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 O₈ of 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 Ca²⁺ atoms are 27-2, 16-6 and 20-9 Å² 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 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 electron density indicates above would be to use FFT techniques through 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.

We thank Ignacio Fita for help in the implementation of the Konnert–Hendrickson least-squares program, and Wayne Hendrickson for discussions relating to the identification of water molecules in the solvent. We have enjoyed discussions with Lars Liljas and Alwyn Jones as to the best refinement procedures throughout the progress of this work. We are grateful to Sharon Wilder for assistance in the preparation of this manuscript. The work was supported by the National Science Foundation and the National Institutes of Health.

References


International Union of Crystallography


Acta Crystallographica Indexes

The indexes to Volume 39 (1983) of Acta Crystallographica have just been distributed to subscribers. The International Union of Crystallography regrets the delay in publishing these indexes, which is due to the introduction of a computerized index-production system. The system will be used to produce the next five-year index to Volumes 39-43. The indexes to Volume 40 (1984) are expected to be distributed on time.

A ten-year compilation of the indexes for Volumes 29-38 (1973-1982) was distributed to subscribers in mid-1984. Further copies are available at a price of Dkr 150 (Dkr 75 for scientists who give an undertaking that the index is for their own personal use).