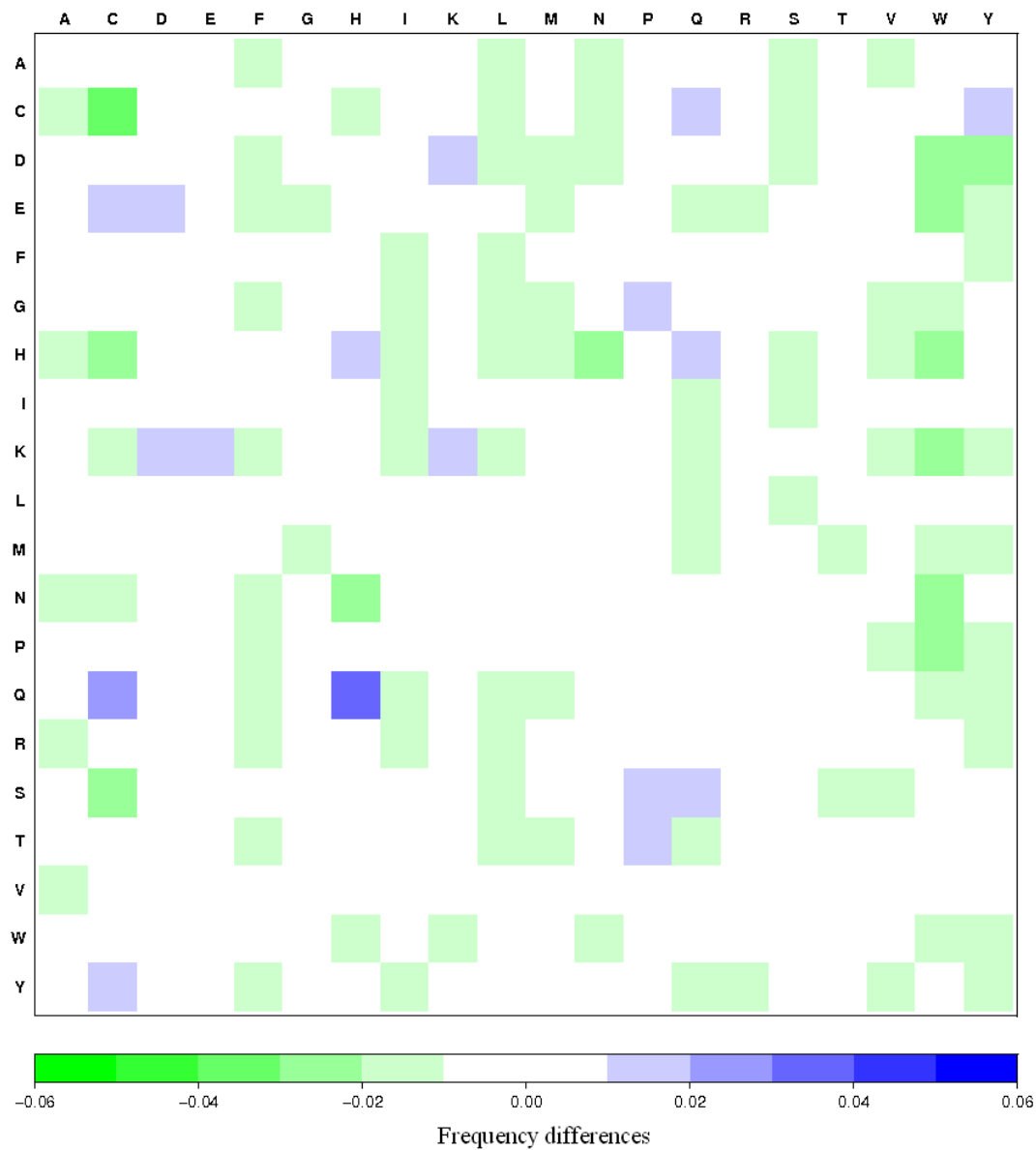


## Supplementary data

**Sup data 1:** *Pearson correlation coefficient (PCC) of (residue volume, contact number) pairs for buried or exposed residues.* The residue exposure to solvent is specified in the top row, “DB” meaning the whole data bank. For Voronoi and Laguerre tessellations, the residue volumes are sums of atomic polyhedral volumes and the contact numbers are VCN or LCN, while for the distance methods, DC (distance between C $\alpha$ ) and DA (distance between all atoms), the residue volumes are Van der Waals volumes given by NACCESS and the contact numbers are CCN and ACN respectively.

	DB	ASA>25	ASA<25	ASA=0	ASA+PIA=0
PCC Laguerre	0.71	0.94	0.96	NA	0.96
PCC Voronoi	0.74	0.94	0.96	NA	0.96
PCC DC	-0.03	0.73	-0.8	-0.76	NA
PCC DA	0.63	0.91	0.96	0.98	NA

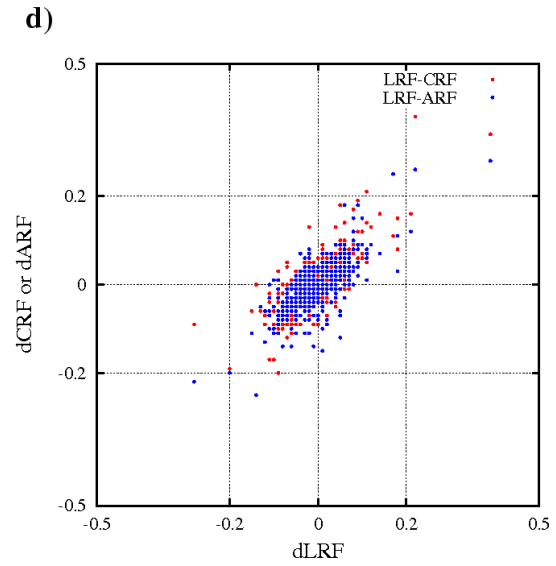
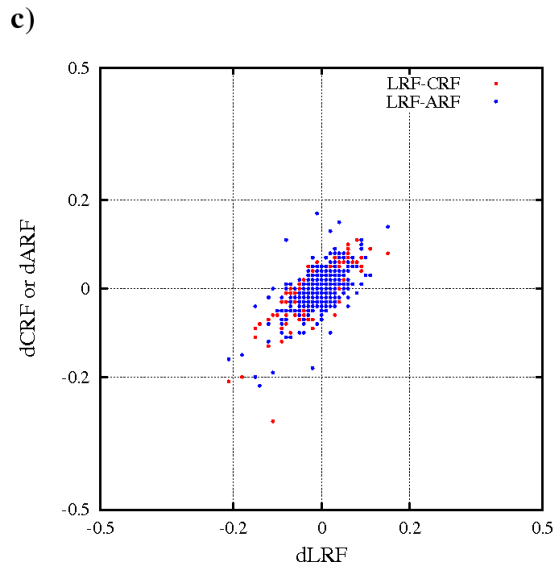
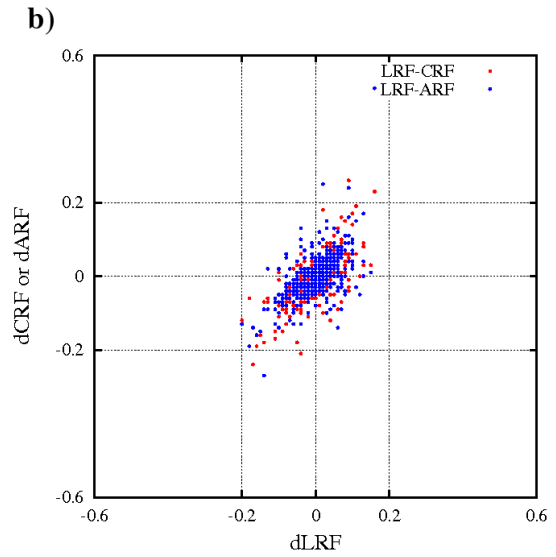
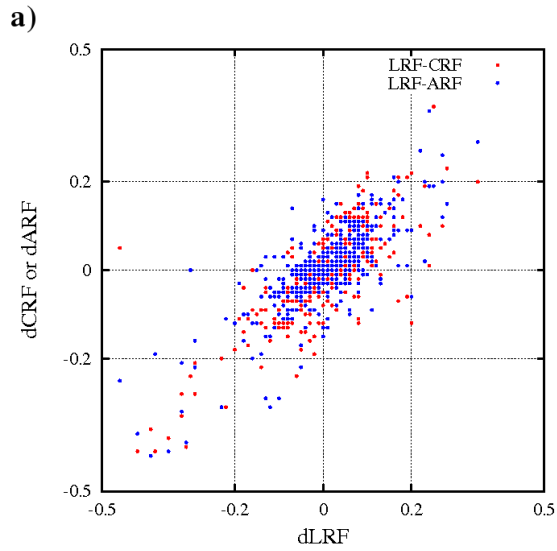
**Sup data 2a:** Matrix of relative frequency differences  $LRF - VRF$ . The statistics are computed on all residues of the databank.



**Sup data 2b:** *Table of relative frequencies from Laguerre method ( LRF).*

ij	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	1.18	1.14	0.56	0.58	1.45	0.73	0.91	1.48	0.62	1.46	1.44	0.67	0.76	0.77	0.90	0.69	0.87	1.42	1.53	1.30
C	0.81	6.47	0.48	0.47	1.71	0.73	1.16	1.34	0.60	1.25	1.46	0.72	0.75	0.62	0.82	0.72	0.93	1.23	1.82	1.41
D	0.77	0.93	0.63	0.55	1.15	0.77	1.48	0.94	1.47	0.91	1.18	1.07	0.83	1.01	1.86	0.89	0.93	0.90	1.64	1.64
E	0.78	0.89	0.54	0.63	1.17	0.63	1.36	1.03	1.55	1.01	1.14	0.88	0.84	0.98	2.00	0.81	0.92	0.99	1.59	1.46
F	0.82	1.34	0.47	0.49	2.10	0.59	0.92	1.68	0.56	1.63	1.59	0.59	0.75	0.65	0.78	0.69	0.82	1.38	1.90	1.57
G	0.95	1.34	0.73	0.62	1.37	0.93	1.11	1.15	0.76	1.11	1.34	0.88	0.93	0.85	1.15	0.89	0.99	1.12	1.63	1.43
H	0.77	1.38	0.92	0.86	1.40	0.72	1.62	1.11	0.62	1.10	1.30	0.82	0.96	0.85	1.09	0.85	0.99	1.03	1.95	1.65
I	0.90	1.14	0.41	0.47	1.83	0.54	0.79	2.03	0.57	1.73	1.54	0.56	0.63	0.58	0.69	0.60	0.84	1.63	1.49	1.38
K	0.75	1.01	1.28	1.39	1.20	0.70	0.87	1.13	0.83	1.05	1.03	0.99	0.77	0.94	0.85	0.85	0.91	1.00	1.41	1.54
L	0.93	1.11	0.42	0.48	1.85	0.54	0.82	1.80	0.55	1.89	1.46	0.52	0.67	0.63	0.79	0.57	0.78	1.54	1.67	1.35
M	0.92	1.30	0.54	0.54	1.81	0.65	0.97	1.62	0.55	1.47	2.16	0.66	0.78	0.67	0.82	0.65	0.83	1.33	1.91	1.51
N	0.78	1.17	0.90	0.76	1.22	0.78	1.11	1.07	0.95	0.94	1.20	1.20	0.90	1.05	1.15	0.99	1.10	0.96	1.70	1.54
P	0.83	1.15	0.66	0.68	1.46	0.77	1.22	1.14	0.70	1.15	1.33	0.85	1.00	0.97	1.19	0.83	0.98	1.08	2.04	1.73
Q	0.84	0.94	0.80	0.80	1.27	0.72	1.10	1.05	0.86	1.09	1.16	1.00	0.97	1.14	1.21	0.91	1.04	1.02	1.76	1.48
R	0.78	1.00	1.18	1.30	1.21	0.77	1.11	0.99	0.62	1.08	1.13	0.86	0.95	0.96	1.12	0.83	0.92	0.96	1.68	1.45
S	0.82	1.18	0.76	0.71	1.46	0.80	1.17	1.17	0.83	1.06	1.21	1.00	0.90	0.98	1.12	0.93	1.04	1.08	1.64	1.47
T	0.84	1.26	0.65	0.67	1.41	0.74	1.13	1.33	0.73	1.19	1.27	0.92	0.87	0.92	1.03	0.86	1.09	1.25	1.60	1.41
V	0.97	1.18	0.45	0.50	1.69	0.59	0.83	1.84	0.57	1.66	1.43	0.57	0.68	0.64	0.76	0.63	0.88	1.64	1.54	1.33
W	0.80	1.33	0.62	0.62	1.77	0.65	1.19	1.28	0.61	1.37	1.57	0.77	0.98	0.84	1.01	0.73	0.86	1.17	2.28	1.59
Y	0.79	1.19	0.72	0.65	1.69	0.66	1.16	1.36	0.77	1.28	1.43	0.80	0.95	0.81	1.00	0.75	0.87	1.16	1.84	1.60

**Sup data 3:** Correlation between  $dLRF$  and  $dCRF$  (or  $dARF$ ) for each protein size class. For the four classes of protein size,  $<150$  (a),  $150-250$  (b),  $2501-400$  (c) and  $>400$  (d), the relative frequency differences  $dCRF$  and  $dARF$  are plotted vs  $dLRF$ .



**Sup data 4:** *Number of cysteine-SS-cysteine contacts found by tessellation methods.* Contacts are counted whenever cysteine sulfurs share a face in the Voronoi or Laguerre diagram. The lines in blue highlight the discrepancies between Voronoi and Laguerre methods.

pdb	Voro	Lag	pdb	Voro	Lag	pdb	Voro	Lag	pdb	Voro	Lag	pdb	Voro	Lag
1a4i	2	2	1f2l	4	4	1jkg	2	2	1n7z	2	2	1szh	14	14
1aqz	4	4	1f6f	6	6	1jly	2	2	1now	6	6	1t0p	2	2
1ayo	2	2	1fiu	2	2	1jql	2	2	1nyk	4	4	1tvx	4	4
1b25	4	4	1fjr	10	10	1jr8	2	2	1oaq	2	2	1twd	2	2
1c7n	2	2	1fn9	3	3	1js8	6	6	<b>1ofd</b>	<b>4</b>	<b>6</b>	1u19	2	2
1cq3	8	8	1fo0	4	4	1kol	4	4	1olz	16	16	1u8v	4	4
1cvu	10	10	1fzc	2	2	1kqn	2	2	1ors	4	4	1uhg	2	2
1d0c	2	2	1gxy	4	4	1kve	2	2	1otv	2	2	1unn	2	2
1d0d	6	6	1h03	8	8	1kzq	12	12	1ozj	3	3	1uuz	2	2
1d0q	3	3	1h21	5	5	1l0s	8	8	1pju	16	16	1vmo	8	8
1d8w	2	2	1h8p	8	8	1l4d	12	12	1pk6	2	2	1vzi	4	4
1dp5	4	4	1iar	6	6	1l5j	6	6	1pz7	2	2	1w94	2	2
1dqe	6	6	1ijy	10	10	1lpb	10	10	1q7z	3	3	1wbh	2	2
1dqt	4	4	1im3	4	4	1lr5	2	2	1qb5	2	2	1wur	2	2
1ece	2	2	1im8	2	2	<b>1m2d</b>	<b>2</b>	<b>3</b>	1qft	4	4	1wwz	2	2
1elk	3	3	1isu	3	3	1m4u	6	6	1ql0	4	4	1x0v	2	2
1ep3	2	2	1itu	4	4	1mkf	10	10	1qu0	2	2	1xiw	2	2
1ext	24	24	1itv	2	2	<b>1n1j</b>	<b>0</b>	<b>2</b>	1qyn	2	2	1xlq	4	4
1ezg	16	16	1jfr	2	2	1n4a	2	2	1sac	2	2	1xs0	2	2
1f0x	2	2	1jh6	2	2	1n69	6	6	1syx	2	2	1xx1	2	2
pdb	Voro	Lag	pdb	Voro	Lag	pdb	Voro	Lag	pdb	Voro	Lag	pdb	Voro	Lag
1yk3	2	2	2clb	2	2	2fp8	2	2	2oa6	2	2	2yww	4	4
1ylk	2	2	2cov	4	4	2g6q	7	7	<b>2pa8</b>	<b>6</b>	<b>9</b>	3b8f	3	3
1ypq	6	6	2cw6	2	2	2gak	8	8	2pkh	2	2	3box	2	2
1ypy	6	6	2czs	2	2	2gel	2	2	2pof	4	4	3c0n	4	4
1zh1	6	6	2d5w	2	2	2ghv	6	6	2psp	14	14	3c3k	2	2
1zps	2	2	2de6	2	2	2gmf	4	4	2q4f	2	2			
1zy7	2	2	2djf	4	4	2gmn	2	2	2q4g	8	8			
2a1k	3	3	2dpf	2	2	2grv	2	2	2q4x	2	2			
2a25	2	2	2e1v	2	2	2hnu	14	14	<b>2q97</b>	<b>0</b>	<b>2</b>			
2afw	2	2	2e79	6	6	2hq4	2	2	2qeb	6	6			
2ag4	8	8	2eab	2	2	2i2x	2	2	2qki	2	2			
2ask	6	6	2ebo	2	2	<b>2inu</b>	<b>0</b>	<b>2</b>	2qsf	2	2			
2b3f	2	2	2f5g	2	2	2iwg	4	4	2qul	2	2			
2bb6	6	6	2f5x	2	2	2jby	4	4	2qyf	2	2			
<b>2bm5</b>	<b>0</b>	<b>2</b>	2fb2	2	2	<b>2jh3</b>	<b>0</b>	<b>2</b>	2rl8	6	6			
<b>2bpt</b>	<b>2</b>	<b>5</b>	<b>2fd6</b>	<b>10</b>	<b>12</b>	2jig	2	2	2tnf	2	2			
2c5u	2	2	2fe8	4	4	2mpr	2	2	2uwa	4	4			
2c7n	4	4	2fh5	2	2	2nt0	4	4	2veo	4	4			
2cjl	4	4	2fkl	6	6	2ntp	2	2	2vgn	2	2			
2ckl	7	7	2foj	2	2	2o70	2	2	2ywi	2	2			

**Sup data 5:** *Contacts found in both, Voronoi and Laguerre, tessellations.* The hatched part counts the contacts occurring in both tessellations.

