

Acta Crystallographica Section D

Volume 70 (2014)

Supporting information for article:

**Flexible torsion angle non-crystallographic symmetry restraints
for improved macromolecular structure refinement**

**Jeffrey J. Headd, Nathaniel Echols, Pavel V. Afonine, Nigel W. Moriarty,
Richard J. Gildea and Paul D. Adams**

Table S1 Moderate Resolution MR Test Set

PDB ID	Resolution	# NCS copies	MR search model PDB ID
1c03	2.30	4	1c02
1ck4	2.20	2	1pt6
1fvj	2.06	2	1dsb
1g83	2.60	2	3uf4
1j2f	2.30	2	3a77
1jbb	2.00	2	2gmi
1ng5	2.00	2	1qwz
1o65	2.33	3	1o67
1pcv	2.30	2	2i0w
1pk5	2.40	2	1zh7
1s5v	2.35	2	3i7q
1xiz	2.00	2	3lf6
1yz1	2.00	4	3ebm
2azo	2.30	2	1azo
2c24	2.27	2	1wmx
2c4p	2.35	2	2yho
2ckg	2.45	2	2xph
2d2z	2.20	3	2ahe
2dps	2.40	2	2cxa
2f6b	2.80	2	1qh6
2fxk	2.54	2	1yd9
2o9f	2.55	2	1rc2
2qw4	2.80	4	1yje
2qxt	2.00	2	1t4m
2vj5	3.00	2	2vix
2vpi	2.40	2	2vx0
2vs6	2.40	2	2jdl
2wqx	2.03	2	2uzx
2x16	2.13	2	2vei
2xee	2.10	4	2xeh
2z16	2.02	2	3md2
2z1i	2.00	2	2z1g
2z8m	2.00	2	2q8y
2ztz	2.00	2	3zye
3amh	2.09	2	3amn
3asg	2.33	2	3as4

3cw0	2.40	4	3efp
3esv	2.00	2	3et9
3gaq	2.25	2	1qft
3gqm	2.10	2	3eir
3hwi	2.29	2	3aay
3im5	2.55	2	3im6
3jwi	2.20	2	3jwg
3k9k	2.55	2	3k9j
3ks4	2.40	2	3l2a
3l2z	2.80	2	2cgh
3l56	2.30	2	3cw4
3ncx	2.60	2	2zqk
3nfh	2.17	2	3nfi
3o9r	2.00	2	3l4q
3omw	2.87	4	3p9y
3p2i	2.40	2	3pb3
3pxj	2.30	4	2yd1
3qyd	2.97	3	3i2x
3t7j	2.04	2	3t7i
3tgz	2.30	2	3p90

Table S2 1.0Å-4.1Å Re-refinement Test Set

PDB ID	Resolution	# NCS Copies
1mn8	1.00	4
3m9j	1.10	2
3d95	1.20	2
1kmt	1.30	2
2ohw	1.40	2
3w3e	1.50	2
4j7w	1.60	2
4dov	1.70	2
4guz	1.80	4
3v3s	1.90	2
4ilj	2.00	2
4gkf	2.10	2
4lq8	2.20	2
4h43	2.30	2
4hu4	2.40	2
4lla	2.50	3
4hl0	2.00	2
4kw3	2.70	2
4ey0	2.80	4
4i6p	2.90	2
4hfy	3.00	2
2etc	3.10	2
2vr9	3.20	3
2etn	3.30	3
3p0l	3.40	4
2xi1	3.50	2
3s0x	3.60	2
2y22	3.70	6
2bbz	3.80	4
1z9x	3.93	3
3bbw	4.00	2
1xdv	4.10	2

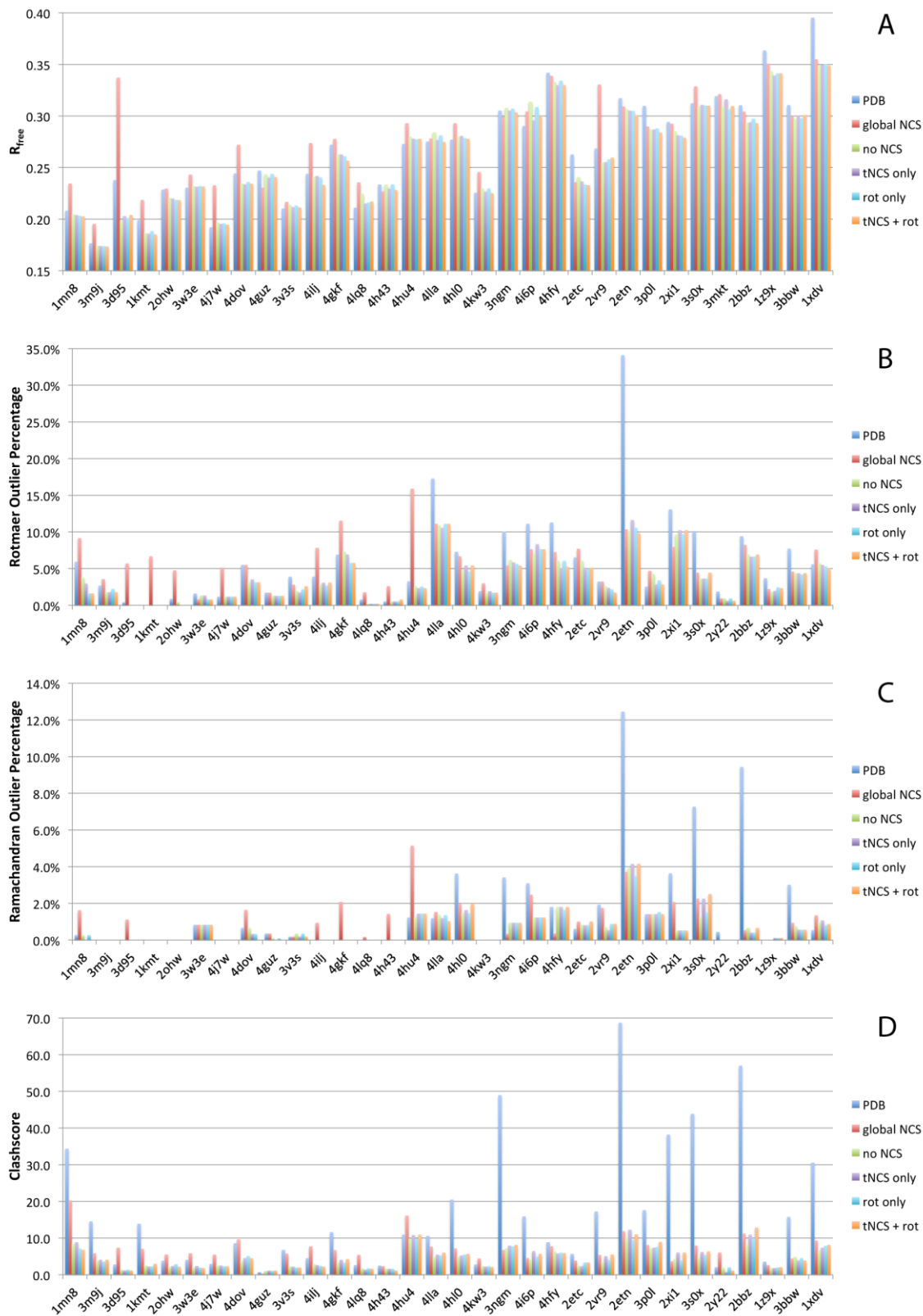


Figure S1 Summary of results of re-refinement tests for deposited PDB structures ranging from 1.0-4.1 Å resolution. For each metric, the value for the deposited PDB model is given in blue, followed by refinement using global NCS (red), no NCS (green), torsion NCS only (purple), NCS-related rotamer correction (light blue), and torsion NCS plus NCS-related rotamer correction (orange). Results are presented from left to right, highest (1.0 Å) to lowest (4.1 Å) resolution. A) R_{free} values. B) Rotamer outlier percentage. C) Ramachandran outlier percentage. D) Clashscore.