

R-free sets chosen by SFTOOLS

PDB-ID	Resoln. (Å)	N mol. / A.U.	Random R-free set		'Shellular' R-free set	
			R (%)	R-free (%)	R (%)	R-free (%)
4p9g	2.2	1	17.1	21.3	17.0	20.1
5pep	2.3	1	18.2	24.0	18.2	26.4
1aw5	2.3	1	18.6	23.1	18.6	24.8
2ccm	1.8	2	16.9	21.9	16.9	21.8
5l9a	1.5	2	12.7	18.1	12.4	17.4
1ids	2.0	4 (222)	13.7	18.8	13.7	18.0
5lc1	2.3	6	14.8	18.9	14.8	19.4
5lzl	3.5	12 (incl. 422)	15.3	22.4	15.0	21.9
2wqt	2.8	20 (532)	20.1	24.3	20.0	23.7

R-free sets chosen by SHELXPRO

PDB-ID	Resoln. (Å)	N mol. / A.U.	Random R-free set		'Shellular' R-free set	
			R (%)	R-free (%)	R (%)	R-free (%)
4p9g	2.2	1	17.2	19.6	17.2	21.7
5pep	2.3	1	18.4	24.5	18.3	24.9
1aw5	2.3	1	18.7	23.4	18.5	22.9
2ccm	1.8	2	16.9	21.2	17.0	22.4
5l9a	1.5	2	12.6	18.4	12.8	19.2
1ids	2.0	4 (222)	13.7	18.2	13.7	18.2
5lc1	2.3	6	14.9	19.4	15.0	20.9
5lzl	3.5	12 (incl. 422)	15.1	22.8	15.1	21.9
2wqt	2.8	20 (532)	20.1	23.7	20.0	23.0

R-free sets chosen by PHENIX

PDB-ID	Resoln. (Å)	N mol. / A.U.	Random R-free set		'Shellular' R-free set	
			R (%)	R-free (%)	R (%)	R-free (%)
4p9g	2.2	1	17.0	21.8	17.1	21.2
5pep	2.3	1	18.2	23.0	18.5	23.7
1aw5	2.3	1	18.6	22.9	18.8	24.3
2ccm	1.8	2	16.9	21.0	16.8	21.9
5l9a	1.5	2	12.5	18.2	12.2	17.0
1ids	2.0	4 (222)	13.7	17.7	13.7	19.1
5lc1	2.3	6	14.9	20.1	14.8	18.6
5lzl	3.5	12 (incl. 422)	15.1	22.1	14.8	21.9
2wqt	2.8	20 (532)	20.2	24.4	20.2	23.6