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Errata to “DiffFit: Visually-Guided Differentiable Fitting of Molecule Structures to a Cryo-EM Map”

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Errata to “DiffFit: Visually-Guided Differentiable Fitting of Molecule Structures to a Cryo-EM Map” by Deng Luo, Zainab Alsuwaykit, Dawar Khan, Ondřej Strnad, Tobias Isenberg, Ivan Viola (Digital Object Identifier no. 10.1109/TVCG.2024.3456404)

The authors would like to make the following errata after correcting the initialization related bugs in the associated program.

On page 1, the last two sentences of Fig. 1’s caption should be “Right: the final composited structure overlaid on the original target volume (RMSD: 0.138). The involved computation takes 10 seconds in total, and the human-in-the-loop interaction takes ≈ 3 minutes.” On page 5, “10-element array” should be “3-element array.” On page 10, in the ACKNOWLEDGMENTS section, the authors add: “The authors also thank Alexandra Irgler for her narration in the submission video.” The authors also make changes to Fig. 3 (c–f), Fig. 4, Table 1–3, which are attached below, and an updated attachment “ExpRes.xlsx” in the supplementary materials.

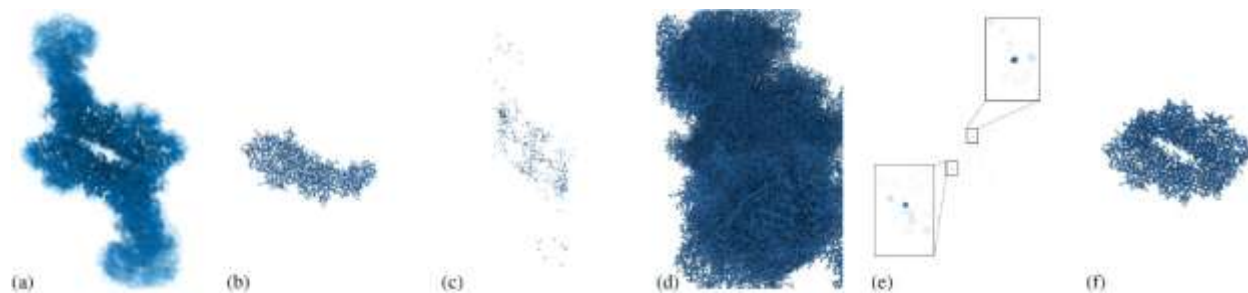


Fig. 3: Clustering and filtering: (a) target volume, (b) atom coordinates of the source structure, (c) positions of 1000 fit results (the dots are clustered, hiding the number of results), (d) 1000 instances of the structure, (e) positions of 1000 fit results with a transparency level set based on an exponential scaling of the sum of sampled density metric (two clusters stand out, as in the zoom-in insets), and (f) instances of the structure at those two clusters.

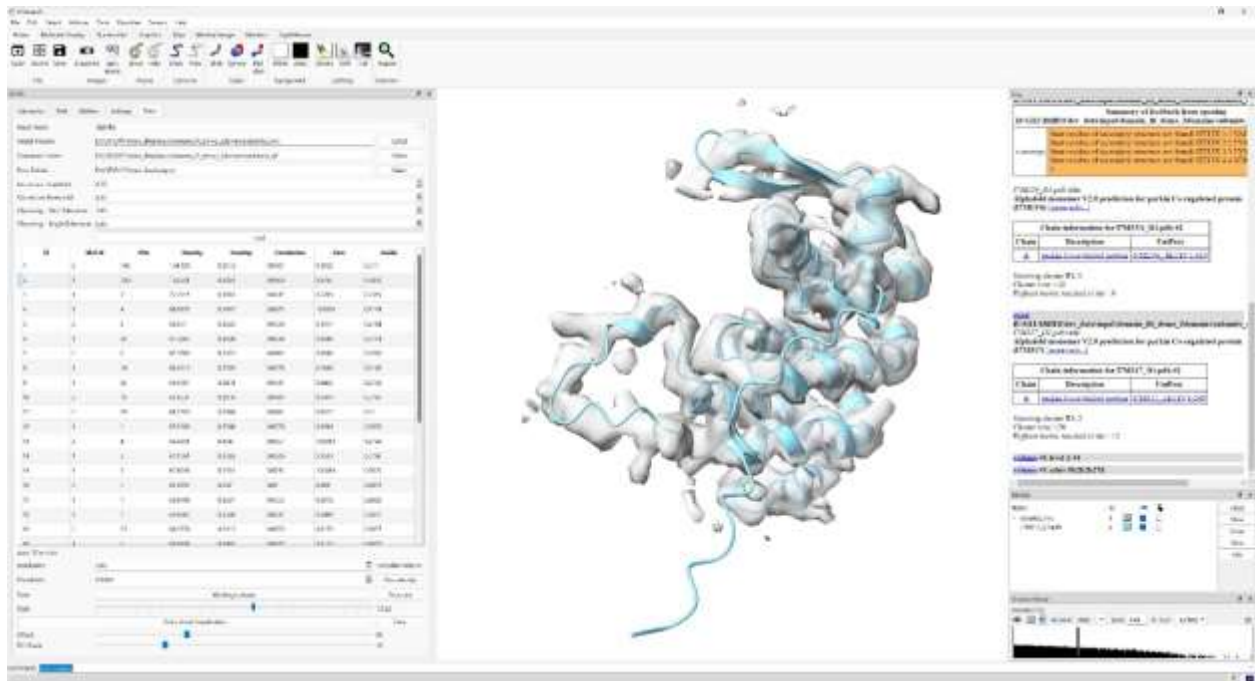


Fig. 4: Visual browser based on ChimeraX. The target volume on the middle is overlaid with a fitted molecule corresponding to the selected fit result in the table on the left (clustered fits, each row is the representative placement with the highest correlation from that cluster). After inspection, users can save the placement and then select “Simulate volume” and “Zero density” to zero out the corresponding voxels from the target volume.

Table 1

PDB	Res	Hit rate			Computing time			RMSD (Å)			
		C	D	G	C	D	G	M	C	D	DC
6WTI	2.38	0.0	136.8	n/a	150.3	3.8	39.7	1.310	n/a	0.942	0.037
7D8X	2.60	0.0	202.0	n/a	196.0	5.2	37.6	1.960	n/a	0.984	0.014
7SP8	2.70	4.6	188	40.9	130.6	2.6	50.5	1.290	0.996	0.969	0.025
7STE	2.73	14.0	110.4	7.9	806.1	12.1	66.6	1.740	0.062	0.662	0.058
7JPO	3.20	5.4	191.8	35.5	250.7	6.7	37.2	2.540	0.017	0.922	0.015
7PM9	3.60	44.0	195.4	4.4	352.4	4.1	86.7	1.640	0.030	0.907	0.024
6M5U	3.80	0.0	105.0	n/a	162.2	4.1	39.2	2.360	n/a	0.912	0.018
6MEO	3.90	7.4	116.0	15.7	128.2	3.2	40.1	1.940	0.489	0.786	0.488
7MGE	3.94	4.8	123.6	25.8	337.6	4.3	78.1	1.870	0.017	0.819	0.017
High-avg		8.9	152.1	21.7	279.3	5.1	52.8	1.850	0.268	0.878	0.077
5NL2	6.60	1.8	163.2	90.7	94.6	2.0	48.0	2.440	0.093	1.124	0.056
7K2V	6.60	49.0	165.6	3.4	240.6	4.1	58.2	25.290	0.338	1.323	0.338
7CA5	7.60	55.8	72.4	1.3	322.6	2.9	110.0	3.290	2.042	1.207	2.042
5VH9	7.70	68.6	158.0	2.3	1147.8	14.1	81.3	0.960	0.085	0.991	0.085
6AR6	9.00	78.0	182.6	2.3	74.9	1.5	49.3	2.200	0.123	2.617	0.117
3J1Z	13.00	138.6	172.2	1.2	64.4	2.0	33.0	32.330	0.396	2.612	0.388
Med-avg		65.3	152.3	16.9	324.1	4.4	63.3	11.085	0.513	1.646	0.504
All-avg		31.5	152.2	19.8	297.3	4.9	57.0	5.544	0.366	1.185	0.248

Table 2

Structure	C Hit	D Hit	Gain
17MLV6_D3	108	254	2.4×
17M317_D1	127	240	1.9×

Table 3

PDB	EMDB	#S	#A	Res	Vs	L	Hit rate			Computing time			RMSD (Å)			
							C	D	G	C	D	G	M	C	D	DC
6WTI	21897	4	9,980	2.38	1.08	0.7660	0.0	136.8	n/a	150.3	3.8	39.7	1.310	n/a	0.942	0.037
7D8X	30614	4	10,928	2.60	1.08	0.0229	0.0	202.0	n/a	196.0	5.2	37.6	1.960	n/a	0.984	0.014
7SP8	25368	3	6,090	2.70	1.08	5.5755	4.6	188	40.9	130.6	2.6	50.5	1.290	0.996	0.969	0.025
7STE	25426	5	14,249	2.73	0.83	0.0963	14.0	110.4	7.9	806.1	12.1	66.6	1.740	0.062	0.662	0.058
7JPO	22417	5	16,087	3.20	1.07	0.0240	5.4	191.8	35.5	250.7	6.7	37.2	2.540	0.017	0.922	0.015
7PM9	13508	3	10,169	3.60	1.10	0.0068	44.0	195.4	4.4	352.4	4.1	86.7	1.640	0.030	0.907	0.024
6M5U	30093	3	10,549	3.80	1.06	0.0350	0.0	105.0	n/a	162.2	4.1	39.2	2.360	n/a	0.912	0.018
6MEO	9108	3	7,465	3.90	1.06	0.0500	7.4	116.0	15.7	128.2	3.2	40.1	1.940	0.489	0.786	0.488
7MGE	23827	4	9,010	3.94	0.94	0.2550	4.8	123.6	25.8	337.6	4.3	78.1	1.870	0.017	0.819	0.017
High-avg		3.78	10,503	3.21	1.03	n/a	8.9	152.1	21.7	279.3	5.1	52.8	1.850	0.268	0.878	0.077
5NL2	3658	2	4,312	6.60	1.35	0.0297	1.8	163.2	90.7	94.6	2.0	48.0	2.440	0.093	1.124	0.056
7K2V	22647	2	5,717	6.60	1.05	0.0050	49.0	165.6	3.4	240.6	4.1	58.2	25.290	0.338	1.323	0.338
7CA5	30324	2	6,484	7.60	1.06	0.0100	55.8	72.4	1.3	322.6	2.9	110.0	3.290	2.042	1.207	2.042
5VH9	8673	2	22,042	7.70	1.20	0.0074	68.6	158.0	2.3	1147.8	14.1	81.3	0.960	0.085	0.991	0.085
6AR6	8898	2	2,395	9.00	3.00	0.0739	78.0	182.6	2.3	74.9	1.5	49.3	2.200	0.123	2.617	0.117
3J1Z	5450	2	4,586	13.00	2.74	3.8989	138.6	172.2	1.2	64.4	2.0	33.0	32.330	0.396	2.612	0.388
Med-avg		2.00	7,589	8.42	1.73	n/a	65.3	152.3	16.9	324.1	4.4	63.3	11.085	0.513	1.646	0.504
All-avg		3.01	9,337	5.29	1.31	n/a	31.5	152.2	19.8	297.3	4.9	57.0	5.544	0.366	1.185	0.248