

NEWS

US human spacefaring questioned

Review panel takes a hard look at NASA's goal of returning astronauts to the Moon.

When it comes to how NASA should spend its money putting people in space, just about everyone has an opinion — some of them strident. But at the moment, the opinions that matter most are those in a ten-person committee that listened quietly as key players pleaded their case at a meeting on 17 June in Washington DC.

Led by retired Lockheed Martin chief executive Norman Augustine, the committee has been tasked by President Barack Obama to review the United States' plans for humans in space. It includes a mix of aerospace executives, astronauts, engineers, a retired general and two scientists: Christopher Chyba, a planetary scientist at Princeton University in New Jersey, and Earth scientist Charles Kennel, chair of the National Academies' Space Studies Board.

The meeting — its first public hearing — showcased the dire budget constraints the agency faces as it struggles to replace the space shuttle, which will be retired by 2010, with rockets that could return astronauts to the Moon. The hearing also made plain the



Panel chair Norman Augustine.

number of people who feel that NASA's existing designs aren't the best way to do it.

Several groups presented alternatives to the committee and said they could be completed faster and more cheaply than the Ares rockets in NASA's planned Moon programme, called Constellation (see graphic). Michael Gass, chief executive of United Launch Alliance in Littleton, Colorado, told the panel that his company's Delta IV cargo rocket could be modified

to carry a crew capsule. Stephen Metschan, representing a group that claims to include NASA engineers working in their spare time, presented designs for a system called Direct, based on existing shuttle hardware.

Steve Cook, Ares project manager at Marshall Space Flight Center in Huntsville, Alabama, says such proposals may reflect lingering bitterness over lost contracts. In 2005, a NASA study selected what became the Constellation system as the best method for getting astronauts past low-Earth orbit and back to the Moon. "When decisions are made, somebody wins and somebody loses," Cook says. "Those that didn't win don't like that."

Budget stretch

Getting beyond low-Earth orbit may be too much of a stretch for NASA's budget, however, regardless of which rocket is used to do so. Cook says that the agency has already spent US\$10 billion of the \$35 billion needed to complete the *Orion* crew capsule and the Ares I rocket, which together could fly astronauts to

P. E. ALERS/NASA/GETTY IMAGES

New protein structures replace the old

Protein structures are getting regular makeovers with the help of 're-refinement' software developed by Dutch structural biologists.

The Protein Data Bank (PDB) holds nearly 53,000 three-dimensional structures of protein molecules and nucleic acids that have mainly been deciphered through X-ray crystallography. Most journals, including *Nature*, require such data to be deposited in the PDB if a paper with a protein structure is to be published.

But some structures are not as accurate as they could be. The data bank began in 1971, and the ability to analyse crystallographic data has improved dramatically since then.

"There are definitely errors in the PDB," says crystallographer Nenad Ban at the Swiss Federal Institute of Technology Zurich.

This has consequences for scientists who want to use the

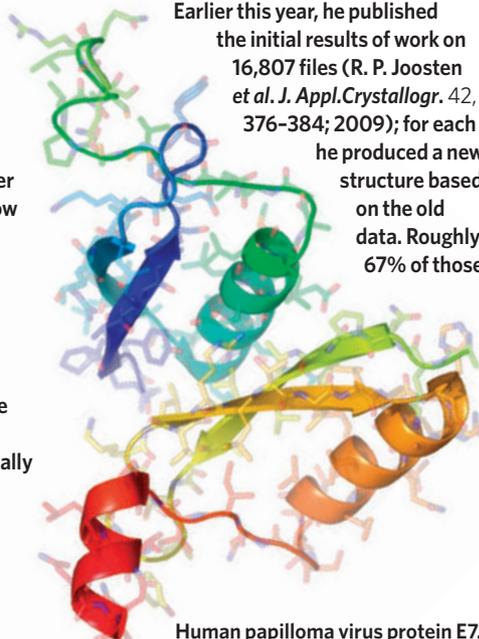
PDB to look for sites on proteins to target with small-molecule drugs, or to feed the data into molecular dynamics simulations. More profoundly, a wrong structure in the data bank could also trigger wrong ideas about how the protein works.

To help, Gert Vriend at Radboud University Medical Centre in Nijmegen, the Netherlands, and his colleagues are writing software that they hope will eventually automatically re-refine, at the click of a mouse, all the data deposited in the PDB.

So far, Vriend has

gone through 38,000 data files with his PDB_REDO program.

Earlier this year, he published the initial results of work on 16,807 files (R. P. Joosten *et al. J. Appl. Crystallogr.* 42, 376–384; 2009); for each he produced a new structure based on the old data. Roughly 67% of those



Human papilloma virus protein E7.

new structures were better than the original structure as measured by a quantity known as *R*-free, used by crystallographers to determine structure quality.

The automated program could also decipher other problems caused by human error: data deposited with the wrong labels, for example, in which intensity of a signal is labelled as amplitude. "If the intensity and amplitude are swapped, the structure doesn't make sense," says collaborator Robbie Joosten.

Vriend runs his program on all new entries in the PDB every two weeks and sends the PDB a monthly report flagging problems. Administrators can correct small problems like names of labels being swapped; bigger problems are added to an ongoing list of things to fix.

Maintenance for the PDB

LAGUNA DESIGN/SPL



APOLLOPLUS40 ON TWITTER
 Nature News relives the Apollo 11 Moon mission.
<http://twitter.com/apolloplus40>

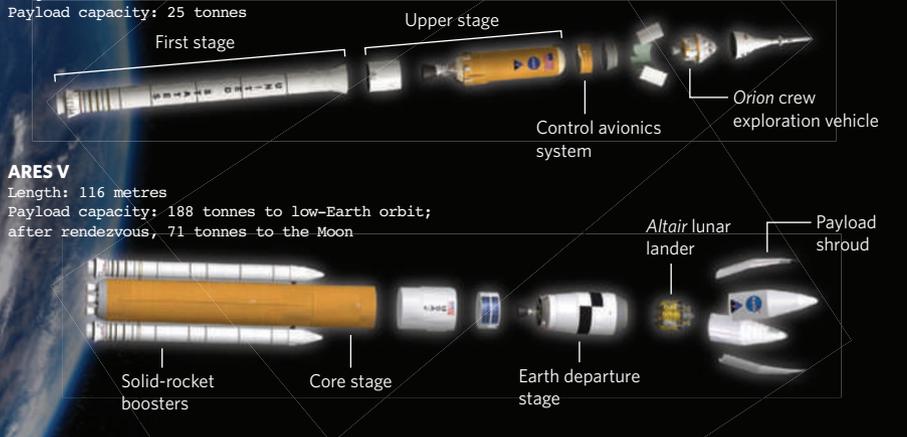
NASA/JPL/USGS

ROCKETS TO RETURN TO THE MOON

NASA's Constellation system, under development, includes the Ares I rocket to bring astronauts to low-Earth orbit and the Ares V, which would rendezvous and carry the crew the rest of the way to the Moon in the mated Orion crew exploration vehicle and Altair lunar lander.

ARES I

Length: 99 metres
 Payload capacity: 25 tonnes



ARES V

Length: 116 metres
 Payload capacity: 188 tonnes to low-Earth orbit; after rendezvous, 71 tonnes to the Moon

as the Planetary Society in Pasadena, California, have lobbied for other destinations, such as near-Earth asteroids, as intermediate steps to the human exploration of Mars. Furthermore, some astronomers believe that astronauts — and the beefier rockets that are needed to carry them beyond low-Earth orbit — will be instrumental in launching large space telescopes, or building and repairing them in space.

Florida Senator Bill Nelson (Democrat), one of NASA's powerful patrons in Congress, told the committee that Obama would probably heed their advice. "You come to the table with extraordinary influence," he says. Nelson, an advocate for increased NASA funding, exhorted them to find the most meaningful programme goals, even if that meant ignoring the budget constraints given to them.

Although the committee members spent most of the day listening rather than talking, Augustine says his group will not be bashful in its report if it finds that NASA can't do much worthwhile within its budget. "Just because something's cheap doesn't mean it's worth doing," he says.

The committee's report is due in August. Former astronaut Charles Bolden, who has been nominated as the next NASA chief, would implement any changes that result from it. ■
Eric Hand

the International Space Station, by 2015. He estimates it will cost \$100 billion to complete the Ares V, which would pick up astronauts in orbit and carry them to the Moon, by 2020.

The committee will examine not only the means of spaceflight but also its ends. Augustine says his team will "look at the full spectrum of possible destinations" other than the

Moon. It has also been asked to evaluate using the space station after 2015.

Augustine says he has received lots of correspondence from scientist friends and acknowledges that many of them feel that putting astronauts on the space station and the Moon isn't all that useful scientifically. But others disagree, he says. Advocacy groups such

is spread over three sites: the Research Collaboratory for Structural Bioinformatics based at Rutgers University in Piscataway, New Jersey; the European Bioinformatics Institute (EBI), in Hinxton, UK; and the Japan Science and Technology Agency in Tokyo.

Helen Berman of Rutgers, who runs the US part of the PDB, says that the data bank welcomes efforts to improve deposited data. "This is exactly the vision we had when we started," she says. Staff at the data bank run a standard set of quality checks before depositing a structure and flag any problems to the researcher who submitted it, but "we're not the data police". The data bank doesn't reject an entry

even if its advice on improving a structure is ignored.

Vriend occasionally contacts the scientists who deposited data that he has refined, with mixed reactions. "Sometimes people are very grateful, and sometimes they are insulted," he says.

Occasionally, the program can cause researchers to change interpretations of their data. Annalisa Pastore, a molecular biologist at the National Institute for Medical Research, London, UK, recalls asking Vriend to validate a protein structure she had worked out from her nuclear magnetic resonance (NMR) data. Vriend

told her she had got it wrong, and she took a closer look. It turned out that she wasn't wrong, but that she had uncovered a histidine residue that was unusually buried within

the protein. "Gert correctly focused our attention to this residue," she says. "In the end we could definitely say the structure

was right."

Pastore says researchers might be more careful about submitting their structures to the data bank if they think re-refinement software might be checking up on it.

Vriend is not the only one looking at data-bank quality. At the Lawrence Berkeley National Laboratory in California, computational biologist Paul Adams is testing the PHENIX crystallography software he develops on PDB data before sharing the software with other academics or licensing it to companies. "We [want to] make

sure the software we are giving to people can do the right thing," he says. Adams doesn't make his results public, but says he has noticed that his software often improves an original structure assignment.

Vriend hopes his re-refinement software will eventually be linked to the PDB so that a user could click through from the data bank to obtain the most up-to-date protein structure. Gerard Kleywegt, who took over the European PDB operations at the EBI last month, says that this will probably be implemented at some point.

Even so, the software is not sophisticated enough to automatically fix problems that are more than cosmetic, Kleywegt says. More serious problems, such as amino-acid side chains that have been assigned to the wrong location, require manual intervention.

"I see this as a first step," he says. ■
 Katharine Sanderson

"Sometimes people are very grateful, and sometimes they are insulted."

Pandemic virus update

ASIA: Australia and the Philippines both report deaths of people infected with the novel H1N1 virus — the first in the Asia-Pacific region.

IRAN: reports its first swine-flu case, a 16-year-old boy visiting from the United States.

CDC