

WP9 Use case: From cells to molecules - integrating structural data









1. Do you currently do any shape fitting?

		Response Percent	Response Count
Yes		80.0%	36
No, but would do if a web-service was available		13.3%	6
No, tools are not mature enough		0.0%	0
No, not enough data available		0.0%	0
No, I don't need it		4.4%	2
No – other reason		2.2%	1
	Comment		3
answered question			45
skipped question			0

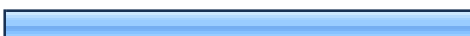






2. If you answered "No" above, please describe what you would be looking for/need in terms of tools, data, web services or other resources.

	Response Count
	5
answered question	5
skipped question	40


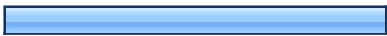












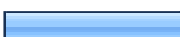



3. What type(s) of shapes do you use?

		Response Percent	Response Count
Volume		80.5%	33
Sub-volume		53.7%	22
Atomic models		82.9%	34
Course-grained models		22.0%	9
Geometric shapes – cube, ellipsoid, drawn by hand, based on feature in volume		14.6%	6
Other (please specify)		9.8%	4
answered question			41
skipped question			4






4. What type(s) of volume data do you fit into?

		Response Percent	Response Count
EM single particle		75.6%	31
EM 2D crystals		4.9%	2
EM Helices		12.2%	5
ET Tomogram		24.4%	10
ET Sub tomogram averages		26.8%	11
SAXS		29.3%	12
SXT		0.0%	0
Other (please specify)		9.8%	4
answered question			41
skipped question			4



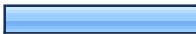



5. Which software are you using for shape matching (select all that you use)? Please note: while this is a long list, we have no doubt forgotten several software packages - please enter any that are missing below in the comments field.

		Response Percent	Response Count
Amira		2.6%	1
Chimera		61.5%	24
CoAn/BBHP		0.0%	0
DireX		5.1%	2
DockEM		7.7%	3
EMAN - foldhunter/helixhunter		12.8%	5
EMFIT		12.8%	5
Flex-EM		5.1%	2
Fold-EM		2.6%	1
MDFP (NAMD/VMD)		23.1%	9
MODELLER		7.7%	3
Mod-EM		2.6%	1
MOLREP		15.4%	6
NMFF		5.1%	2
NORMA		5.1%	2
Situs - CoLoRes/qplasty		28.2%	11
3SOM		2.6%	1
Veda/Urox		12.8%	5
Yup.scx		0.0%	0
Other (please specify)		46.2%	18
answered question			39
skipped question			6


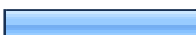

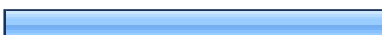

6. Do you use a GUI or a command line script? Do you follow a documented or published protocol, or do you use an in-house protocol?

		Response Percent	Response Count
Use GUI		68.3%	28
Use command line script		65.9%	27
Follow documented or published protocol		31.7%	13
Follow in-house protocol		31.7%	13
No, each case is different		24.4%	10
	Comment		2
answered question			41
skipped question			4




7. What, if any, meta data does the software need (select all that apply)?

		Response Percent	Response Count
Resolution		66.7%	24
Density level representing surface (contour level)		38.9%	14
Density level above background scattering and/or masks		30.6%	11
Symmetry		61.1%	22
Grid sampling		55.6%	20
Other (please specify)		19.4%	7
answered question			36
skipped question			9




8. Any options/feature that is particularly useful with the software that you use?

		Response Percent	Response Count
Ease of use		61.1%	22
Features available - please use comment field		30.6%	11
Scriptable		44.4%	16
Availability		61.1%	22
Developed in-house		22.2%	8
	Comment		8
answered question			36
skipped question			9





9. What type of matching do you do (select all that apply)?

		Response Percent	Response Count
Manual fit		56.1%	23
Rigid body		90.2%	37
Flexible		58.5%	24
	Comment		2
answered question			41
skipped question			4








10. If your volume data have symmetry elements, such as in viruses, chaperons, helices etc., how do you handle the symmetry (select all that apply)?

		Response Percent	Response Count
Ignore symmetry		29.0%	9
Fit into each symmetry position		54.8%	17
Only fit into one symmetry position		51.6%	16
	Comment		11
		answered question	31
		skipped question	14

11. How do you evaluate the results (select all that apply)?

		Response Percent	Response Count
Visual inspection		80.0%	32
Cross correlation score		72.5%	29
Atom inclusion score		22.5%	9
Special scoring function different from matching/fitting function		25.0%	10
	Comment		1
		answered question	40
		skipped question	5

12. What is your role?

		Response Percent	Response Count
Principal investigator		54.5%	24
Staff scientist		18.2%	8
Postdoc		11.4%	5
Graduate student		15.9%	7
Undergraduate student		2.3%	1
Industry		0.0%	0
Government		2.3%	1
Management		0.0%	0
Other (please specify)		4.5%	2
		answered question	44
		skipped question	1