The only well defined metal-ion sites are those mediating subunit contacts between Asp 138 and Asp 141 of one subunit and O 199, O 260, O 259 and $O_{\delta 1}$ Asn 259 of the other. This means that two charges are provided by one subunit and a third by the terminal carboxyl of the other. Temperature factors for the Ca^{2+} atoms are 27·2, 16·6 and 20·9 $Å^2$ at the *A–B*, *B–C* and *C–A* interface, respectively.

The electron density inside the viral capsid is in general very low and discontinuous. A continuous region of low density can be observed at the internal surface near the quasi-threefold axis. It is close to a series of basic residues (Lys 195, Arg 196, Arg 249 of all three subunits). This density could be interpreted as an RNA strand of at least six nucleotides, but these were not included in the present model.

This is the first time that the structure of a complete virus has been refined by a reciprocal-space method. The explicit use of non-crystallographic symmetry in reciprocal and direct space made possible this process, which considerably simplifies the refinement of large macromolecular assemblies. Nevertheless, the procedure used here taxed the limits of the computing power of the Cyber 205. Further improvements as indicated above would be to use FFT techniques throughout for the calculations of structure factors and their derivatives. However, the most demanding part of the process is the recurring visual inspection of the model in the graphics system. This is caused by the intrinsic weakness in the least-squares method which cannot surmount local minima. A possible solution would be the systematic exploration of different local minima by rotating side chains and peptide bonds while checking contacts and normal stereochemistry.

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