99%) | 3 (1%) | 78 | 87 |
| 3 | a | 233/295 (79%) | 230 (99%) | 3 (1%) | 69 | 82 |
| 3 | b | 244/295 (83%) | 241 (99%) | 3 (1%) | 71 | 83 |
| 3 | c | 235/295 (80%) | 232 (99%) | 3 (1%) | 69 | 82 |
| 3 | d | 238/295 (81%) | 234 (98%) | 4 (2%) | 60 | 78 |
| 3 | e | 234/295 (79%) | 231 (99%) | 3 (1%) | 69 | 82 |
| 3 | f | 238/295 (81%) | 235 (99%) | 3 (1%) | 69 | 82 |
| 3 | g | 244/295 (83%) | 240 (98%) | 4 (2%) | 62 | 79 |
| 3 | h | 233/295 (79%) | 230 (99%) | 3 (1%) | 69 | 82 |
| 3 | i | 244/295 (83%) | 238 (98%) | 6 (2%) | 47 | 72 |
| 3 | j | 244/295 (83%) | 237 (97%) | 7 (3%) | 42 | 69 |
| 3 | k | 238/295 (81%) | 234 (98%) | 4 (2%) | 60 | 78 |
| 3 | l | 238/295 (81%) | 231 (97%) | 7 (3%) | 42 | 69 |
| 3 | m | 244/295 (83%) | 240 (98%) | 4 (2%) | 62 | 79 |
| 3 | n | 238/295 (81%) | 234 (98%) | 4 (2%) | 60 | 78 |
| 3 | o | 238/295 (81%) | 232 (98%) | 6 (2%) | 47 | 72 |
| 3 | p | 244/295 (83%) | 237 (97%) | 7 (3%) | 42 | 69 |
| 3 | q | 233/295 (79%) | 228 (98%) | 5 (2%) | 53 | 75 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 3 | r | 244/295 (83%) | 240 (98%) | 4 (2%) | 62 | 79 |
| All | All | 11327/13674 (83%) | 11145 (98%) | 182 (2%) | 64 | 79 |

All (182) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 307 | ARG |
| 1 | 1 | 323 | MET |
| 1 | 1 | 413 | THR |
| 1 | 1 | 423 | SER |
| 1 | 1 | 443 | ARG |
| 1 | 1 | 473 | LEU |
| 1 | 2 | 307 | ARG |
| 1 | 2 | 312 | VAL |
| 1 | 2 | 335 | THR |
| 1 | 2 | 349 | SER |
| 1 | 2 | 423 | SER |
| 1 | 2 | 477 | ASN |
| 1 | 3 | 270 | ASP |
| 1 | 3 | 323 | MET |
| 1 | 3 | 413 | THR |
| 1 | 3 | 423 | SER |
| 1 | 3 | 473 | LEU |
| 1 | 3 | 477 | ASN |
| 2 | A | 186 | SER |
| 2 | A | 238 | ILE |
| 2 | A | 342 | MET |
| 2 | B | 7 | LEU |
| 2 | B | 231 | ARG |
| 2 | B | 264 | LEU |
| 2 | B | 301 | THR |
| 2 | B | 312 | GLN |
| 2 | B | 342 | MET |
| 2 | C | 7 | LEU |
| 2 | C | 179 | THR |
| 2 | C | 207 | GLN |
| 2 | C | 239 | ASN |
| 2 | C | 319 | THR |
| 2 | C | 342 | MET |
| 2 | D | 74 | ASP |
| 2 | D | 179 | THR |
| 2 | D | 207 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | D | 319 | THR |
| 2 | D | 342 | MET |
| 2 | E | 301 | THR |
| 2 | E | 319 | THR |
| 2 | E | 337 | ASP |
| 2 | E | 342 | MET |
| 2 | F | 7 | LEU |
| 2 | F | 86 | ASP |
| 2 | F | 131 | ASN |
| 2 | F | 238 | ILE |
| 2 | F | 255 | ARG |
| 2 | F | 312 | GLN |
| 2 | F | 342 | MET |
| 2 | G | 7 | LEU |
| 2 | G | 69 | THR |
| 2 | G | 234 | PHE |
| 2 | G | 272 | THR |
| 2 | G | 342 | MET |
| 2 | H | 6 | SER |
| 2 | H | 7 | LEU |
| 2 | H | 234 | PHE |
| 2 | H | 239 | ASN |
| 2 | H | 264 | LEU |
| 2 | H | 272 | THR |
| 2 | H | 342 | MET |
| 2 | I | 6 | SER |
| 2 | I | 7 | LEU |
| 2 | I | 342 | MET |
| 2 | J | 7 | LEU |
| 2 | J | 207 | GLN |
| 2 | J | 239 | ASN |
| 2 | J | 337 | ASP |
| 2 | K | 7 | LEU |
| 2 | K | 264 | LEU |
| 2 | L | 62 | ASP |
| 2 | L | 182 | LEU |
| 2 | L | 207 | GLN |
| 2 | L | 234 | PHE |
| 2 | L | 264 | LEU |
| 2 | L | 315 | GLU |
| 2 | L | 319 | THR |
| 2 | M | 7 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | M | 238 | ILE |
| 2 | M | 239 | ASN |
| 2 | N | 7 | LEU |
| 2 | N | 238 | ILE |
| 2 | N | 264 | LEU |
| 2 | O | 69 | THR |
| 2 | O | 90 | ASP |
| 2 | O | 186 | SER |
| 2 | O | 207 | GLN |
| 2 | O | 234 | PHE |
| 2 | O | 239 | ASN |
| 2 | O | 342 | MET |
| 2 | P | 234 | PHE |
| 2 | P | 264 | LEU |
| 2 | P | 272 | THR |
| 2 | P | 315 | GLU |
| 2 | P | 337 | ASP |
| 2 | P | 370 | LEU |
| 2 | Q | 207 | GLN |
| 2 | Q | 239 | ASN |
| 2 | Q | 301 | THR |
| 2 | R | 7 | LEU |
| 2 | R | 264 | LEU |
| 2 | R | 286 | ASP |
| 3 | a | 186 | SER |
| 3 | a | 207 | CYS |
| 3 | a | 281 | THR |
| 3 | b | 202 | THR |
| 3 | b | 281 | THR |
| 3 | b | 284 | MET |
| 3 | c | 174 | TYR |
| 3 | c | 179 | ASP |
| 3 | c | 281 | THR |
| 3 | d | 73 | GLU |
| 3 | d | 149 | GLN |
| 3 | d | 185 | ILE |
| 3 | d | 281 | THR |
| 3 | e | 202 | THR |
| 3 | e | 209 | THR |
| 3 | e | 281 | THR |
| 3 | f | 150 | LEU |
| 3 | f | 220 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | f | 281 | THR |
| 3 | g | 180 | GLU |
| 3 | g | 281 | THR |
| 3 | g | 318 | ASN |
| 3 | g | 324 | TYR |
| 3 | h | 231 | ASP |
| 3 | h | 244 | CYS |
| 3 | h | 281 | THR |
| 3 | i | 87 | THR |
| 3 | i | 176 | GLN |
| 3 | i | 186 | SER |
| 3 | i | 231 | ASP |
| 3 | i | 281 | THR |
| 3 | i | 324 | TYR |
| 3 | j | 150 | LEU |
| 3 | j | 176 | GLN |
| 3 | j | 185 | ILE |
| 3 | j | 237 | LEU |
| 3 | j | 277 | THR |
| 3 | j | 281 | THR |
| 3 | j | 284 | MET |
| 3 | k | 60 | THR |
| 3 | k | 74 | GLU |
| 3 | k | 208 | LEU |
| 3 | k | 281 | THR |
| 3 | l | 162 | GLU |
| 3 | l | 186 | SER |
| 3 | l | 202 | THR |
| 3 | l | 209 | THR |
| 3 | l | 274 | ASP |
| 3 | l | 281 | THR |
| 3 | l | 283 | ARG |
| 3 | m | 151 | ASP |
| 3 | m | 185 | ILE |
| 3 | m | 281 | THR |
| 3 | m | 324 | TYR |
| 3 | n | 131 | PRO |
| 3 | n | 169 | ASP |
| 3 | n | 207 | CYS |
| 3 | n | 281 | THR |
| 3 | o | 73 | GLU |
| 3 | o | 74 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | o | 133 | LEU |
| 3 | o | 176 | GLN |
| 3 | o | 209 | THR |
| 3 | o | 284 | MET |
| 3 | p | 133 | LEU |
| 3 | p | 149 | GLN |
| 3 | p | 176 | GLN |
| 3 | p | 209 | THR |
| 3 | p | 237 | LEU |
| 3 | p | 281 | THR |
| 3 | p | 324 | TYR |
| 3 | q | 87 | THR |
| 3 | q | 202 | THR |
| 3 | q | 231 | ASP |
| 3 | q | 244 | CYS |
| 3 | q | 281 | THR |
| 3 | r | 180 | GLU |
| 3 | r | 185 | ILE |
| 3 | r | 186 | SER |
| 3 | r | 231 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 345 | ASN |
| 2 | A | 383 | GLN |
| 2 | B | 383 | GLN |
| 2 | D | 383 | GLN |
| 2 | E | 383 | GLN |
| 2 | F | 383 | GLN |
| 2 | G | 383 | GLN |
| 2 | H | 383 | GLN |
| 2 | Q | 257 | ASN |
| 2 | Q | 293 | GLN |
| 2 | Q | 383 | GLN |
| 3 | c | 305 | GLN |
| 3 | d | 149 | GLN |
| 3 | d | 176 | GLN |
| 3 | d | 234 | ASN |
| 3 | f | 149 | GLN |
| 3 | g | 132 | GLN |
| 3 | g | 149 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | g | 176 | GLN |
| 3 | g | 234 | ASN |
| 3 | h | 149 | GLN |
| 3 | h | 182 | ASN |
| 3 | h | 248 | ASN |
| 3 | j | 132 | GLN |
| 3 | j | 248 | ASN |
| 3 | j | 305 | GLN |
| 3 | k | 305 | GLN |
| 3 | l | 248 | ASN |
| 3 | n | 288 | ASN |
| 3 | n | 305 | GLN |
| 3 | r | 182 | ASN |
| 3 | r | 248 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 54 are monoatomic - leaving 18 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAG | g | 401 | 3 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.44 | 0 |
| 4 | NAG | b | 401 | - | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.48 | 0 |
| 4 | NAG | h | 401 | 3 | 14,14,15 | 0.59 | 1 (7%) | 17,19,21 | 0.72 | 1 (5%) |
| 4 | NAG | d | 401 | 3 | 14,14,15 | 0.39 | 0 | 17,19,21 | 0.38 | 0 |
| 4 | NAG | m | 401 | 3 | 14,14,15 | 0.57 | 0 | 17,19,21 | 0.71 | 1 (5%) |
| 4 | NAG | k | 401 | 3 | 14,14,15 | 0.60 | 1 (7%) | 17,19,21 | 0.79 | 1 (5%) |
| 4 | NAG | p | 401 | 3 | 14,14,15 | 0.51 | 0 | 17,19,21 | 0.74 | 1 (5%) |
| 4 | NAG | o | 401 | 3 | 14,14,15 | 0.49 | 0 | 17,19,21 | 0.45 | 0 |
| 4 | NAG | a | 401 | 3 | 14,14,15 | 0.63 | 1 (7%) | 17,19,21 | 0.76 | 1 (5%) |
| 4 | NAG | f | 401 | 3 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.43 | 0 |
| 4 | NAG | q | 401 | 3 | 14,14,15 | 0.43 | 0 | 17,19,21 | 0.70 | 1 (5%) |
| 4 | NAG | j | 401 | 3 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.36 | 0 |
| 4 | NAG | l | 401 | 3 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.45 | 0 |
| 4 | NAG | r | 401 | 3 | 14,14,15 | 0.60 | 1 (7%) | 17,19,21 | 0.76 | 1 (5%) |
| 4 | NAG | n | 401 | 3 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.34 | 0 |
| 4 | NAG | i | 401 | 3 | 14,14,15 | 0.60 | 1 (7%) | 17,19,21 | 0.72 | 1 (5%) |
| 4 | NAG | e | 401 | 3 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.56 | 0 |
| 4 | NAG | c | 401 | 3 | 14,14,15 | 0.58 | 0 | 17,19,21 | 0.70 | 1 (5%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4 | NAG | g | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | b | 401 | - | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | h | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | d | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | m | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | k | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | p | 401 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | o | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | a | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | f | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | q | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | j | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | l | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | r | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | n | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4 | NAG | i | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | e | 401 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | c | 401 | 3 | - | 2/6/23/26 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4 | a | 401 | NAG | C1-C2 | 2.11 | 1.55 | 1.52 |
| 4 | r | 401 | NAG | C1-C2 | 2.03 | 1.55 | 1.52 |
| 4 | h | 401 | NAG | C1-C2 | 2.02 | 1.55 | 1.52 |
| 4 | k | 401 | NAG | C1-C2 | 2.02 | 1.55 | 1.52 |
| 4 | i | 401 | NAG | C1-C2 | 2.00 | 1.55 | 1.52 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 4 | k | 401 | NAG | C1-O5-C5 | 2.84 | 116.04 | 112.19 |
| 4 | r | 401 | NAG | C1-O5-C5 | 2.72 | 115.88 | 112.19 |
| 4 | a | 401 | NAG | C1-O5-C5 | 2.69 | 115.83 | 112.19 |
| 4 | p | 401 | NAG | C1-O5-C5 | 2.58 | 115.68 | 112.19 |
| 4 | i | 401 | NAG | C1-O5-C5 | 2.55 | 115.65 | 112.19 |
| 4 | h | 401 | NAG | C1-O5-C5 | 2.54 | 115.64 | 112.19 |
| 4 | m | 401 | NAG | C1-O5-C5 | 2.50 | 115.58 | 112.19 |
| 4 | c | 401 | NAG | C1-O5-C5 | 2.43 | 115.48 | 112.19 |
| 4 | q | 401 | NAG | C1-O5-C5 | 2.38 | 115.41 | 112.19 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 4 | c | 401 | NAG | C4-C5-C6-O6 |
| 4 | c | 401 | NAG | O5-C5-C6-O6 |
| 4 | p | 401 | NAG | O5-C5-C6-O6 |
| 4 | p | 401 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

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

This section contains visualisations of the EMDB entry EMD-21957. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.