This example shows how the "frc" module can be used to compute the potential energy of a charge or a group of charges placed in the electrostatic field of a molecule. This can be used to compute the electrostatic component of the interaction energy of molecules.

How to run:
Check that you have the following files before running:
barstar.pqr frc.in param.txt

To run it, type:
<path>/delphi param_protein.prm > protein.log
Press enter key, you should get the results.

Output files: frc.out (contains information about the)
*Note: <path> is the full path where the delphi executable is located.

Details of the run:
This is a new feature in Delphi which extends the uility of the FRC module. By supplying the input FRC in PQR format, the user provides the location of certain charges whose potential energy in the field of the "source" molecule is to be computed. E.g. The potential energy of charge 'q_2', placed at some 3D point 'r' in the field of a molecule of charge 'q_1' is given by q_2*phi(due to q_1 at r). By using FRC in PQR format, you get exactly this number.

'barstar.pqr' is the source molecule written in PQR format.
'frc.in' is a PQR format file indicating the positions of the charges (Column 55-62).

NOTE: TO USE PQR FORMAT FRC INPUT, THE SOURCE FILE SHOULD ALSO BE PROVIDED IN PQR FORMAT. IF PDB FORMAT IS USED ONSTEAD (INCONJUNCTION WITH CRG AND SIZ FILES), FRC AS PQR OPTION WILL FAIL. ALSO BY USING PQR FORMAT FOR BOTH, SOURCE AND FRC, ONE BYPASSES THE USE OF CRG/SIZ FILES ALTOGETHER.

NOTE: THOUGH FRC INPUT AS A PQR FILE ALSO CONTAINS RADIUS, IT IS NOT USED AT ALL. ONLY THE RADIUS VALUES IN THE SOURCE MOLECULE'S PQR FILE IS NECESSARY.

After the run, 'frc.out' file is produced which contains the following information:

ATOM	DESCRIPTOR		CHARGE	GRID PT.	GRID FIELDS: (Ex,	Ey,	Ez)
N	ASP	39	-0.5163	3.9613	0.1819	-0.2827	-0.1480
CA	ASP	39	0.0381	4.4289	0.1610	-0.3904	-0.3397
C	ASP	39	0.5366	4.2541	0.3588	-0.3546	-0.2997
O	ASP	39	-0.5819	4.6631	0.5404	-0.3084	-0.3554
CB	ASP	39	-0.0303	4.4390	0.0066	-0.4222	-0.4936
CG	ASP	39	0.7994	5.9174	0.3548	-0.5789	-1.2382
OD1	ASP	39	-0.8014	7.3401	0.2780	0.4640	1.4681
OD2	ASP	39	-0.8014	6.0159	1.3547	-1.2546	-0.7645
H	ASP	39	0.2936	3.7884	0.1675	-0.2661	-0.0450
HA	ASP	39	0.0880	4.9010	0.1473	-0.5017	-0.4157
HB3	ASP	39	-0.0122	3.9842	0.1063	-0.5456	-0.2646
HB2	ASP	39	-0.0122	4.1149	-0.3134	-0.2029	-0.3474

total energy = -3.48505 kt

The 'total energy' indicates the electrostatic potential energy of the group of charges presented in the 'frc.in' file. One can see that for each charge in the input FRC file, there is a corresponding value of grid potential ('GRID PT.') and electric field vector (GRID FIELDS: (Ex, Ey, Ez)). The 'total energy' is computed by multiplying a charge with the grid-potential and summing all the products.