

**Supplementary Material for:**  
**Weak data do not make a free lunch, but only a cheap meal**

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Refinement protocols:

All data sets, with or without randomization, were refined using the same protocol at incremental resolutions, analogously to that of Karplus & Diederichs (2012). All water molecules were deleted from the initial models and were acquired automatically during refinement by phenix.refine. All ligand CIF files were obtained from the monomer library. TLS parameters for each PDB model were obtained by phenix.find\_tls\_groups. Only isotropic refinement was used.

The Phenix.refine options were kept the same as those used by Karplus & Diederichs:

```
“strategy=individual_sites+individual_adp+tls \
tls_group_selections.params \
ordered_solvent=true \
fix_rotamers=true \
xray_data.high_resolution=1.8”
```

To calculate R values at a resolution lower than that at which the model was refined, the options were listed as follows:

```
“main.number_of_macro_cycles=1 \
strategy=none \
ordered_solvent=False \
fix_rotamers=False \
xray_data.high_resolution=1.9”
```

## Supplementary Table S1

Diffraction data statistics.

a) 3E4F				P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>		a = 36.31		b = 108.05		c = 132.81 Å								
dmin (Å)	dmax (Å)	dopt (Å)	refl. meas.	refl. unique	mult.	compl. (%)	<I>	<I>/<σ(I)>		R <sub>merge</sub>	R <sub>meas</sub>	R <sub>pim</sub>	CC <sub>1/2</sub>	CC*	CC <sub>work</sub>	CC <sub>free</sub>	R <sub>work</sub>	R <sub>free</sub>
29.39	4.61	3.04	13810	3128	4.41	98.61	2239.8	43.8	39.6	0.048	0.054	0.025	0.997	0.999	0.921	0.925	0.185	0.219
4.61	3.66	2.46	14304	3012	4.75	99.83	2037.2	44.0	38.0	0.055	0.062	0.029	0.996	0.999	0.956	0.967	0.145	0.155
3.66	3.20	2.19	14809	3008	4.92	99.97	1030.8	37.0	30.1	0.066	0.074	0.033	0.995	0.999	0.952	0.927	0.160	0.195
3.20	2.91	2.03	14857	2954	5.03	99.97	521.7	28.6	22.8	0.076	0.085	0.038	0.995	0.999	0.929	0.876	0.185	0.228
2.91	2.70	1.96	14848	2940	5.05	100.00	316.3	21.8	17.6	0.094	0.105	0.046	0.994	0.999	0.930	0.828	0.191	0.270
2.70	2.54	1.87	14912	2948	5.06	100.00	211.9	16.8	13.7	0.120	0.134	0.059	0.992	0.998	0.935	0.919	0.188	0.234
2.54	2.41	1.80	14576	2881	5.06	100.00	170.5	14.0	11.8	0.144	0.161	0.071	0.988	0.997	0.938	0.810	0.175	0.228
2.41	2.31	1.76	15078	2956	5.10	100.00	134.0	11.3	9.7	0.177	0.198	0.087	0.981	0.995	0.939	0.865	0.179	0.223
2.31	2.22	1.71	14778	2913	5.07	100.00	111.6	9.4	8.0	0.215	0.240	0.106	0.976	0.994	0.952	0.915	0.170	0.226
2.22	2.14	1.69	14587	2877	5.07	100.00	88.0	7.4	6.5	0.269	0.301	0.132	0.966	0.991	0.944	0.945	0.174	0.184
2.14	2.07	1.66	14961	2930	5.11	100.00	70.1	5.7	5.2	0.343	0.384	0.169	0.949	0.987	0.946	0.886	0.186	0.229
2.07	2.02	1.64	14535	2874	5.06	100.00	52.1	4.3	4.0	0.451	0.505	0.223	0.893	0.971	0.919	0.809	0.206	0.255
2.02	1.96	1.62	14893	2923	5.10	100.00	39.8	3.3	3.1	0.595	0.665	0.293	0.832	0.953	0.901	0.781	0.223	0.266
1.96	1.91	1.60	14414	2852	5.06	100.00	31.6	2.5	2.4	0.787	0.881	0.389	0.795	0.941	0.888	0.798	0.246	0.316
1.91	1.87	1.59	14112	2937	4.80	100.00	25.2	1.8	1.8	0.987	1.112	0.504	0.711	0.912	0.855	0.804	0.265	0.318
1.87	1.83	1.57	11061	2823	3.92	98.05	19.9	1.2	1.3	1.158	1.340	0.663	0.491	0.812	0.767	0.838	0.295	0.281
1.83	1.79	1.56	9408	2769	3.40	95.98	16.4	0.9	0.9	1.475	1.743	0.910	0.274	0.656	0.623	0.430	0.328	0.384
1.79	1.76	1.55	8247	2744	3.01	94.62	15.6	0.7	0.8	1.583	1.902	1.033	0.256	0.638	0.554	0.533	0.351	0.362
1.76	1.73	1.53	6730	2605	2.58	91.82	12.5	0.5	0.6	1.919	2.353	1.340	0.168	0.537	0.433	0.272	0.374	0.416
1.73	1.70	1.52	6328	2555	2.48	88.13	10.2	0.4	0.4	2.284	2.812	1.603	0.132	0.483	0.360	0.469	0.401	0.382
29.39	1.70	1.52	261248	57629	4.53	98.36	375.5	19.3	11.3	0.094	0.107	0.049	0.997	0.997	0.961	0.959	0.188	0.225

b) 3N0S

P2<sub>1</sub>

a = 72.04

b = 109.44

c = 74.05 Å    β = 111.9

dmin (Å)	dmax (Å)	dopt (Å)	refl. meas.	refl. unique	mult.	compl. (%)	<D>	<I>/<σ(I)> <I/σ(I)>	R <sub>merge</sub>	R <sub>meas</sub>	R <sub>pim</sub>	CC <sub>1/2</sub>	CC <sup>*</sup>	CC <sub>work</sub>	CC <sub>free</sub>	R <sub>work</sub>	R <sub>free</sub>	
27.38	4.87	3.22	19770	5007	3.95	99.29	1049.0	45.6	35.6	0.055	0.063	0.031	0.997	0.999	0.956	0.932	0.170	0.198
4.87	3.87	2.50	19996	4966	4.03	99.34	1172.0	42.0	34.4	0.057	0.065	0.032	0.996	0.999	0.961	0.925	0.136	0.169
3.87	3.38	2.30	20542	4961	4.14	99.60	760.1	32.2	26.0	0.074	0.085	0.041	0.995	0.999	0.957	0.950	0.144	0.181
3.38	3.07	2.12	20987	4948	4.24	99.92	408.1	22.1	18.1	0.108	0.123	0.059	0.989	0.997	0.933	0.897	0.174	0.229
3.07	2.85	2.00	21060	4934	4.27	99.84	229.3	14.6	12.8	0.158	0.179	0.085	0.981	0.995	0.922	0.814	0.186	0.234
2.85	2.68	1.94	21173	4963	4.27	99.86	154.0	10.3	9.4	0.216	0.246	0.117	0.967	0.992	0.927	0.875	0.183	0.211
2.68	2.55	1.86	20865	4924	4.24	99.70	116.1	7.8	7.3	0.290	0.330	0.157	0.949	0.987	0.931	0.859	0.182	0.249
2.55	2.44	1.81	20777	4963	4.19	99.64	95.4	6.1	5.9	0.375	0.427	0.203	0.931	0.982	0.930	0.884	0.184	0.251
2.44	2.35	1.76	20308	4910	4.14	99.31	80.5	4.7	4.8	0.507	0.577	0.275	0.876	0.966	0.911	0.856	0.194	0.252
2.35	2.26	1.73	19876	4861	4.09	99.02	73.2	3.9	4.0	0.632	0.719	0.342	0.854	0.960	0.928	0.857	0.192	0.252
2.26	2.19	1.69	19886	4893	4.06	98.57	62.5	3.0	3.3	0.842	0.958	0.455	0.733	0.920	0.897	0.834	0.202	0.251
2.19	2.13	1.67	19574	4832	4.05	98.03	50.8	2.3	2.6	1.149	1.307	0.620	0.585	0.859	0.862	0.722	0.216	0.263
2.13	2.07	1.65	19388	4803	4.04	97.46	46.0	1.9	2.2	1.441	1.639	0.777	0.504	0.818	0.830	0.800	0.228	0.261
2.07	2.01	1.63	19409	4820	4.03	97.24	37.0	1.4	1.7	1.875	2.132	1.010	0.358	0.726	0.750	0.720	0.246	0.290
2.02	1.98	1.61	19367	4815	4.02	97.27	30.3	1.1	1.4	2.574	2.927	1.387	0.276	0.657	0.692	0.527	0.274	0.312
1.98	1.94	1.60	19244	4785	4.02	97.08	24.9	0.9	1.2	3.553	4.040	1.914	0.162	0.528	0.627	0.464	0.291	0.336
1.94	1.90	1.59	19002	4731	4.02	96.89	21.5	0.8	1.0	4.850	5.515	2.612	0.106	0.437	0.564	0.410	0.296	0.350
1.90	1.86	1.57	19267	4815	4.00	97.21	17.3	0.6	0.7	5.595	6.362	3.015	0.083	0.392	0.548	0.512	0.309	0.376
1.86	1.83	1.55	19121	4794	3.99	96.75	14.3	0.5	0.6	5.524	6.284	2.981	0.049	0.306	0.525	0.375	0.318	0.354
1.83	1.80	1.53	18500	4648	3.98	94.59	12.6	0.4	0.5	10.107	11.501	5.463	0.026	0.223	0.504	0.415	0.342	0.372
27.38	1.80	1.53	398112	97373	4.09	98.33	26.8	10.1	8.9	0.342	0.389	0.185	0.990	0.998	0.968	0.951	0.230	0.230

c) 2FXQ

C222<sub>1</sub>

a = 51.1

b = 163.77

c = 60.16 Å

dmin (Å)	dmax (Å)	dopt (Å)	refl. meas.	refl. unique	mult.	compl. (%)	<I>	<I>/<σ(I)>	R <sub>merge</sub>	R <sub>meas</sub>	R <sub>pim</sub>	CC <sub>1/2</sub>	CC*	CC <sub>work</sub>	CC <sub>free</sub>	R <sub>work</sub>	R <sub>free</sub>	
						<I>/<σ(I)>												
40.96	4.40	2.91	11981	1756	6.82	99.72	1154.8	59.7	52.7	0.024	0.026	0.010	0.999	1.000	0.925	0.952	0.198	0.197
4.40	3.49	2.38	12100	1674	7.23	100.00	776.7	55.4	45.2	0.031	0.033	0/0.012	0.999	1.000	0.947	0.900	0.173	0.190
3.49	3.05	2.14	12142	1660	7.31	100.00	359.3	42.1	33.5	0.054	0.059	0.021	0.998	1.000	0.931	0.881	0.186	0.221
3.05	2.77	2.00	12014	1640	7.33	100.00	144.7	27.8	21.8	0.074	0.079	0.029	0.998	0.999	0.912	0.884	0.214	0.231
2.77	2.57	1.91	12020	1634	7.36	100.00	81.1	19.1	15.9	0.098	0.105	0.039	0.996	0.999	0.913	0.934	0.201	0.231
2.57	2.42	1.85	11932	1624	7.35	100.00	53.4	13.8	11.9	0.136	0.146	0.053	0.994	0.998	0.906	0.866	0.212	0.227
2.42	2.30	1.79	12005	1637	7.33	100.00	40.9	10.7	9.4	0.179	0.193	0.071	0.989	0.997	0.908	0.764	0.209	0.335
2.30	2.20	1.75	11804	1601	7.37	100.00	32.8	8.5	7.6	0.233	0.251	0.092	0.985	0.996	0.919	0.811	0.202	0.246
2.20	2.12	1.70	11945	1630	7.33	100.00	27.2	6.8	6.2	0.293	0.315	0.116	0.976	0.994	0.925	0.882	0.202	0.260
2.12	2.04	1.68	11819	1608	7.35	100.00	21.2	5.3	4.9	0.385	0.415	0.152	0.965	0.991	0.941	0.790	0.199	0.263
2.04	1.98	1.66	11816	1616	7.31	100.00	17.6	4.2	4.0	0.469	0.505	0.185	0.959	0.990	0.933	0.921	0.217	0.241
1.98	1.92	1.65	11805	1614	7.31	100.00	12.6	3.1	3.0	0.642	0.691	0.253	0.925	0.980	0.927	0.876	0.217	0.266
1.92	1.87	1.63	11557	1581	7.31	100.00	7.8	2.0	2.0	0.967	1.040	0.382	0.841	0.956	0.891	0.868	0.245	0.269
1.87	1.83	1.62	11976	1630	7.35	100.00	5.4	1.4	1.5	1.447	1.556	0.569	0.732	0.919	0.841	0.915	0.287	0.273
1.83	1.79	1.61	11781	1622	7.26	100.00	4.0	1.1	1.1	1.918	2.065	0.760	0.582	0.858	0.786	0.628	0.321	0.401
1.79	1.75	1.59	11526	1586	7.27	100.00	3.1	0.8	0.8	2.473	2.662	0.978	0.440	0.781	0.728	0.547	0.375	0.418
1.75	1.71	1.58	11703	1615	7.25	100.00	2.4	0.6	0.6	3.130	3.370	1.239	0.347	0.717	0.622	0.511	0.368	0.391
1.71	1.68	1.57	11438	1594	7.18	100.00	2.1	0.5	0.5	3.529	3.802	1.403	0.215	0.595	0.522	0.756	0.379	0.413
1.68	1.65	1.56	11319	1586	7.14	100.00	1.8	0.4	0.4	4.213	4.540	1.682	0.144	0.502	0.430	0.378	0.418	0.407
1.65	1.62	1.54	9445	1579	5.98	96.52	1.9	0.4	0.4	4.185	4.587	1.841	0.020	0.200	0.340	0.165	0.432	0.493
40.96	1.62	1.54	234128	32487	7.21	99.81	143.9	25.3	11.5	0.074	0.080	0.030	0.999	1.000	0.954	0.960	0.208	0.233

d) Thaumatin

P4<sub>1</sub>2<sub>1</sub>2

a = b = 57.72

c = 149.88 Å

dmin (Å)	dmax (Å)	dopt (Å)	refl. meas.	refl. unique	mult.	compl. (%)	<I>	<I>/<σ(I)>		R <sub>merge</sub>	R <sub>meas</sub>	R <sub>pim</sub>	CC <sub>1/2</sub>	CC*	CC <sub>work</sub>	CC <sub>free</sub>	R <sub>work</sub>	R <sub>free</sub>
						<I>/<σ(I)>			<I>/<σ(I)>									
26.91	3.53	2.32	46555	3472	13.41	99.94	1928.5	53.2	42.2	0.046	0.048	0.013	0.999	1.000	0.959	0.950	0.156	0.156
3.53	2.80	1.92	46510	3265	14.25	100.00	1165.5	41.6	33.0	0.068	0.071	0.019	0.999	1.000	0.945	0.933	0.160	0.180
2.80	2.45	1.74	46456	3234	14.36	100.00	520.9	25.0	20.4	0.117	0.121	0.032	0.997	0.999	0.944	0.924	0.171	0.171
2.45	2.22	1.61	45783	3179	14.40	100.00	397.5	20.1	16.8	0.153	0.159	0.041	0.995	0.999	0.943	0.887	0.160	0.174
2.22	2.06	1.54	45786	3186	14.37	100.00	315.0	16.1	13.6	0.201	0.209	0.055	0.992	0.998	0.948	0.962	0.160	0.176
2.06	1.94	1.46	45549	3169	14.37	100.00	223.5	12.0	10.5	0.252	0.261	0.068	0.988	0.997	0.948	0.936	0.158	0.172
1.96	1.85	1.43	45237	3157	14.33	100.00	149.9	8.7	7.7	0.331	0.343	0.090	0.983	0.996	0.951	0.935	0.160	0.170
1.85	1.76	1.38	45196	3143	14.38	100.00	105.0	6.2	5.8	0.438	0.454	0.119	0.969	0.992	0.942	0.932	0.167	0.201
1.76	1.70	1.35	44882	3132	14.33	100.00	79.7	4.8	4.5	0.570	0.591	0.155	0.953	0.988	0.933	0.907	0.182	0.198
1.70	1.64	1.33	45112	3150	14.32	100.00	61.0	3.6	3.5	0.744	0.771	0.202	0.933	0.983	0.941	0.918	0.183	0.212
1.64	1.59	1.31	44977	3147	14.29	100.00	51.9	3.0	2.9	0.897	0.930	0.244	0.920	0.979	0.943	0.901	0.191	0.223
1.59	1.54	1.29	44442	3113	14.28	100.00	42.0	2.4	2.4	1.110	1.150	0.302	0.865	0.963	0.919	0.888	0.202	0.235
1.54	1.50	1.27	44572	3124	14.27	100.00	33.8	1.9	1.9	1.375	1.425	0.374	0.794	0.941	0.903	0.855	0.221	0.255
1.50	1.46	1.26	44157	3109	14.20	100.00	29.3	1.5	1.6	1.615	1.675	0.440	0.780	0.936	0.902	0.831	0.236	0.236
1.46	1.43	1.25	44186	3114	14.19	100.00	24.8	1.3	1.3	1.952	2.024	0.532	0.737	0.921	0.869	0.825	0.259	0.289
1.43	1.40	1.24	44010	3103	14.18	100.00	20.2	1.0	1.0	2.440	2.530	0.664	0.540	0.837	0.807	0.715	0.272	0.310
1.40	1.37	1.23	43807	3101	14.13	100.00	17.5	0.8	0.9	2.872	2.978	0.783	0.503	0.818	0.735	0.819	0.303	0.322
1.37	1.35	1.22	43965	3118	14.10	100.00	15.9	0.7	0.8	3.179	3.297	0.868	0.412	0.764	0.711	0.699	0.306	0.324
1.35	1.32	1.21	43952	3122	14.08	100.00	13.4	0.6	0.6	3.794	3.935	1.037	0.343	0.715	0.669	0.654	0.313	0.303
1.32	1.30	1.21	42261	3023	13.98	98.18	11.9	0.5	0.5	4.338	4.501	1.190	0.258	0.641	0.595	0.669	0.325	0.327
28.86	1.30	1.21	897395	63161	14.21	99.91	272.6	13.2	8.9	0.212	0.058	0.058	0.999	1.000	0.970	0.964	0.180	0.194



**Supplementary Table S2**

Distribution of the highest resolution  $I/\sigma(I)$  values in all PDB submissions reporting this parameter. In the June 2013 version of the PDB, among 80,939 X-ray structures, this value is provided in 49,589 (61.3%) submissions.

$I/\sigma(I)$ range	# of contributors	$I/\sigma(I)$ limit	# of contributors	
>1000	10	$\geq 1000$	10	0.02 %
1000 - 100	15	$\geq 100$	25	0.05 %
100 - 10	1,910	$\geq 10$	1,935	3.9 %
10 - 5	7,354	$\geq 5$	9,289	18.7 %
5 - 3	15,132	$\geq 3$	24,421	48.2 %
3 - 2	16,255	$\geq 2$	40,676	82.0 %
2.0 - 1.5	4,437	< 2.0	8,913	18.0 %
1.5 - 1.0	2,586	< 1.5	3,350	6.8 %
1.0 - 0.5	680	< 1.0	736	1.5 %
0.5 - 0.1	38	< 0.5	56	0.1 %
< 0.1	18	< 0.1	18	0.03 %

### Supplementary Table S3

Correlation coefficients between the  $2F_o - F_c$  map corresponding to the models refined at resolution  $d$  and the map simulated at the same resolution from the 'best' model refined at the maximum nominal resolution  $d_{\text{nominal}}$ .

#### 3E4F

Resolution d ( $\text{\AA}$ )	2.2	2.1	2.0	1.9	1.8	1.7
Data without randomization						
Refined and calculated at $d$	0.910	0.910	0.915	0.915	0.911	0.916
Refined at $d-0.1$ , calculated at $d$	0.911	0.914	0.916	0.914	0.912	
Data randomized beyond $d+0.1$						
Refined and calculated at $d$	0.888	0.891	0.896	0.898	0.898	0.905

#### 3N0S

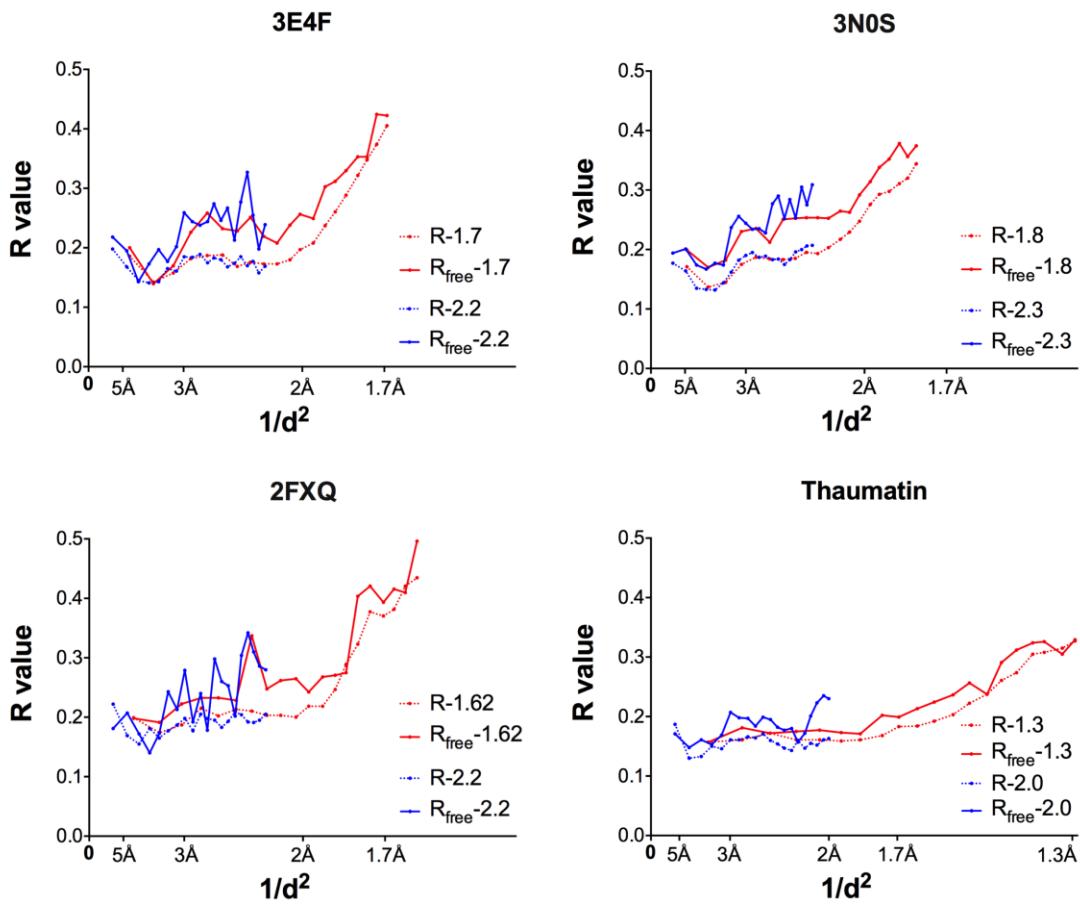
Resolution d ( $\text{\AA}$ )	2.3	2.2	2.1	2.0	1.9	1.8
Data without randomization						
Refined and calculated at $d$	0.898	0.903	0.905	0.911	0.909	0.911
Refined at $d-0.1$ , calculated at $d$	0.901	0.904	0.905	0.912	0.912	
Data randomized beyond $d+0.1$						
Refined and calculated at $d$	0.894	0.899	0.898	0.903	0.898	0.897

#### 2FXQ

Resolution d ( $\text{\AA}$ )	2.2	2.1	2.0	1.9	1.8	1.7	1.62
Data without randomization							
Refined and calculated at $d$	0.918	0.916	0.917	0.918	0.917	0.915	0.917
Refined at $d-0.1$ , calculated at $d$	0.919	0.916	0.918	0.919	0.916	0.917	
Data randomized beyond $d+0.1$							
Refined and calculated at $d$	0.906	0.905	0.903	0.904	0.902	0.895	0.893

#### Thaumatin

Resolution d ( $\text{\AA}$ )	2.0	1.9	1.8	1.7	1.6	1.5	1.4	1.3
Data without randomization								
Refined and calculated at $d$	0.916	0.922	0.923	0.926	0.932	0.930	0.928	0.935
Refined at $d-0.1$ , calculated at $d$	0.918	0.923	0.923	0.926	0.930	0.931	0.930	
Data randomized beyond $d+0.1$								
Refined and calculated at $d$	0.906	0.911	0.912	0.919	0.025	0.923	0.922	0.930



### Supplementary Fig.S1

R and R<sub>free</sub> factors (solid and dashed lines, respectively) obtained for four investigated structures after refinement at the highest available resolution (red) and the limit lower by 0.5 Å (blue).