Overall statement for reviews a total of 8 TRPV1 maps:

101, 115, 133, 135, 146, 156, 161, 163

1) FSC curves for all maps were calculated by using the same spherical mask (by Jean-Paul Armache). Ranking of all maps based on FSC indicated resolution is as follows:

* 5 of 8 (101,115, 133, 135, 161) maps have similar resolution estimated from FSC curve, which also have reasonable shapes. Note that the mask includes all un-structured density contributed by amphipols, so that the nominal resolution is lower.

* Map 156 has the highest nominal resolution based on FSC = 0.143 criterion, as well as FSC = 0.5 criterion, 3.3Å/3.4Å. However, the shape of the FSC is very strange. The map is also very noisy, although mostly correct. There is a sign of over-refinement of some kind. Not clear what was the cause of the map.

* Map 146 has a normal FSC curve, but significantly different from others FSC curves. The map is also extremely noisy, and almost un-interpretable. Either over-sharpened or over-refined.

* It is apparently that some provided masks used for calculating FSC are too tight, beyond reasonable (115, 161, for example), which may boost the nominal resolution.

2) All maps and atomic models are fitted using “Fit in map” option in Chimera and evaluated by EMRinger. EMRinger does not judge map quality per se, but it evaluates how well is side chain fitted to the map. Therefore, it provides an indirect evaluation of the map quality. The ranking of EMRinger fitting was listed in the Table.

3) Using our most recent atomic model as a starting point, we did a round of refinement in Phenix. Again, this is not a good way to evaluate map, however, the MolProbity score matches reasonably well with the visual inspection of the map, aside from map 146.

4) All maps were visually evaluated by 4 persons separately and independently. The evaluation comments from individuals are included. Overall, there is a consensus about the ranking:

161 best

115 good
101

133
135 Used super-resolution pixel. The map looks over-smooth, but otherwise normal if binned by 2.

163 not impressive. Outer helices (S3) are smooth without side chains.

156

146 uninterpretable/over-refined

Conclusion:

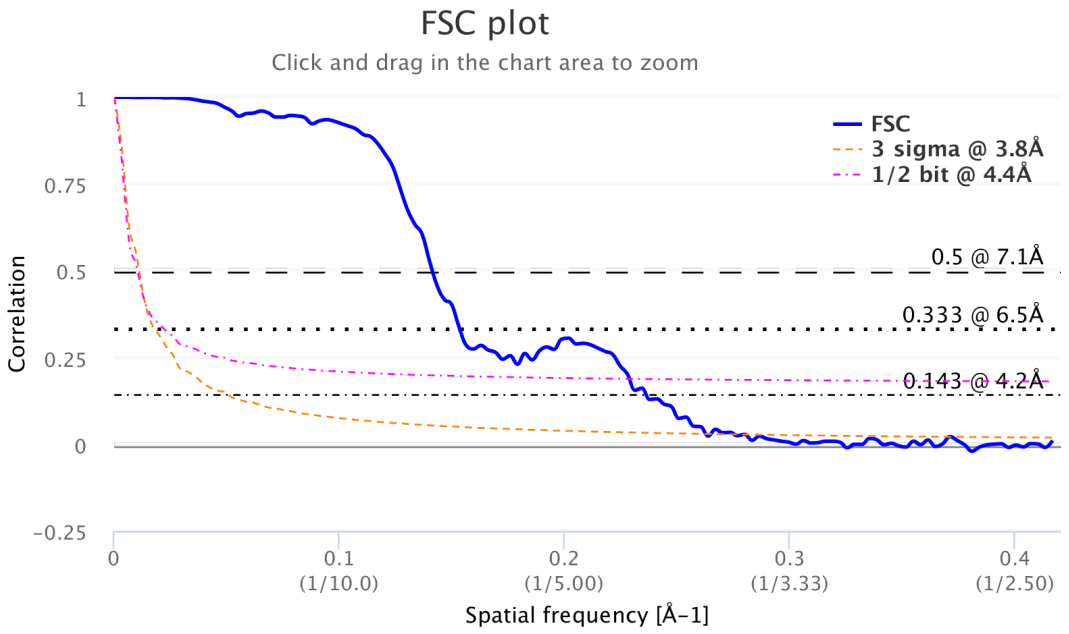
FSC curve alone cannot judge map quality. EMRing and Phenix refinement all provide useful information about the map quality. The best judge, unfortunately, is still visual inspection of the maps.

EMRinger

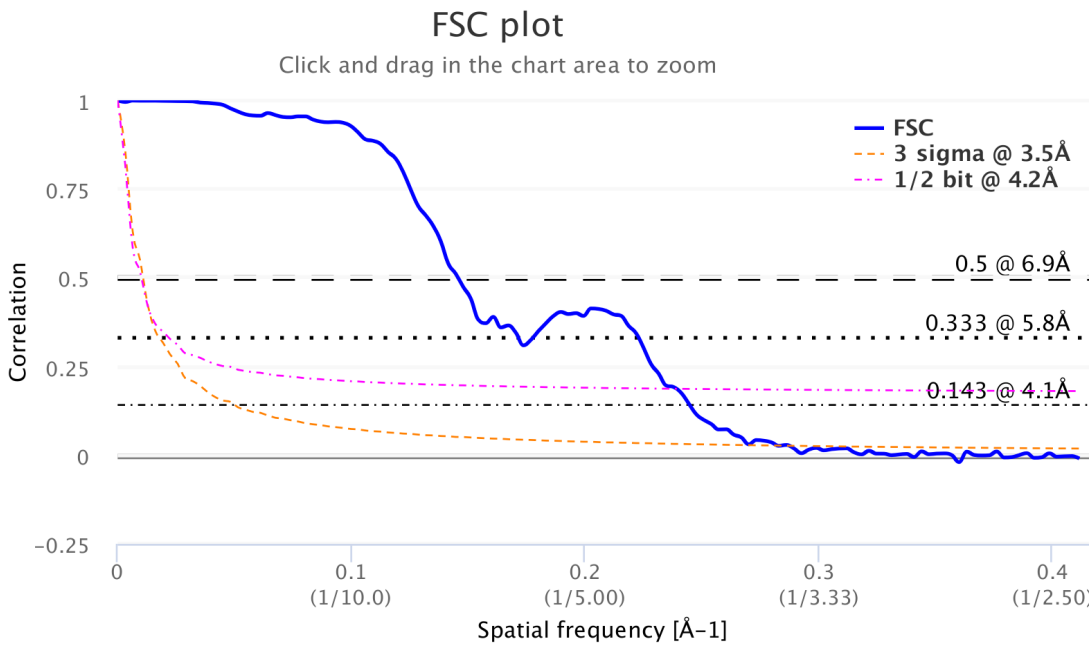
	(Higher is better)	(Higher is better)	(Lower is better)	
Entry number	**EMRinger (unfilt)**	**EMRinger (filt)**	**Subjective rank**	**Comment**
101	2.02	2.58	3	Good S2-S3 linker, very poor lipids
115	3.5	3.92	1	Good bound and weakly bound lipids
133	0.22	0.22	5/6	Overly smooth density, unfiltered map looks filtered
135	0	0.65	5/6	Perceptually identical to map 133
146	0.43	0.43	8	Extremely overrefined, map is uninterpretable
156	2.37	2.37	7	Extremely noisy, but the structure is correct
161	3.65	4.03	2	S2-S3 linker absent, lipid weak, 'spikey' density
163	1.9	2.29	4	Acceptable, strangely masked out amphipol

FSCs : applied spherical mask to half-maps using e2proc3d with a radius = box/2 and plotted using FSC validation server (http://www.ebi.ac.uk/pdbe/emdb/validation/fsc/)

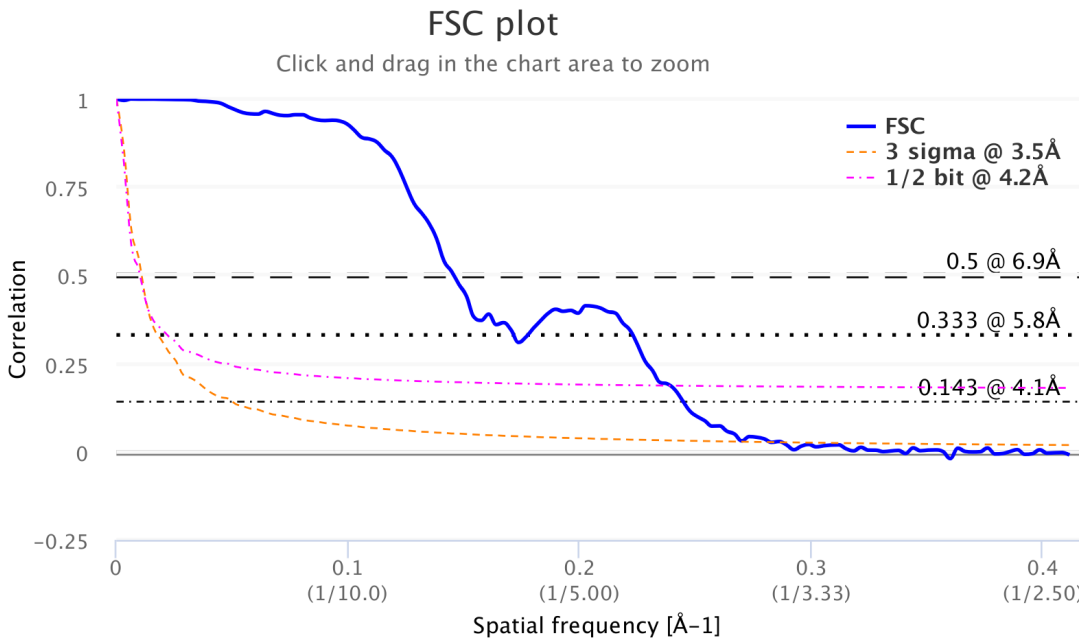
101 (box 256, pix 1.2)



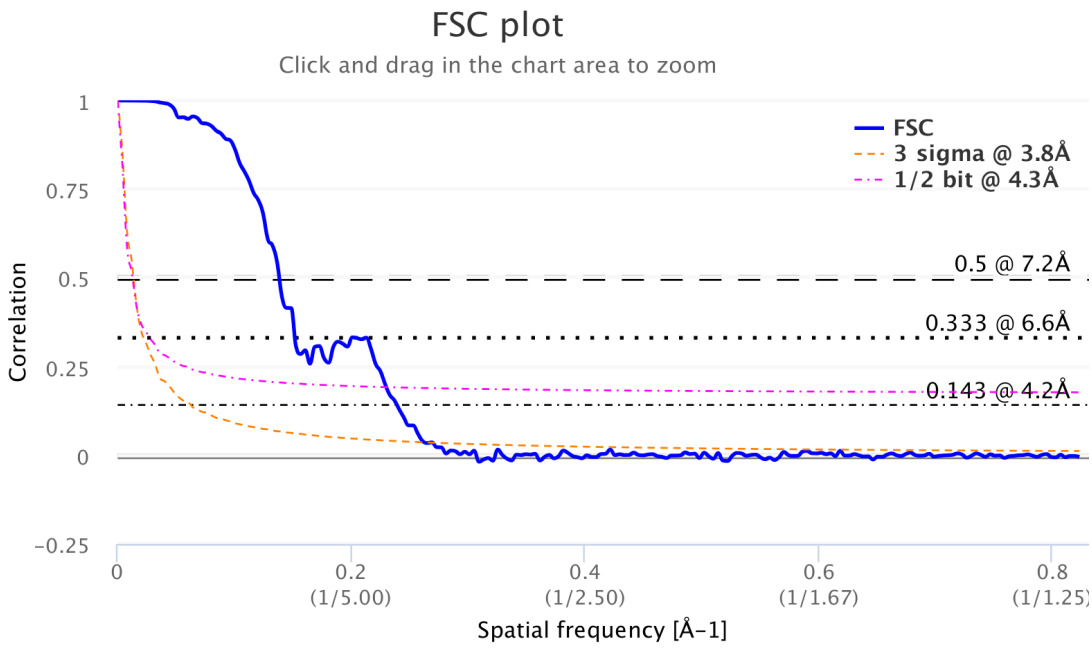
115 (box 256, pix 1.2156)



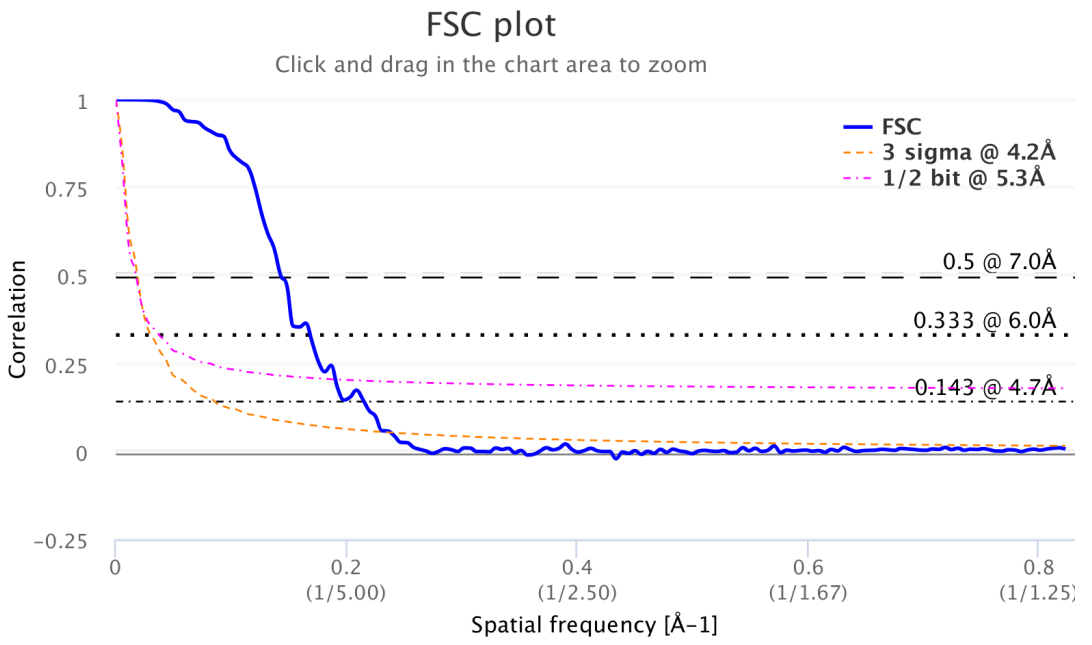
133 (box 410, pix 0.6078)



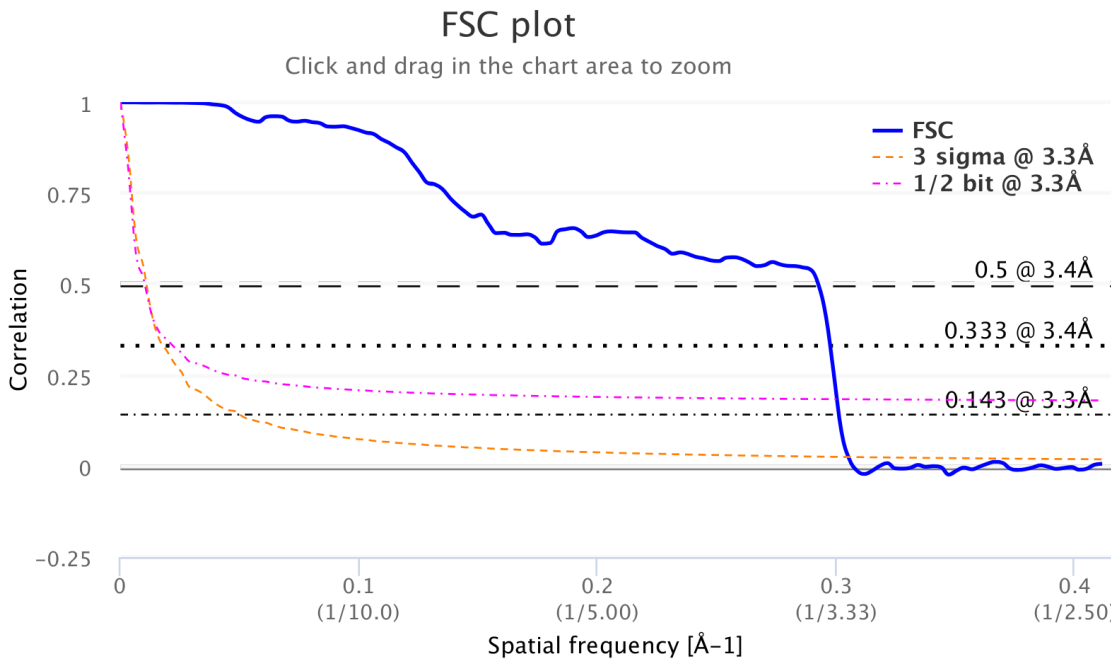
135 (box 410, pix 0.6078)



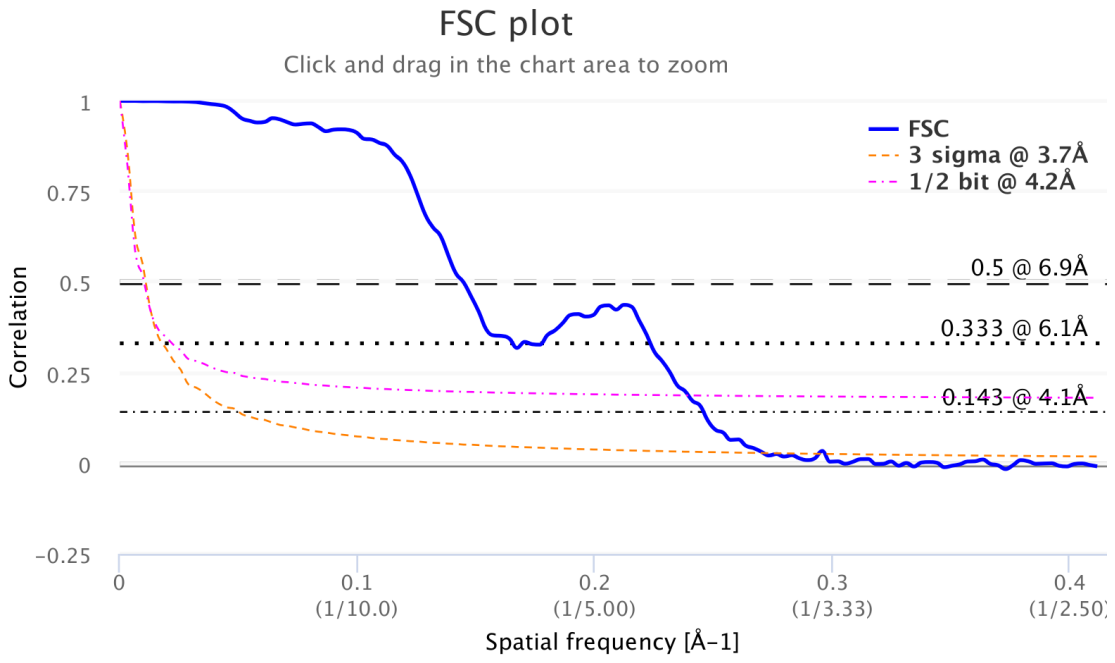
146 (box 300, pix 0.6078)



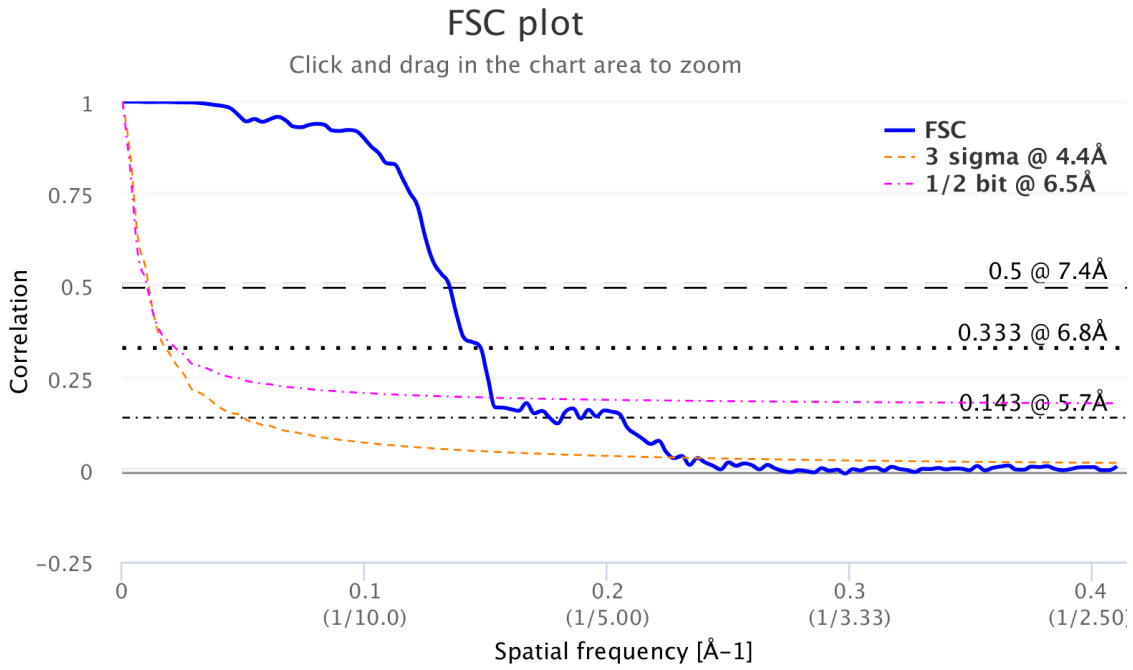
156 (box 256, pix 1.2156)



161 (box 256, pix 1.2156)



163 (box 256, pix 1.22)



Summary: Resolution (from FSC) is the highest in 156, but this is not true - a question should be asked, what happened. There are then three other maps, 115, 133 and 161 which seem to be of similar resolution. The worst one, according to FSC is 163. One needs to review the maps.

Rank based on filtered provided by the people submitting:
115 and 161 (best overall), 101 (nterm weaker), 156, 133, 135 (weak Nterm, good transmembrane), 163 (not great resolved transmembrane, but better resolved nterm than 135), 146 (something went wrong with filtering ?)
So,
RANK:
101 2
115 1 (FSC too)
133 4
135 5
146 6
156 3
161 1 (FSC too)
163 7

Method: I did a round of refinement in Phenix using Yuan's recent APO-trpv1 structure.

Results:

	Ramachandran	MolProbity		RMSD		Map CC		Visual
Model	Favored	Score	Clashscore	Bonds	Angles	unit cell	atoms	rank
101	0.896	1.78	4.44	0.012	1.379	0.463	0.811	3
115	0.926	1.74	5.18	0.006	1.198	0.455	0.81	2
133	0.9311	1.73	5.4	0.005	1.145	0.073	0.034	6
135	0.919	1.88	7.06	0.007	1.368	0.073	0.052	7
146	0.9247	1.67	4.22	0.004	1.105	-0.047	0	8
156	0.9082	1.79	5.01	0.008	1.284	0.418	0.722	5
161	0.9133	1.71	4.18	0.007	1.251	0.503	0.803	1
163	0.9158	1.84	6.18	0.01	1.32	0.503	0.788	4

Summary:
Refinement statistics from Phenix refine is not a good way to judge map quality. However, if we ignore the worst three maps (133, 135, 146), the MolProbity score seems somewhat correlated to my visual ranking. I thought 161 was the best visually, followed by 115 and 101, 163 and 156 were not impressive, while 133 and 135 looks strange, 146 is uninterpretable. My visual ranking is based solely on how the density looks (ie. I didn't inspect bound lipids).

Rank	Visual	MolProbity
161	1	1.71
115	2	1.74
101	3	1.78
163	4	1.84

156	5	1.79
133	6	1.73
135	7	1.88
146	8	1.67