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Table S1 Complete feature list for all features investigated in this publication.

Name	Explanation
I/σ	$\langle I/\sigma \rangle_{\text{obs}}$, Signal (intensity I) to noise (uncertainty or measurement error σ) ratio (Wilson, 1949; Srinivasan & Parthasarathy, 1976) ¹
$CC_{1/2}$	$CC_{1/2}$ (Karplus & Diederichs, 2012; Diederichs & Karplus, 2013; Evans & Murshudov, 2013)
$R_{\text{merge}I}$	R_{sym} or R_{merge} (Arndt <i>et al.</i> , 1968; Wilson, 1950). Determined by treating Friedel pair I^+ and I^- as equivalent measurements.
$R_{\text{merge}(I^+/I^-)}$	R_{merge} determined by treating Friedel pair I^+ and I^- as independent measurements.
$R_{\text{meas}I}$	R_{meas} or $R_{r.i.m.}$ (Diederichs & Karplus, 1997; Weiss, 2001). Determined by treating Friedel pair I^+ and I^- as equivalent measurements.
$R_{\text{meas}(I^+/I^-)}$	R_{meas} determined by treating Friedel pair I^+ and I^- as independent measurements.
$R_{p.i.m.I}$	$R_{p.i.m.}$ (Weiss, 2001). Determined by treating Friedel pair I^+ and I^- as equivalent measurements.
$R_{p.i.m.}(I^+/I^-)$	$R_{p.i.m.}$ determined by treating Friedel pair I^+ and I^- as independent measurements.
N_{obstotal}	Total number of observations
$N_{\text{obsunique}}$	Total number of unique observations
M	Multiplicity; Number of observations for each reflection
T	Completeness; Representation of missing data
d_{max}	Low resolution limit found by integration software
d_{min}	High resolution limit found by integration software
B	Wilson B-factor (Wilson, 1942)
m_{anom}	Anomalous slope (Howell & Smith, 1992)
CC_{anom}	CC_{anom} (Schneider & Sheldrick, 2002)
M_{anom}	Anomalous multiplicity; Number of observations for each anomalous reflection
T_{anom}	Anomalous Completeness; Representation of missing anomalous data
$\Delta I/\sigma I$	Signal to noise ratio for the anomalous differences

$\Delta F/F$	structure factors for the anomalous differences (Bijvoet <i>et al.</i> , 1951)
f^* _{theor}	Calculated with CROSSEC (Winn <i>et al.</i> , 2011)
V_{cell}	Unit cell volume
N_{sg}	Space group number from data reduction
a	Unit cell parameter a
b	Unit cell parameter b
c	Unit cell parameter c
α	Unit cell parameter alpha
β	Unit cell parameter beta
γ	Unit cell parameter gamma
V_m	Matthews coefficient
V_s	Expected solvent content determined using Matthews coefficient
N_{cell}	Defined in (6)
N_{molASU}	Expected number of molecules in the asymmetric unit determined using Matthews coefficient
MW_{ASU}	Defined in (1)
N_{sitesASU}	Defined in (2)
MW_{chain}	Molecular weight of the protein based on its sequence
$N_{\text{atomchain}}$	Number of atoms in the protein based on its sequence
MWS_{ASU}	Defined in (3)
$MWS_{\text{ASU}Vs}$	Defined in (4)
AV_z	Defined in (5)
I_{ASU}	Defined in (7)
d_{inv}	Defined in (8)
L	Defined in (9)

¹ where I is the observed intensity and σ its associated uncertainty provided $\chi^2 \sim 1$ for observed and estimated differences between symmetry-related observations

Table S2 Hyperparameter settings for the best classifier, a decision tree with AdaBoost, based on performance statistics.

Decision tree with AdaBoost	Base_estimator: class_weight = balanced criterion = entropy max_depth = 3 max_features = 2 max_leaf_nodes = 17 min_samples_leaf = 8 min_samples_split = 18 random_state = 0
	AdaBoostClassifier: n_estimators = 5694 learning_rate = 0.6355 algorithm = SAMME.R random_state = 5

Table S3 Numerical results for Pearson's correlation coefficient.

Feature	Feature	r	p	r2
I/σ	CC _{1/2}	0.204099	0.000001	0.041657
I/σ	R _{mergeI}	-0.461005	0	0.212525
I/σ	R _{merge(I+/I-)}	-0.406516	0	0.165255
I/σ	R _{measI}	-0.524406	0	0.275002
I/σ	R _{meas(I+/I-)}	-0.51533	0	0.265565
I/σ	R _{p.i.m.I}	-0.658338	0	0.433409
I/σ	R _{p.i.m.(I+/I-)}	-0.684956	0	0.469164
I/σ	N _{obstotal}	0.05358	0.204695	0.002871
I/σ	N _{obsunique}	-0.215612	0	0.046489
I/σ	M	0.327343	0	0.107153
I/σ	T	-0.319765	0	0.10225
I/σ	d _{max}	-0.004266	0.919627	0.000018

I/σ	d _{min}	-0.03209	0.447704	0.00103
I/σ	B	0.088631	0.035677	0.007855
I/σ	d _{inv}	0.082296	0.051186	0.006773
I/σ	m _{anom}	0.317502	0	0.100807
I/σ	CC _{anom}	0.254705	0	0.064875
I/σ	M _{anom}	0.340871	0	0.116193
I/σ	T _{anom}	-0.161448	0.000121	0.026065
I/σ	ΔI/σI	0.372491	0	0.13875
I/σ	ΔF/F	-0.673614	0	0.453755
I/σ	f' _{theor}	-0.1989	0.000002	0.039561
I/σ	V _{cell}	-0.005937	0.888309	0.000035
I/σ	N _{sg}	0.389966	0	0.152073
I/σ	a	-0.021461	0.611666	0.000461
I/σ	b	-0.043566	0.30254	0.001898
I/σ	c	-0.006508	0.877662	0.000042
I/σ	α	-0.164493	0.000089	0.027058
I/σ	β	-0.151351	0.000317	0.022907
I/σ	γ	0.228871	0	0.052382
I/σ	V _s	-0.04504	0.286468	0.002029
I/σ	N _{cell}	-0.004917	0.907409	0.000024
I/σ	L	0.028798	0.495661	0.000829
I/σ	V _m	-0.016452	0.697139	0.000271
I/σ	MWS _{ASUVs}	0.072105	0.087679	0.005199
I/σ	MW _{chain}	-0.246298	0	0.060663
I/σ	N _{atomchain}	-0.245889	0	0.060461
I/σ	N _{molASU}	-0.204453	0.000001	0.041801
I/σ	MW _{ASU}	-0.290423	0	0.084346
I/σ	N _{sitesASU}	-0.281477	0	0.07923
I/σ	MWS _{ASU}	0.044644	0.290734	0.001993
I/σ	I _{ASU}	0.699194	0	0.488872

I/σ	AV _z	0.022952	0.587147	0.000527
CC _{1/2}	R _{merge} I	-0.364135	0	0.132594
CC _{1/2}	R _{merge} (I+/I-)	-0.164214	0.000092	0.026966
CC _{1/2}	R _{meas} I	-0.451295	0	0.203667
CC _{1/2}	R _{meas} (I+/I-)	-0.204826	0.000001	0.041954
CC _{1/2}	R _{p.i.m.} I	-0.621068	0	0.385726
CC _{1/2}	R _{p.i.m.} (I+/I-)	-0.256568	0	0.065827
CC _{1/2}	N _{obstotal}	0.069437	0.100089	0.004821
CC _{1/2}	N _{obsunique}	-0.02572	0.542869	0.000662
CC _{1/2}	M	0.075758	0.072728	0.005739
CC _{1/2}	T	0.138029	0.001036	0.019052
CC _{1/2}	d _{max}	-0.037902	0.369796	0.001437
CC _{1/2}	d _{min}	-0.216243	0	0.046761
CC _{1/2}	B	0.09398	0.025886	0.008832
CC _{1/2}	d _{inv}	0.140168	0.000862	0.019647
CC _{1/2}	m _{anom}	0.171091	0.000046	0.029272
CC _{1/2}	CC _{anom}	0.133635	0.001497	0.017858
CC _{1/2}	M _{anom}	0.070818	0.0935	0.005015
CC _{1/2}	T _{anom}	0.204663	0.000001	0.041887
CC _{1/2}	ΔI/σI	0.091764	0.029618	0.008421
CC _{1/2}	ΔF/F	-0.498313	0	0.248316
CC _{1/2}	f' _{theor}	-0.023131	0.584235	0.000535
CC _{1/2}	V _{cell}	-0.014342	0.734414	0.000206
CC _{1/2}	N _{sg}	0.104343	0.013329	0.010888
CC _{1/2}	a	-0.011953	0.777372	0.000143
CC _{1/2}	b	-0.041557	0.325411	0.001727
CC _{1/2}	c	-0.046993	0.266058	0.002208
CC _{1/2}	α	-0.275457	0	0.075877
CC _{1/2}	β	-0.038344	0.36424	0.00147

CC _{1/2}	γ	0.059401	0.159637	0.003528
CC _{1/2}	V _s	0.00842	0.842123	0.000071
CC _{1/2}	N _{cell}	-0.013873	0.742795	0.000192
CC _{1/2}	L	-0.002407	0.954594	0.000006
CC _{1/2}	V _m	0.016777	0.691467	0.000281
CC _{1/2}	MWS _{ASUVs}	0.036719	0.384942	0.001348
CC _{1/2}	MW _{chain}	-0.068916	0.102669	0.004749
CC _{1/2}	N _{atomchain}	-0.068311	0.105729	0.004666
CC _{1/2}	N _{molASU}	-0.286824	0	0.082268
CC _{1/2}	MW _{ASU}	-0.277251	0	0.076868
CC _{1/2}	N _{sitesASU}	-0.325971	0	0.106257
CC _{1/2}	MWS _{ASU}	0.035462	0.401431	0.001258
CC _{1/2}	I _{ASU}	0.130181	0.001985	0.016947
CC _{1/2}	AV _z	0.002417	0.954413	0.000006
R _{mergeI}	R _{merge(I+/I-)}	0.915797	0	0.838685
R _{mergeI}	R _{measI}	0.986226	0	0.972642
R _{mergeI}	R _{meas(I+/I-)}	0.896073	0	0.802947
R _{mergeI}	R _{p.i.m.I}	0.697979	0	0.487175
R _{mergeI}	R _{p.i.m.(I+/I-)}	0.66775	0	0.445891
R _{mergeI}	N _{obstotal}	0.231511	0	0.053597
R _{mergeI}	N _{obsunique}	0.009718	0.818191	0.000094
R _{mergeI}	M	0.321401	0	0.103299
R _{mergeI}	T	0.203856	0.000001	0.041557
R _{mergeI}	d _{max}	0.233883	0	0.054701
R _{mergeI}	d _{min}	0.22442	0	0.050364
R _{mergeI}	B	-0.042683	0.312457	0.001822
R _{mergeI}	d _{inv}	-0.225517	0	0.050858
R _{mergeI}	m _{anom}	-0.1013	0.016292	0.010262
R _{mergeI}	CC _{anom}	-0.126364	0.002691	0.015968

R _{mergeI}	M _{anom}	0.317057	0	0.100525
R _{mergeI}	T _{anom}	0.21886	0	0.0479
R _{mergeI}	ΔI/σI	-0.117	0.005486	0.013689
R _{mergeI}	ΔF/F	0.692511	0	0.479571
R _{mergeI}	f' _{theor}	0.042779	0.311371	0.00183
R _{mergeI}	V _{cell}	0.243134	0	0.059114
R _{mergeI}	N _{sg}	0.06547	0.121074	0.004286
R _{mergeI}	a	0.133692	0.00149	0.017874
R _{mergeI}	b	0.195158	0.000003	0.038087
R _{mergeI}	c	0.255679	0	0.065372
R _{mergeI}	α	0.191732	0.000005	0.036761
R _{mergeI}	β	-0.017561	0.67783	0.000308
R _{mergeI}	γ	0.033298	0.430792	0.001109
R _{mergeI}	V _s	0.045625	0.280249	0.002082
R _{mergeI}	N _{cell}	0.22952	0	0.052679
R _{mergeI}	L	-0.031771	0.452241	0.001009
R _{mergeI}	V _m	0.045035	0.286519	0.002028
R _{mergeI}	MWS _{ASUVs}	-0.010808	0.798219	0.000117
R _{mergeI}	MW _{chain}	0.245374	0	0.060208
R _{mergeI}	N _{atomchain}	0.248079	0	0.061543
R _{mergeI}	N _{molASU}	0.144846	0.000572	0.02098
R _{mergeI}	MW _{ASU}	0.258505	0	0.066825
R _{mergeI}	N _{sitesASU}	0.209098	0.000001	0.043722
R _{mergeI}	MWS _{ASU}	0.005793	0.891002	0.000034
R _{mergeI}	I _{ASU}	-0.360897	0	0.130247
R _{mergeI}	AV _z	-0.048875	0.247363	0.002389
R _{merge(I+/I-)}	R _{measI}	0.872964	0	0.762067
R _{merge(I+/I-)}	R _{meas(I+/I-)}	0.977293	0	0.955101
R _{merge(I+/I-)}	R _{p.i.m.I}	0.508323	0	0.258392

$R_{\text{merge}}(I+/I-)$	$R_{\text{p.i.m.}}(I+/I-)$	0.723511	0	0.523468
$R_{\text{merge}}(I+/I-)$	N_{obstotal}	0.271626	0	0.073781
$R_{\text{merge}}(I+/I-)$	$N_{\text{obsunique}}$	0.028581	0.498925	0.000817
$R_{\text{merge}}(I+/I-)$	M	0.386217	0	0.149163
$R_{\text{merge}}(I+/I-)$	T	0.203553	0.000001	0.041434
$R_{\text{merge}}(I+/I-)$	d_{max}	0.287031	0	0.082387
$R_{\text{merge}}(I+/I-)$	d_{min}	0.211205	0	0.044608
$R_{\text{merge}}(I+/I-)$	B	0.016579	0.694915	0.000275
$R_{\text{merge}}(I+/I-)$	d_{inv}	-0.221175	0	0.048918
$R_{\text{merge}}(I+/I-)$	m_{anom}	-0.200151	0.000002	0.04006
$R_{\text{merge}}(I+/I-)$	CC_{anom}	-0.232355	0	0.053989
$R_{\text{merge}}(I+/I-)$	M_{anom}	0.383715	0	0.147237
$R_{\text{merge}}(I+/I-)$	T_{anom}	0.184825	0.00001	0.03416
$R_{\text{merge}}(I+/I-)$	$\Delta I/\sigma I$	-0.211527	0	0.044744
$R_{\text{merge}}(I+/I-)$	$\Delta F/F$	0.517815	0	0.268132
$R_{\text{merge}}(I+/I-)$	f'_{theor}	0.001603	0.969757	0.000003
$R_{\text{merge}}(I+/I-)$	V_{cell}	0.262157	0	0.068726
$R_{\text{merge}}(I+/I-)$	N_{sg}	0.107384	0.010853	0.011531
$R_{\text{merge}}(I+/I-)$	a	0.152656	0.000281	0.023304
$R_{\text{merge}}(I+/I-)$	b	0.170265	0.00005	0.02899
$R_{\text{merge}}(I+/I-)$	c	0.255633	0	0.065348
$R_{\text{merge}}(I+/I-)$	α	0.068077	0.106929	0.004634
$R_{\text{merge}}(I+/I-)$	β	-0.070144	0.09667	0.00492
$R_{\text{merge}}(I+/I-)$	γ	0.040317	0.34006	0.001625
$R_{\text{merge}}(I+/I-)$	V_s	0.071711	0.089429	0.005142
$R_{\text{merge}}(I+/I-)$	N_{cell}	0.246402	0	0.060714
$R_{\text{merge}}(I+/I-)$	L	-0.026914	0.524305	0.000724
$R_{\text{merge}}(I+/I-)$	V_m	0.072527	0.085833	0.00526
$R_{\text{merge}}(I+/I-)$	MWS_{ASUVs}	0.017661	0.6761	0.000312
$R_{\text{merge}}(I+/I-)$	MW_{chain}	0.227518	0	0.051764

$R_{\text{merge}}(I+/I-)$	$N_{\text{atomchain}}$	0.232133	0	0.053886
$R_{\text{merge}}(I+/I-)$	N_{molASU}	0.10473	0.012988	0.010968
$R_{\text{merge}}(I+/I-)$	MW_{ASU}	0.203019	0.000001	0.041217
$R_{\text{merge}}(I+/I-)$	N_{sitesASU}	0.133579	0.001504	0.017843
$R_{\text{merge}}(I+/I-)$	MWS_{ASU}	0.038638	0.360577	0.001493
$R_{\text{merge}}(I+/I-)$	I_{ASU}	-0.323916	0	0.104922
$R_{\text{merge}}(I+/I-)$	AV_z	-0.061284	0.14679	0.003756
R_{measI}	$R_{\text{meas}}(I+/I-)$	0.88109	0	0.77632
R_{measI}	$R_{\text{p.i.m.I}}$	0.805114	0	0.648208
R_{measI}	$R_{\text{p.i.m.}}(I+/I-)$	0.72241	0	0.521876
R_{measI}	N_{obstotal}	0.170748	0.000047	0.029155
R_{measI}	$N_{\text{obsunique}}$	0.025188	0.551248	0.000634
R_{measI}	M	0.219009	0	0.047965
R_{measI}	T	0.167228	0.000068	0.027965
R_{measI}	d_{max}	0.192321	0.000004	0.036987
R_{measI}	d_{min}	0.238619	0	0.056939
R_{measI}	B	-0.083135	0.048855	0.006911
R_{measI}	d_{inv}	-0.237285	0	0.056304
R_{measI}	m_{anom}	-0.128236	0.00232	0.016444
R_{measI}	CC_{anom}	-0.15076	0.000335	0.022729
R_{measI}	M_{anom}	0.214824	0	0.046149
R_{measI}	T_{anom}	0.156749	0.000191	0.02457
R_{measI}	$\Delta I/\sigma I$	-0.144988	0.000565	0.021021
R_{measI}	$\Delta F/F$	0.777715	0	0.60484
R_{measI}	f'_{theor}	0.056476	0.181247	0.003189
R_{measI}	V_{cell}	0.208189	0.000001	0.043343
R_{measI}	N_{sg}	-0.014872	0.724994	0.000221
R_{measI}	a	0.109518	0.009368	0.011994
R_{measI}	b	0.171806	0.000042	0.029517

R _{meas} I	c	0.224827	0	0.050547
R _{meas} I	α	0.227705	0	0.05185
R _{meas} I	β	0.00499	0.906035	0.000025
R _{meas} I	γ	-0.023322	0.581135	0.000544
R _{meas} I	V _s	0.030983	0.463528	0.00096
R _{meas} I	N _{cell}	0.196883	0.000003	0.038763
R _{meas} I	L	-0.029689	0.482426	0.000881
R _{meas} I	V _m	0.026196	0.535429	0.000686
R _{meas} I	MWS _{ASUVs}	-0.014152	0.7378	0.0002
R _{meas} I	MW _{chain}	0.251862	0	0.063435
R _{meas} I	N _{atomchain}	0.253493	0	0.064259
R _{meas} I	N _{molASU}	0.187036	0.000008	0.034983
R _{meas} I	MW _{ASU}	0.296993	0	0.088205
R _{meas} I	N _{sitesASU}	0.258252	0	0.066694
R _{meas} I	MWS _{ASU}	0.001005	0.981026	0.000001
R _{meas} I	I _{ASU}	-0.401506	0	0.161207
R _{meas} I	AV _z	-0.044427	0.293085	0.001974
R _{meas} (I+/I-)	R _{p.i.m.} I	0.622879	0	0.387978
R _{meas} (I+/I-)	R _{p.i.m.} (I+/I-)	0.852228	0	0.726293
R _{meas} (I+/I-)	N _{obstotal}	0.188124	0.000007	0.035391
R _{meas} (I+/I-)	N _{obsunique}	0.059154	0.161384	0.003499
R _{meas} (I+/I-)	M	0.23533	0	0.05538
R _{meas} (I+/I-)	T	0.186294	0.000009	0.034706
R _{meas} (I+/I-)	d _{max}	0.22784	0	0.051911
R _{meas} (I+/I-)	d _{min}	0.222298	0	0.049416
R _{meas} (I+/I-)	B	-0.02576	0.542244	0.000664
R _{meas} (I+/I-)	d _{inv}	-0.239272	0	0.057251
R _{meas} (I+/I-)	m _{anom}	-0.23946	0	0.057341
R _{meas} (I+/I-)	CC _{anom}	-0.277271	0	0.076879

$R_{\text{meas}}(I+/I-)$	M_{anom}	0.23217	0	0.053903
$R_{\text{meas}}(I+/I-)$	T_{anom}	0.132299	0.001671	0.017503
$R_{\text{meas}}(I+/I-)$	$\Delta I/\sigma I$	-0.258223	0	0.066679
$R_{\text{meas}}(I+/I-)$	$\Delta F/F$	0.622482	0	0.387484
$R_{\text{meas}}(I+/I-)$	f'_{theor}	0.028456	0.500797	0.00081
$R_{\text{meas}}(I+/I-)$	V_{cell}	0.215539	0	0.046457
$R_{\text{meas}}(I+/I-)$	N_{sg}	-0.011153	0.791926	0.000124
$R_{\text{meas}}(I+/I-)$	a	0.130941	0.001867	0.017146
$R_{\text{meas}}(I+/I-)$	b	0.135218	0.001313	0.018284
$R_{\text{meas}}(I+/I-)$	c	0.212645	0	0.045218
$R_{\text{meas}}(I+/I-)$	α	0.077456	0.066522	0.005999
$R_{\text{meas}}(I+/I-)$	β	-0.026945	0.523824	0.000726
$R_{\text{meas}}(I+/I-)$	γ	-0.041936	0.321008	0.001759
$R_{\text{meas}}(I+/I-)$	V_s	0.052772	0.211621	0.002785
$R_{\text{meas}}(I+/I-)$	N_{cell}	0.202852	0.000001	0.041149
$R_{\text{meas}}(I+/I-)$	L	-0.023343	0.580798	0.000545
$R_{\text{meas}}(I+/I-)$	V_m	0.047229	0.263665	0.002231
$R_{\text{meas}}(I+/I-)$	MWS_{ASUVs}	0.019086	0.651631	0.000364
$R_{\text{meas}}(I+/I-)$	MW_{chain}	0.244632	0	0.059845
$R_{\text{meas}}(I+/I-)$	$N_{\text{atomchain}}$	0.247478	0	0.061245
$R_{\text{meas}}(I+/I-)$	N_{molASU}	0.148335	0.000418	0.022003
$R_{\text{meas}}(I+/I-)$	MW_{ASU}	0.243234	0	0.059163
$R_{\text{meas}}(I+/I-)$	N_{sitesASU}	0.181835	0.000014	0.033064
$R_{\text{meas}}(I+/I-)$	MWS_{ASU}	0.039004	0.356038	0.001521
$R_{\text{meas}}(I+/I-)$	I_{ASU}	-0.398936	0	0.15915
$R_{\text{meas}}(I+/I-)$	AV_z	-0.053703	0.203656	0.002884
$R_{\text{p.i.m.I}}$	$R_{\text{p.i.m.}}(I+/I-)$	0.77852	0	0.606093
$R_{\text{p.i.m.I}}$	N_{obstotal}	-0.125573	0.002863	0.015769
$R_{\text{p.i.m.I}}$	$N_{\text{obsunique}}$	0.079253	0.060437	0.006281

R _{p.i.m.I}	M	-0.264174	0	0.069788
R _{p.i.m.I}	T	0.023045	0.585627	0.000531
R _{p.i.m.I}	d _{max}	-0.016903	0.689267	0.000286
R _{p.i.m.I}	d _{min}	0.227469	0	0.051742
R _{p.i.m.I}	B	-0.205812	0.000001	0.042359
R _{p.i.m.I}	d _{inv}	-0.223638	0	0.050014
R _{p.i.m.I}	m _{anom}	-0.186272	0.000009	0.034697
R _{p.i.m.I}	CC _{anom}	-0.200395	0.000002	0.040158
R _{p.i.m.I}	M _{anom}	-0.267631	0	0.071626
R _{p.i.m.I}	T _{anom}	-0.070019	0.097265	0.004903
R _{p.i.m.I}	ΔI/σI	-0.210635	0	0.044367
R _{p.i.m.I}	ΔF/F	0.911637	0	0.831082
R _{p.i.m.I}	f' _{theor}	0.110413	0.008801	0.012191
R _{p.i.m.I}	V _{cell}	0.017425	0.680201	0.000304
R _{p.i.m.I}	N _{sg}	-0.317886	0	0.101052
R _{p.i.m.I}	a	-0.00415	0.921799	0.000017
R _{p.i.m.I}	b	0.042599	0.313416	0.001815
R _{p.i.m.I}	c	0.059814	0.156746	0.003578
R _{p.i.m.I}	α	0.290484	0	0.084381
R _{p.i.m.I}	β	0.101562	0.016016	0.010315
R _{p.i.m.I}	γ	-0.21991	0	0.048361
R _{p.i.m.I}	V _s	-0.03449	0.414462	0.00119
R _{p.i.m.I}	N _{cell}	0.019206	0.649593	0.000369
R _{p.i.m.I}	L	-0.015183	0.719479	0.000231
R _{p.i.m.I}	V _m	-0.053071	0.209036	0.002817
R _{p.i.m.I}	MWS _{ASUVs}	-0.0234	0.579873	0.000548
R _{p.i.m.I}	MW _{chain}	0.22464	0	0.050463
R _{p.i.m.I}	N _{atomchain}	0.221729	0	0.049164
R _{p.i.m.I}	N _{molASU}	0.288049	0	0.082972
R _{p.i.m.I}	MW _{ASU}	0.363838	0	0.132378

R _{p.i.m.I}	N _{sitesASU}	0.369649	0	0.13664
R _{p.i.m.I}	MWS _{ASU}	-0.017649	0.676312	0.000311
R _{p.i.m.I}	I _{ASU}	-0.472569	0	0.223322
R _{p.i.m.I}	AV _z	-0.017299	0.682389	0.000299
R _{p.i.m.(I+/I-)}	N _{obstotal}	-0.078875	0.061679	0.006221
R _{p.i.m.(I+/I-)}	N _{obsunique}	0.122534	0.003622	0.015015
R _{p.i.m.(I+/I-)}	M	-0.218326	0	0.047666
R _{p.i.m.(I+/I-)}	T	0.115008	0.006344	0.013227
R _{p.i.m.(I+/I-)}	d _{max}	0.03876	0.359055	0.001502
R _{p.i.m.(I+/I-)}	d _{min}	0.204123	0.000001	0.041666
R _{p.i.m.(I+/I-)}	B	-0.120539	0.004215	0.01453
R _{p.i.m.(I+/I-)}	d _{inv}	-0.234282	0	0.054888
R _{p.i.m.(I+/I-)}	m _{anom}	-0.283278	0	0.080247
R _{p.i.m.(I+/I-)}	CC _{anom}	-0.328675	0	0.108027
R _{p.i.m.(I+/I-)}	M _{anom}	-0.222573	0	0.049539
R _{p.i.m.(I+/I-)}	T _{anom}	-0.009289	0.826082	0.000086
R _{p.i.m.(I+/I-)}	ΔI/σI	-0.317837	0	0.10102
R _{p.i.m.(I+/I-)}	ΔF/F	0.754161	0	0.568759
R _{p.i.m.(I+/I-)}	f' _{theor}	0.097987	0.02016	0.009601
R _{p.i.m.(I+/I-)}	V _{cell}	0.048119	0.254767	0.002315
R _{p.i.m.(I+/I-)}	N _{sg}	-0.292046	0	0.085291
R _{p.i.m.(I+/I-)}	a	0.047292	0.263028	0.002237
R _{p.i.m.(I+/I-)}	b	0.021151	0.616832	0.000447
R _{p.i.m.(I+/I-)}	c	0.071138	0.092025	0.005061
R _{p.i.m.(I+/I-)}	α	0.086378	0.040658	0.007461
R _{p.i.m.(I+/I-)}	β	0.077106	0.067766	0.005945
R _{p.i.m.(I+/I-)}	γ	-0.219592	0	0.048221
R _{p.i.m.(I+/I-)}	V _s	-0.005094	0.904101	0.000026
R _{p.i.m.(I+/I-)}	N _{cell}	0.047421	0.261733	0.002249

R _{p.i.m.} (I+/I-)	L	-0.011156	0.79187	0.000124
R _{p.i.m.} (I+/I-)	V _m	-0.023568	0.577155	0.000555
R _{p.i.m.} (I+/I-)	MWS _{ASUVs}	0.017605	0.677071	0.00031
R _{p.i.m.} (I+/I-)	MW _{chain}	0.240245	0	0.057718
R _{p.i.m.} (I+/I-)	N _{atomchain}	0.238626	0	0.056942
R _{p.i.m.} (I+/I-)	N _{molASU}	0.222534	0	0.049521
R _{p.i.m.} (I+/I-)	MW _{ASU}	0.294963	0	0.087003
R _{p.i.m.} (I+/I-)	N _{sitesASU}	0.262585	0	0.068951
R _{p.i.m.} (I+/I-)	MWS _{ASU}	0.030437	0.47145	0.000926
R _{p.i.m.} (I+/I-)	I _{ASU}	-0.503697	0	0.25371
R _{p.i.m.} (I+/I-)	AV _z	-0.028296	0.503215	0.000801
N _{obstotal}	N _{obsunique}	0.551436	0	0.304081
N _{obstotal}	M	0.646415	0	0.417853
N _{obstotal}	T	0.135979	0.001232	0.01849
N _{obstotal}	d _{max}	0.353478	0	0.124946
N _{obstotal}	d _{min}	-0.264105	0	0.069751
N _{obstotal}	B	-0.157408	0.000179	0.024777
N _{obstotal}	d _{inv}	0.312384	0	0.097584
N _{obstotal}	m _{anom}	-0.007891	0.851925	0.000062
N _{obstotal}	CC _{anom}	-0.034142	0.419198	0.001166
N _{obstotal}	M _{anom}	0.631109	0	0.398299
N _{obstotal}	T _{anom}	0.182437	0.000013	0.033283
N _{obstotal}	ΔI/σI	-0.015412	0.715425	0.000238
N _{obstotal}	ΔF/F	-0.115216	0.00625	0.013275
N _{obstotal}	f' _{theor}	-0.038106	0.367234	0.001452
N _{obstotal}	V _{cell}	0.321535	0	0.103385
N _{obstotal}	N _{sg}	0.092174	0.028896	0.008496
N _{obstotal}	a	0.189737	0.000006	0.036
N _{obstotal}	b	0.267943	0	0.071793

N_{obstotal}	c	0.240543	0	0.057861
N_{obstotal}	α	0.057847	0.170859	0.003346
N_{obstotal}	β	-0.031299	0.45899	0.00098
N_{obstotal}	γ	0.007018	0.868158	0.000049
N_{obstotal}	V_s	0.032405	0.44326	0.00105
N_{obstotal}	N_{cell}	0.322035	0	0.103707
N_{obstotal}	L	-0.00295	0.944364	0.000009
N_{obstotal}	V_m	0.011746	0.781126	0.000138
N_{obstotal}	$\text{MWS}_{\text{ASUVs}}$	-0.028153	0.505373	0.000793
N_{obstotal}	MW_{chain}	0.257968	0	0.066548
N_{obstotal}	$N_{\text{atomchain}}$	0.258263	0	0.0667
N_{obstotal}	N_{molASU}	0.118339	0.004969	0.014004
N_{obstotal}	MW_{ASU}	0.302447	0	0.091474
N_{obstotal}	N_{sitesASU}	0.255817	0	0.065442
N_{obstotal}	MWS_{ASU}	-0.01409	0.738917	0.000199
N_{obstotal}	I_{ASU}	-0.168933	0.000057	0.028538
N_{obstotal}	ΔV_z	0.003146	0.940673	0.00001
$N_{\text{obsunique}}$	M	-0.088718	0.035496	0.007871
$N_{\text{obsunique}}$	T	0.023936	0.571226	0.000573
$N_{\text{obsunique}}$	d_{\max}	0.180039	0.000018	0.032414
$N_{\text{obsunique}}$	d_{\min}	-0.356636	0	0.12719
$N_{\text{obsunique}}$	B	-0.294421	0	0.086684
$N_{\text{obsunique}}$	d_{inv}	0.38273	0	0.146482
$N_{\text{obsunique}}$	m_{anom}	-0.05534	0.190196	0.003062
$N_{\text{obsunique}}$	CC_{anom}	-0.090669	0.031627	0.008221
$N_{\text{obsunique}}$	M_{anom}	-0.100341	0.017338	0.010068
$N_{\text{obsunique}}$	T_{anom}	-0.065131	0.123018	0.004242
$N_{\text{obsunique}}$	$\Delta I/\sigma I$	-0.077915	0.064922	0.006071
$N_{\text{obsunique}}$	$\Delta F/F$	0.090956	0.031089	0.008273

$N_{\text{obsunique}}$	f'_{theor}	0.017673	0.675899	0.000312
$N_{\text{obsunique}}$	V_{cell}	0.120036	0.004377	0.014409
$N_{\text{obsunique}}$	N_{sg}	-0.275638	0	0.075976
$N_{\text{obsunique}}$	a	0.081425	0.053704	0.00663
$N_{\text{obsunique}}$	b	0.170157	0.00005	0.028953
$N_{\text{obsunique}}$	c	0.129025	0.002179	0.016647
$N_{\text{obsunique}}$	α	0.061382	0.146147	0.003768
$N_{\text{obsunique}}$	β	0.101793	0.015776	0.010362
$N_{\text{obsunique}}$	γ	-0.182822	0.000013	0.033424
$N_{\text{obsunique}}$	V_s	-0.03354	0.427446	0.001125
$N_{\text{obsunique}}$	N_{cell}	0.129106	0.002164	0.016668
$N_{\text{obsunique}}$	L	0.026789	0.526234	0.000718
$N_{\text{obsunique}}$	V_m	-0.072491	0.085988	0.005255
$N_{\text{obsunique}}$	MWS_{ASUVs}	-0.065234	0.122422	0.004256
$N_{\text{obsunique}}$	MW_{chain}	0.29067	0	0.084489
$N_{\text{obsunique}}$	$N_{\text{atomchain}}$	0.286156	0	0.081885
$N_{\text{obsunique}}$	N_{molASU}	0.400323	0	0.160259
$N_{\text{obsunique}}$	MW_{ASU}	0.584764	0	0.341949
$N_{\text{obsunique}}$	N_{sitesASU}	0.606049	0	0.367296
$N_{\text{obsunique}}$	MWS_{ASU}	-0.058886	0.163292	0.003468
$N_{\text{obsunique}}$	I_{ASU}	-0.354903	0	0.125956
$N_{\text{obsunique}}$	AV_z	0.029377	0.487033	0.000863
M	T	0.166753	0.000071	0.027807
M	d_{\max}	0.305498	0	0.093329
M	d_{\min}	0.024924	0.555438	0.000621
M	B	0.155796	0.000209	0.024272
M	d_{inv}	-0.01109	0.793067	0.000123
M	m_{anom}	0.077951	0.064799	0.006076
M	CC_{anom}	0.07128	0.091374	0.005081

M	M_{anom}	0.999032	0	0.998066
M	T_{anom}	0.270732	0	0.073296
M	$\Delta I/\sigma I$	0.110597	0.008688	0.012232
M	$\Delta F/F$	-0.25161	0	0.063308
M	f'_{theor}	-0.127224	0.002514	0.016186
M	V_{cell}	0.33255	0	0.110589
M	N_{sg}	0.492219	0	0.242279
M	a	0.202638	0.000001	0.041062
M	b	0.224775	0	0.050524
M	c	0.204517	0.000001	0.041827
M	α	0.008914	0.833006	0.000079
M	β	-0.157153	0.000184	0.024697
M	γ	0.241474	0	0.05831
M	V_s	0.089529	0.033841	0.008015
M	N_{cell}	0.31625	0	0.100014
M	L	-0.024627	0.560155	0.000606
M	V_m	0.10453	0.013163	0.010926
M	MWS_{ASUVs}	0.038382	0.363761	0.001473
M	MW_{chain}	-0.013897	0.742364	0.000193
M	$N_{\text{atomchain}}$	-0.009079	0.829948	0.000082
M	N_{molASU}	-0.10708	0.011081	0.011466
M	MW_{ASU}	-0.084371	0.045579	0.007119
M	N_{sitesASU}	-0.129419	0.002111	0.016749
M	MWS_{ASU}	0.050204	0.23473	0.00252
M	I_{ASU}	0.18451	0.000011	0.034044
M	AV_z	-0.018837	0.655883	0.000355
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T	d_{max}	0.052198	0.216641	0.002725
T	d_{min}	0.000208	0.996083	0
T	B	0.237291	0	0.056307

T	d_{inv}	-0.022172	0.599923	0.000492
T	m_{anom}	0.016474	0.696764	0.000271
T	CC_{anom}	0.160459	0.000133	0.025747
T	M_{anom}	0.15169	0.000307	0.02301
T	T_{anom}	0.91627	0	0.839551
T	$\Delta I/\sigma I$	0.065607	0.120298	0.004304
T	$\Delta F/F$	0.127357	0.002488	0.01622
T	f'_{theor}	0.198564	0.000002	0.039428
T	V_{cell}	0.122901	0.003521	0.015105
T	N_{sg}	0.223603	0	0.049998
T	a	0.19638	0.000003	0.038565
T	b	0.135561	0.001276	0.018377
T	c	0.074207	0.078798	0.005507
T	α	0.149666	0.000371	0.0224
T	β	0.119754	0.004471	0.014341
T	γ	0.201588	0.000001	0.040638
T	V_s	0.100854	0.016772	0.010172
T	N_{cell}	0.115718	0.006025	0.013391
T	L	-0.057616	0.172574	0.00332
T	V_m	0.10749	0.010774	0.011554
T	MWS_{ASUVs}	-0.031348	0.458277	0.000983
T	MW_{chain}	0.038519	0.362052	0.001484
T	$N_{\text{atomchain}}$	0.039749	0.346923	0.00158
T	N_{molASU}	-0.068473	0.104902	0.004688
T	MW_{ASU}	-0.032581	0.440779	0.001062
T	N_{sitesASU}	-0.054785	0.194687	0.003001
T	MWS_{ASU}	-0.008932	0.832663	0.00008
T	I_{ASU}	-0.1611	0.000125	0.025953
T	AV_z	0.003269	0.938366	0.000011

d_{\max}	d_{\min}	0.238624	0	0.056941
d_{\max}	B	0.239818	0	0.057513
d_{\max}	d_{inv}	-0.154255	0.000242	0.023795
d_{\max}	m_{anom}	-0.227894	0	0.051936
d_{\max}	CC_{anom}	-0.279757	0	0.078264
d_{\max}	M_{anom}	0.303223	0	0.091944
d_{\max}	T_{anom}	0.06481	0.12488	0.0042
d_{\max}	$\Delta I/\sigma I$	-0.230896	0	0.053313
d_{\max}	$\Delta F/F$	-0.092999	0.027486	0.008649
d_{\max}	f'_{theor}	-0.155897	0.000207	0.024304
d_{\max}	V_{cell}	0.274667	0	0.075442
d_{\max}	N_{sg}	0.065751	0.119486	0.004323
d_{\max}	a	0.265838	0	0.07067
d_{\max}	b	0.320792	0	0.102907
d_{\max}	c	0.158885	0.000155	0.025244
d_{\max}	α	0.032275	0.445096	0.001042
d_{\max}	β	-0.04434	0.294032	0.001966
d_{\max}	γ	0.054788	0.194664	0.003002
d_{\max}	V_s	0.063551	0.132391	0.004039
d_{\max}	N_{cell}	0.270183	0	0.072999
d_{\max}	L	-0.016183	0.701859	0.000262
d_{\max}	V_m	0.058751	0.164259	0.003452
d_{\max}	MWS_{ASUVs}	0.024391	0.56392	0.000595
d_{\max}	MW_{chain}	0.270356	0	0.073092
d_{\max}	$N_{\text{atomchain}}$	0.272707	0	0.074369
d_{\max}	N_{molASU}	0.232678	0	0.054139
d_{\max}	MW_{ASU}	0.360482	0	0.129947
d_{\max}	N_{sitesASU}	0.288042	0	0.082968
d_{\max}	MWS_{ASU}	0.037945	0.369257	0.00144
d_{\max}	I_{ASU}	-0.222251	0	0.049395

d_{\max}	AV_z	-0.049444	0.241897	0.002445
d_{\min}	B	0.712693	0	0.507931
d_{\min}	d_{inv}	-0.89546	0	0.801848
d_{\min}	m_{anom}	-0.197555	0.000002	0.039028
d_{\min}	CC_{anom}	-0.155283	0.000219	0.024113
d_{\min}	M_{anom}	0.035015	0.407388	0.001226
d_{\min}	T_{anom}	-0.01012	0.810814	0.000102
d_{\min}	$\Delta I/\sigma I$	-0.186242	0.000009	0.034686
d_{\min}	$\Delta F/F$	0.168133	0.000062	0.028269
d_{\min}	f'_{theor}	-0.058386	0.166898	0.003409
d_{\min}	V_{cell}	0.259587	0	0.067386
d_{\min}	N_{sg}	0.091779	0.029592	0.008423
d_{\min}	a	0.313014	0	0.097978
d_{\min}	b	0.320795	0	0.102909
d_{\min}	c	0.177204	0.000024	0.031401
d_{\min}	α	0.014747	0.727206	0.000217
d_{\min}	β	-0.105029	0.01273	0.011031
d_{\min}	γ	0.044761	0.289461	0.002004
d_{\min}	V_s	0.098065	0.020061	0.009617
d_{\min}	N_{cell}	0.256021	0	0.065547
d_{\min}	L	-0.019485	0.644851	0.00038
d_{\min}	V_m	0.118401	0.004946	0.014019
d_{\min}	MWS_{ASUVs}	0.051045	0.226975	0.002606
d_{\min}	MW_{chain}	0.186497	0.000009	0.034781
d_{\min}	$N_{\text{atomchain}}$	0.198642	0.000002	0.039459
d_{\min}	N_{molASU}	0.315845	0	0.099758
d_{\min}	MW_{ASU}	0.350999	0	0.1232
d_{\min}	N_{sitesASU}	0.250284	0	0.062642
d_{\min}	MWS_{ASU}	0.062357	0.139835	0.003888

d_{\min}	I_{ASU}	-0.236572	0	0.055967
d_{\min}	ΔV_z	-0.093395	0.02683	0.008723
B	d_{inv}	-0.630203	0	0.397155
B	m_{anom}	-0.057055	0.176801	0.003255
B	CC_{anom}	0.030042	0.47723	0.000903
B	M_{anom}	0.160948	0.000127	0.025904
B	T_{anom}	0.248517	0	0.061761
B	$\Delta I/\sigma I$	-0.01298	0.758808	0.000168
B	$\Delta F/F$	-0.199803	0.000002	0.039921
B	f'_{theor}	-0.011354	0.788251	0.000129
B	V_{cell}	0.247103	0	0.06106
B	N_{sg}	0.26422	0	0.069812
B	a	0.294362	0	0.086649
B	b	0.295481	0	0.087309
B	c	0.159801	0.000142	0.025536
B	α	-0.082918	0.049447	0.006875
B	β	-0.111136	0.008365	0.012351
B	γ	0.178384	0.000021	0.031821
B	V_s	0.132184	0.001687	0.017473
B	N_{cell}	0.242467	0	0.05879
B	L	-0.113426	0.00711	0.012865
B	V_m	0.148195	0.000424	0.021962
B	MWS_{ASUVs}	0.040149	0.342084	0.001612
B	MW_{chain}	0.083043	0.049106	0.006896
B	$N_{\text{atomchain}}$	0.097186	0.021208	0.009445
B	N_{molASU}	0.134501	0.001394	0.018091
B	MW_{ASU}	0.170832	0.000047	0.029183
B	N_{sitesASU}	0.062274	0.140363	0.003878
B	MWS_{ASU}	0.057835	0.170951	0.003345

B	I _{ASU}	-0.106191	0.011771	0.011277
B	AV _z	-0.094782	0.02464	0.008984
d _{inv}	m _{anom}	0.150091	0.000356	0.022527
d _{inv}	CC _{anom}	0.120397	0.00426	0.014496
d _{inv}	M _{anom}	-0.020693	0.624478	0.000428
d _{inv}	T _{anom}	-0.00731	0.862727	0.000053
d _{inv}	ΔI/σI	0.156677	0.000192	0.024548
d _{inv}	ΔF/F	-0.183938	0.000011	0.033833
d _{inv}	f' _{theor}	0.031887	0.450579	0.001017
d _{inv}	V _{cell}	-0.238005	0	0.056646
d _{inv}	N _{sg}	-0.095115	0.024138	0.009047
d _{inv}	a	-0.305115	0	0.093095
d _{inv}	b	-0.314627	0	0.09899
d _{inv}	c	-0.168877	0.000057	0.028519
d _{inv}	α	0.01719	0.684268	0.000296
d _{inv}	β	0.062457	0.139195	0.003901
d _{inv}	γ	-0.063424	0.133168	0.004023
d _{inv}	V _s	-0.079407	0.05994	0.006305
d _{inv}	N _{cell}	-0.235043	0	0.055245
d _{inv}	L	0.006382	0.880014	0.000041
d _{inv}	V _m	-0.095678	0.023307	0.009154
d _{inv}	MWS _{ASUVs}	-0.048945	0.246692	0.002396
d _{inv}	MW _{chain}	-0.158109	0.000168	0.024998
d _{inv}	N _{atomchain}	-0.166832	0.000071	0.027833
d _{inv}	N _{molASU}	-0.271065	0	0.073476
d _{inv}	MW _{ASU}	-0.29409	0	0.086489
d _{inv}	N _{sitesASU}	-0.219255	0	0.048073
d _{inv}	MWS _{ASU}	-0.056065	0.184445	0.003143
d _{inv}	I _{ASU}	0.288625	0	0.083304

d_{inv}	AV_z	0.067755	0.108605	0.004591
m_{anom}	CC_{anom}	0.800133	0	0.640213
m_{anom}	M_{anom}	0.080777	0.055643	0.006525
m_{anom}	T_{anom}	0.11594	0.005929	0.013442
m_{anom}	$\Delta I/\sigma I$	0.908074	0	0.824598
m_{anom}	$\Delta F/F$	0.019654	0.641976	0.000386
m_{anom}	f'_{theor}	0.140219	0.000859	0.019661
m_{anom}	V_{cell}	-0.065598	0.120347	0.004303
m_{anom}	N_{sg}	0.212855	0	0.045307
m_{anom}	a	-0.091723	0.029692	0.008413
m_{anom}	b	-0.040559	0.337167	0.001645
m_{anom}	c	0.002067	0.961014	0.000004
m_{anom}	α	-0.165057	0.000085	0.027244
m_{anom}	β	-0.106245	0.011727	0.011288
m_{anom}	γ	0.09023	0.032465	0.008141
m_{anom}	V_s	-0.061657	0.144342	0.003802
m_{anom}	N_{cell}	-0.062861	0.136653	0.003952
m_{anom}	L	-0.065829	0.119042	0.004334
m_{anom}	V_m	-0.05219	0.216709	0.002724
m_{anom}	$\text{MWS}_{\text{ASUVs}}$	-0.0887	0.035533	0.007868
m_{anom}	MW_{chain}	-0.109288	0.009519	0.011944
m_{anom}	$N_{\text{atomchain}}$	-0.115287	0.006217	0.013291
m_{anom}	N_{molASU}	-0.187929	0.000007	0.035317
m_{anom}	MW_{ASU}	-0.212722	0	0.04525
m_{anom}	N_{sitesASU}	-0.154886	0.000228	0.02399
m_{anom}	MWS_{ASU}	-0.111186	0.008336	0.012362
m_{anom}	I_{ASU}	0.235855	0	0.055627
m_{anom}	AV_z	0.066551	0.115042	0.004429

CC _{anom}	M _{anom}	0.07226	0.086995	0.005222
CC _{anom}	T _{anom}	0.229073	0	0.052474
CC _{anom}	ΔI/σI	0.840959	0	0.707212
CC _{anom}	ΔF/F	0.028364	0.502194	0.000804
CC _{anom}	f' _{theor}	0.190764	0.000005	0.036391
CC _{anom}	V _{cell}	-0.061816	0.143306	0.003821
CC _{anom}	N _{sg}	0.252862	0	0.063939
CC _{anom}	a	-0.071869	0.088722	0.005165
CC _{anom}	b	-0.040514	0.337713	0.001641
CC _{anom}	c	-0.006942	0.869573	0.000048
CC _{anom}	α	-0.053495	0.205415	0.002862
CC _{anom}	β	-0.073704	0.080852	0.005432
CC _{anom}	γ	0.163337	0.0001	0.026679
CC _{anom}	V _s	-0.02532	0.549163	0.000641
CC _{anom}	N _{cell}	-0.060561	0.151626	0.003668
CC _{anom}	L	-0.057209	0.175637	0.003273
CC _{anom}	V _m	-0.009174	0.828212	0.000084
CC _{anom}	MWS _{ASUVs}	-0.073263	0.082692	0.005367
CC _{anom}	MW _{chain}	-0.136024	0.001227	0.018503
CC _{anom}	N _{atomchain}	-0.142805	0.000686	0.020393
CC _{anom}	N _{molASU}	-0.190402	0.000005	0.036253
CC _{anom}	MW _{ASU}	-0.235652	0	0.055532
CC _{anom}	N _{sitesASU}	-0.190411	0.000005	0.036256
CC _{anom}	MWS _{ASU}	-0.085325	0.043183	0.00728
CC _{anom}	I _{ASU}	0.218658	0	0.047811
CC _{anom}	AV _z	0.073283	0.082607	0.00537
M _{anom}	T _{anom}	0.253586	0	0.064306
M _{anom}	ΔI/σI	0.113366	0.007141	0.012852
M _{anom}	ΔF/F	-0.253977	0	0.064504

M _{anom}	f' theor	-0.134308	0.001416	0.018039
M _{anom}	V _{cell}	0.330603	0	0.109298
M _{anom}	N _{sg}	0.497825	0	0.24783
M _{anom}	a	0.196693	0.000003	0.038688
M _{anom}	b	0.218902	0	0.047918
M _{anom}	c	0.210497	0	0.044309
M _{anom}	α	0.007421	0.860651	0.000055
M _{anom}	β	-0.164615	0.000088	0.027098
M _{anom}	γ	0.241017	0	0.058089
M _{anom}	V _s	0.085216	0.04345	0.007262
M _{anom}	N _{cell}	0.314442	0	0.098874
M _{anom}	L	-0.02469	0.559153	0.00061
M _{anom}	V _m	0.101309	0.016283	0.010263
M _{anom}	MWS _{ASUVs}	0.042867	0.310375	0.001838
M _{anom}	MW _{chain}	-0.021568	0.609895	0.000465
M _{anom}	N _{atomchain}	-0.017253	0.683174	0.000298
M _{anom}	N _{molASU}	-0.110011	0.009052	0.012102
M _{anom}	MW _{ASU}	-0.092449	0.028419	0.008547
M _{anom}	N _{sitesASU}	-0.136137	0.001215	0.018533
M _{anom}	MWS _{ASU}	0.053101	0.208781	0.00282
M _{anom}	I _{ASU}	0.198424	0.000002	0.039372
M _{anom}	AV _z	-0.016574	0.69501	0.000275
T _{anom}	$\Delta I/\sigma I$	0.149563	0.000374	0.022369
T _{anom}	$\Delta F/F$	0.036982	0.381539	0.001368
T _{anom}	f' theor	0.172731	0.000038	0.029836
T _{anom}	V _{cell}	0.146609	0.000489	0.021494
T _{anom}	N _{sg}	0.300844	0	0.090507
T _{anom}	a	0.198065	0.000002	0.03923
T _{anom}	b	0.149603	0.000373	0.022381

T _{anom}	c	0.118616	0.004868	0.01407
T _{anom}	α	0.145874	0.000522	0.021279
T _{anom}	β	0.08812	0.03676	0.007765
T _{anom}	γ	0.260381	0	0.067798
T _{anom}	V _s	0.110153	0.008963	0.012134
T _{anom}	N _{cell}	0.138585	0.000988	0.019206
T _{anom}	L	-0.062278	0.140339	0.003878
T _{anom}	V _m	0.121616	0.003884	0.01479
T _{anom}	MWS _{ASUVs}	-0.038524	0.361995	0.001484
T _{anom}	MW _{chain}	0.030034	0.477342	0.000902
T _{anom}	N _{atomchain}	0.031695	0.453323	0.001005
T _{anom}	N _{molASU}	-0.148821	0.0004	0.022148
T _{anom}	MW _{ASU}	-0.095676	0.023311	0.009154
T _{anom}	N _{sitesASU}	-0.14072	0.000822	0.019802
T _{anom}	MWS _{ASU}	-0.013983	0.74082	0.000196
T _{anom}	I _{ASU}	-0.060139	0.154501	0.003617
T _{anom}	AV _z	-0.001143	0.978423	0.000001
$\Delta I/\sigma I$	$\Delta F/F$	0.007089	0.866838	0.00005
$\Delta I/\sigma I$	f' theor	0.121395	0.00395	0.014737
$\Delta I/\sigma I$	V _{cell}	-0.076729	0.069122	0.005887
$\Delta I/\sigma I$	N _{sg}	0.258124	0	0.066628
$\Delta I/\sigma I$	a	-0.08895	0.035015	0.007912
$\Delta I/\sigma I$	b	-0.082709	0.050027	0.006841
$\Delta I/\sigma I$	c	-0.006849	0.871303	0.000047
$\Delta I/\sigma I$	α	-0.07934	0.060155	0.006295
$\Delta I/\sigma I$	β	-0.092786	0.027844	0.008609
$\Delta I/\sigma I$	γ	0.14307	0.00067	0.020469
$\Delta I/\sigma I$	V _s	-0.04011	0.34255	0.001609
$\Delta I/\sigma I$	N _{cell}	-0.076706	0.069209	0.005884

$\Delta I/\sigma I$	L	-0.041574	0.325213	0.001728
$\Delta I/\sigma I$	V_m	-0.027889	0.509377	0.000778
$\Delta I/\sigma I$	MWS _{ASUVs}	-0.098651	0.019327	0.009732
$\Delta I/\sigma I$	MW _{chain}	-0.163314	0.000101	0.026672
$\Delta I/\sigma I$	N _{atomchain}	-0.168819	0.000058	0.0285
$\Delta I/\sigma I$	N _{molASU}	-0.186158	0.000009	0.034655
$\Delta I/\sigma I$	MW _{ASU}	-0.23311	0	0.05434
$\Delta I/\sigma I$	N _{sitesASU}	-0.16585	0.000078	0.027506
$\Delta I/\sigma I$	MWS _{ASU}	-0.117513	0.005282	0.013809
$\Delta I/\sigma I$	I _{ASU}	0.310995	0	0.096718
$\Delta I/\sigma I$	AV _z	0.063918	0.130165	0.004086
$\Delta F/F$	f' theor	0.154232	0.000242	0.023787
$\Delta F/F$	V_{cell}	0.012174	0.773376	0.000148
$\Delta F/F$	N _{sg}	-0.268056	0	0.071854
$\Delta F/F$	a	-0.007734	0.854852	0.00006
$\Delta F/F$	b	0.041687	0.323901	0.001738
$\Delta F/F$	c	0.085014	0.043951	0.007227
$\Delta F/F$	α	0.242717	0	0.058912
$\Delta F/F$	β	0.069695	0.09883	0.004857
$\Delta F/F$	γ	-0.196271	0.000003	0.038522
$\Delta F/F$	V_s	-0.037428	0.37582	0.001401
$\Delta F/F$	N _{cell}	0.011349	0.788351	0.000129
$\Delta F/F$	L	-0.039192	0.353727	0.001536
$\Delta F/F$	V_m	-0.050528	0.231717	0.002553
$\Delta F/F$	MWS _{ASUVs}	-0.044446	0.292872	0.001975
$\Delta F/F$	MW _{chain}	0.241983	0	0.058556
$\Delta F/F$	N _{atomchain}	0.236739	0	0.056045
$\Delta F/F$	N _{molASU}	0.209418	0.000001	0.043856
$\Delta F/F$	MW _{ASU}	0.28788	0	0.082875

$\Delta F/F$	N_{sitesASU}	0.297038	0	0.088231
$\Delta F/F$	MWS_{ASU}	-0.0412	0.329587	0.001697
$\Delta F/F$	I_{ASU}	-0.478383	0	0.228851
$\Delta F/F$	AV_z	0.010913	0.796305	0.000119
f''_{theor}	V_{cell}	-0.009302	0.825845	0.000087
f''_{theor}	N_{sg}	-0.03976	0.346783	0.001581
f''_{theor}	a	0.047069	0.265293	0.002215
f''_{theor}	b	0.008539	0.839931	0.000073
f''_{theor}	c	-0.074957	0.075813	0.005619
f''_{theor}	α	0.036867	0.383018	0.001359
f''_{theor}	β	0.072591	0.085556	0.005269
f''_{theor}	γ	-0.007523	0.858759	0.000057
f''_{theor}	V_s	0.067058	0.112295	0.004497
f''_{theor}	N_{cell}	-0.0082	0.846196	0.000067
f''_{theor}	L	0.025183	0.551326	0.000634
f''_{theor}	V_m	0.061181	0.147471	0.003743
f''_{theor}	MWS_{ASUVs}	0.015304	0.717344	0.000234
f''_{theor}	MW_{chain}	0.03384	0.423315	0.001145
f''_{theor}	$N_{\text{atomchain}}$	0.036793	0.383979	0.001354
f''_{theor}	N_{molASU}	-0.011001	0.794694	0.000121
f''_{theor}	MW_{ASU}	0.004696	0.911545	0.000022
f''_{theor}	N_{sitesASU}	-0.003745	0.929412	0.000014
f''_{theor}	MWS_{ASU}	0.03332	0.430491	0.00111
f''_{theor}	I_{ASU}	-0.125508	0.002878	0.015752
f''_{theor}	AV_z	-0.013218	0.754536	0.000175
V_{cell}	N_{sg}	0.241783	0	0.058459
V_{cell}	a	0.545946	0	0.298057
V_{cell}	b	0.571229	0	0.326303

V_{cell}	c	0.447857	0	0.200576
V_{cell}	α	0.01966	0.641883	0.000386
V_{cell}	β	-0.073708	0.080837	0.005433
V_{cell}	γ	0.040894	0.333193	0.001672
V_{cell}	V_s	0.063002	0.135776	0.003969
V_{cell}	N_{cell}	0.98942	0	0.978952
V_{cell}	L	-0.021566	0.609926	0.000465
V_{cell}	V_m	0.056692	0.179577	0.003214
V_{cell}	$\text{MWS}_{\text{ASUVs}}$	-0.019675	0.64162	0.000387
V_{cell}	MW_{chain}	0.257373	0	0.066241
V_{cell}	$N_{\text{atomchain}}$	0.250397	0	0.062699
V_{cell}	N_{molASU}	0.229531	0	0.052684
V_{cell}	MW_{ASU}	0.363624	0	0.132223
V_{cell}	N_{sitesASU}	0.293865	0	0.086357
V_{cell}	MWS_{ASU}	-0.00729	0.863085	0.000053
V_{cell}	I_{ASU}	-0.209725	0.000001	0.043985
V_{cell}	AV_z	0.044102	0.296633	0.001945
N_{sg}	a	0.258303	0	0.06672
N_{sg}	b	0.172685	0.000039	0.02982
N_{sg}	c	0.235977	0	0.055685
N_{sg}	α	0.014151	0.737821	0.0002
N_{sg}	β	-0.299188	0	0.089513
N_{sg}	γ	0.788098	0	0.621098
N_{sg}	V_s	0.149871	0.000364	0.022461
N_{sg}	N_{cell}	0.223436	0	0.049924
N_{sg}	L	-0.041302	0.328393	0.001706
N_{sg}	V_m	0.194975	0.000003	0.038015
N_{sg}	$\text{MWS}_{\text{ASUVs}}$	0.012842	0.761297	0.000165
N_{sg}	MW_{chain}	-0.14786	0.000437	0.021862

N _{sg}	N _{atomchain}	-0.155773	0.00021	0.024265
N _{sg}	N _{molASU}	-0.254922	0	0.064985
N _{sg}	MW _{ASU}	-0.281318	0	0.07914
N _{sg}	N _{sitesASU}	-0.272	0	0.073984
N _{sg}	MWS _{ASU}	0.020569	0.626554	0.000423
N _{sg}	I _{ASU}	0.378535	0	0.143289
N _{sg}	AV _z	0.069301	0.100755	0.004803
a	b	0.45929	0	0.210947
a	c	0.022581	0.593212	0.00051
a	α	0.028085	0.506397	0.000789
a	β	0.09411	0.02568	0.008857
a	γ	0.190354	0.000006	0.036235
a	V _s	0.088	0.037017	0.007744
a	N _{cell}	0.535843	0	0.287128
a	L	-0.023075	0.585146	0.000532
a	V _m	0.081339	0.053958	0.006616
a	MWS _{ASUVs}	-0.039856	0.345616	0.001589
a	MW _{chain}	0.13004	0.002008	0.01691
a	N _{atomchain}	0.122915	0.003517	0.015108
a	N _{molASU}	0.368116	0	0.135509
a	MW _{ASU}	0.368248	0	0.135607
a	N _{sitesASU}	0.347348	0	0.12065
a	MWS _{ASU}	-0.026693	0.527719	0.000712
a	I _{ASU}	-0.228881	0	0.052386
a	AV _z	0.051902	0.219255	0.002694
b	c	0.030263	0.473993	0.000916
b	α	0.059638	0.157971	0.003557
b	β	-0.077287	0.067121	0.005973

b	γ	0.116371	0.005745	0.013542
b	V_s	0.126579	0.002646	0.016022
b	N_{cell}	0.556852	0	0.310084
b	L	-0.033652	0.425904	0.001132
b	V_m	0.110849	0.008536	0.012287
b	MWS_{ASUVs}	0.020814	0.622456	0.000433
b	MW_{chain}	0.300809	0	0.090486
b	$N_{atomchain}$	0.296805	0	0.088093
b	N_{molASU}	0.233494	0	0.054519
b	MW_{ASU}	0.385423	0	0.148551
b	$N_{sitesASU}$	0.285058	0	0.081258
b	MWS_{ASU}	0.046933	0.266675	0.002203
b	I_{ASU}	-0.313664	0	0.098385
b	AV_z	0.02524	0.550428	0.000637
c	α	0.043707	0.300981	0.00191
c	β	-0.173822	0.000034	0.030214
c	γ	0.104834	0.012898	0.01099
c	V_s	0.122232	0.003706	0.014941
c	N_{cell}	0.440174	0	0.193753
c	L	-0.031297	0.45901	0.00098
c	V_m	0.123016	0.00349	0.015133
c	MWS_{ASUVs}	-0.028376	0.502008	0.000805
c	MW_{chain}	0.309184	0	0.095595
c	$N_{atomchain}$	0.301647	0	0.090991
c	N_{molASU}	0.08724	0.038688	0.007611
c	MW_{ASU}	0.281907	0	0.079472
c	$N_{sitesASU}$	0.236133	0	0.055759
c	MWS_{ASU}	-0.004259	0.919758	0.000018
c	I_{ASU}	-0.193271	0.000004	0.037354

c	AV _z	0.039555	0.349279	0.001565
α	β	0.262442	0	0.068876
α	γ	0.144278	0.000602	0.020816
α	V _s	0.024854	0.556552	0.000618
α	N _{cell}	0.006533	0.877193	0.000043
α	L	0.149864	0.000364	0.022459
α	V _m	0.02947	0.485664	0.000868
α	MWS _{ASUVs}	0.031646	0.454013	0.001001
α	MW _{chain}	0.051479	0.223038	0.00265
α	N _{atomchain}	0.012685	0.764128	0.000161
α	N _{molASU}	0.04101	0.331825	0.001682
α	MW _{ASU}	0.095668	0.023323	0.009152
α	N _{sitesASU}	0.07754	0.066226	0.006013
α	MWS _{ASU}	0.037851	0.370446	0.001433
α	I _{ASU}	-0.070104	0.09686	0.004915
α	AV _z	0.204286	0.000001	0.041733
β	γ	-0.101749	0.015821	0.010353
β	V _s	-0.070717	0.093969	0.005001
β	N _{cell}	-0.067338	0.110801	0.004534
β	L	0.119587	0.004527	0.014301
β	V _m	-0.088173	0.036646	0.007774
β	MWS _{ASUVs}	0.010238	0.808654	0.000105
β	MW _{chain}	-0.043646	0.301657	0.001905
β	N _{atomchain}	-0.04607	0.275574	0.002122
β	N _{molASU}	0.121619	0.003883	0.014791
β	MW _{ASU}	0.076998	0.068151	0.005929
β	N _{sitesASU}	0.068162	0.106489	0.004646
β	MWS _{ASU}	0.00429	0.919174	0.000018

β	I _{ASU}	-0.162619	0.000108	0.026445
β	AV _z	0.01949	0.644757	0.00038
γ	V _s	0.120902	0.004101	0.014617
γ	N _{cell}	0.032609	0.440395	0.001063
γ	L	-0.008805	0.83501	0.000078
γ	V _m	0.156946	0.000187	0.024632
γ	MWS _{ASUVs}	0.027395	0.516915	0.00075
γ	MW _{chain}	-0.07815	0.064115	0.006107
γ	N _{atomchain}	-0.089577	0.033745	0.008024
γ	N _{molASU}	-0.190764	0.000005	0.036391
γ	MW _{ASU}	-0.177849	0.000022	0.03163
γ	N _{sitesASU}	-0.181147	0.000016	0.032814
γ	MWS _{ASU}	0.035345	0.402979	0.001249
γ	I _{ASU}	0.262256	0	0.068778
γ	AV _z	0.079655	0.05914	0.006345
V _s	N _{cell}	-0.026379	0.532583	0.000696
V _s	L	0.010444	0.804868	0.000109
V _s	V _m	0.981723	0	0.96378
V _s	MWS _{ASUVs}	-0.218282	0	0.047647
V _s	MW _{chain}	0.188559	0.000007	0.035555
V _s	N _{atomchain}	0.190301	0.000006	0.036214
V _s	N _{molASU}	-0.184098	0.000011	0.033892
V _s	MW _{ASU}	-0.102866	0.014702	0.010581
V _s	N _{sitesASU}	-0.090073	0.032768	0.008113
V _s	MWS _{ASU}	-0.011714	0.781708	0.000137
V _s	I _{ASU}	-0.006824	0.87176	0.000047
V _s	AV _z	-0.018585	0.66019	0.000345

N _{cell}	L	-0.021441	0.611998	0.00046
N _{cell}	V _m	-0.033625	0.426276	0.001131
N _{cell}	MWS _{ASUVs}	-0.000396	0.992525	0
N _{cell}	MW _{chain}	0.227687	0	0.051841
N _{cell}	N _{atomchain}	0.229467	0	0.052655
N _{cell}	N _{molASU}	0.268045	0	0.071848
N _{cell}	MW _{ASU}	0.385302	0	0.148457
N _{cell}	N _{sitesASU}	0.314736	0	0.099059
N _{cell}	MWS _{ASU}	-0.006158	0.884193	0.000038
N _{cell}	I _{ASU}	-0.21786	0	0.047463
N _{cell}	AV _z	-0.003262	0.93849	0.000011
L	V _m	0.0041	0.922748	0.000017
L	MWS _{ASUVs}	-0.003895	0.926585	0.000015
L	MW _{chain}	-0.046772	0.26832	0.002188
L	N _{atomchain}	-0.046885	0.267166	0.002198
L	N _{molASU}	0.089477	0.033945	0.008006
L	MW _{ASU}	0.017661	0.676099	0.000312
L	N _{sitesASU}	0.006967	0.869105	0.000049
L	MWS _{ASU}	-0.000601	0.988654	0
L	I _{ASU}	-0.021659	0.608386	0.000469
L	AV _z	0.002224	0.958053	0.000005
V _m	MWS _{ASUVs}	-0.203766	0.000001	0.041521
V _m	MW _{chain}	0.201296	0.000002	0.04052
V _m	N _{atomchain}	0.201937	0.000001	0.040779
V _m	N _{molASU}	-0.224485	0	0.050393
V _m	MW _{ASU}	-0.138245	0.001017	0.019112
V _m	N _{sitesASU}	-0.127118	0.002536	0.016159
V _m	MWS _{ASU}	-0.008994	0.831529	0.000081

V_m	I_{ASU}	0.041175	0.329879	0.001695
V_m	AV_z	-0.010268	0.808101	0.000105
MWS_{ASUVs}	MW_{chain}	-0.038341	0.36428	0.00147
MWS_{ASUVs}	$N_{atomchain}$	-0.042745	0.311761	0.001827
MWS_{ASUVs}	N_{molASU}	0.025671	0.543645	0.000659
MWS_{ASUVs}	MW_{ASU}	0.02911	0.491013	0.000847
MWS_{ASUVs}	$N_{sitesASU}$	-0.212131	0	0.045
MWS_{ASUVs}	MWS_{ASU}	0.972152	0	0.94508
MWS_{ASUVs}	I_{ASU}	-0.008908	0.833121	0.000079
MWS_{ASUVs}	AV_z	0.028064	0.506728	0.000788
MW_{chain}	$N_{atomchain}$	0.985546	0	0.971301
MW_{chain}	N_{molASU}	-0.149828	0.000365	0.022448
MW_{chain}	MW_{ASU}	0.412332	0	0.170018
MW_{chain}	$N_{sitesASU}$	0.300168	0	0.090101
MW_{chain}	MWS_{ASU}	-0.001508	0.971542	0.000002
MW_{chain}	I_{ASU}	-0.462634	0	0.21403
MW_{chain}	AV_z	0.065703	0.119755	0.004317
$N_{atomchain}$	N_{molASU}	-0.118776	0.00481	0.014108
$N_{atomchain}$	MW_{ASU}	0.419023	0	0.17558
$N_{atomchain}$	$N_{sitesASU}$	0.311617	0	0.097105
$N_{atomchain}$	MWS_{ASU}	-0.005414	0.898095	0.000029
$N_{atomchain}$	I_{ASU}	-0.466452	0	0.217577
$N_{atomchain}$	AV_z	-0.096753	0.021793	0.009361
N_{molASU}	MW_{ASU}	0.737891	0	0.544483
N_{molASU}	$N_{sitesASU}$	0.734071	0	0.53886
N_{molASU}	MWS_{ASU}	0.002663	0.949769	0.000007

N _{molASU}	I _{ASU}	-0.395268	0	0.156237
N _{molASU}	AV _z	-0.167278	0.000068	0.027982
MW _{ASU}	N _{sitesASU}	0.888157	0	0.788822
MW _{ASU}	MWS _{ASU}	0.019884	0.638091	0.000395
MW _{ASU}	I _{ASU}	-0.516341	0	0.266608
MW _{ASU}	AV _z	-0.041099	0.330776	0.001689
N _{sitesASU}	MWS _{ASU}	-0.223483	0	0.049945
N _{sitesASU}	I _{ASU}	-0.44862	0	0.20126
N _{sitesASU}	AV _z	-0.066459	0.115544	0.004417
MWS _{ASU}	I _{ASU}	-0.025491	0.546472	0.00065
MWS _{ASU}	AV _z	0.021793	0.606167	0.000475
I _{ASU}	AV _z	0.048071	0.255243	0.002311

Table S4 Highest scoring features found for different classifiers in the initial training step using the full feature set.

Linear SVM	Decision tree	Decision tree with Bagging	Decision tree with AdaBoost	Random forest	Extreme randomized forest
I/σ	CC _{anom}	m _{anom}	CC _{anom}	m _{anom}	CC _{anom}
CC _{anom}	ΔF/F	CC _{anom}	m _{anom}	CC _{anom}	Δ I/σI
m _{anom}	CC _{1/2}	Δ I/σI	d _{max}	Δ I/σI	f' _{theor}
CC _{1/2}	d _{max}	f' _{theor}	f' _{theor}	f' _{theor}	m _{anom}
ΔI/σI	m _{anom}	d _{max}	CC _{1/2}	d _{max}	d _{max}
d _{max}	R _{p.i.m.(I+/I-)}	ΔF/F	N _{sg}	ΔF/F	ΔF/F
		f' _{theor}	N _{obstotal}		T _{anom}
			N _{atomchain}		MW _{ASU}
					T
			Δ I/σI		

Table S5 Scores for the classification outcomes and performance metrics found for different classifiers in the initial training step using the full feature set.

	SVM linear	SVM rbf kernel	Decision tree	Decision tree with Bagging	Decision tree with AdaBoost	Random forest	Extreme randomiz ed forest
ACC (%)	95	96	88	94	98	94	94
Class Error (%)	5	4	12	6	2	6	6
Sensitivity (%)	94	96	88	96	97	96	90
Specificity (%)	98	96	87	91	100	91	100
FPR (%)	2	4	13	9	0	9	0
Precision (%)	99	98	93	96	100	96	100
F1 score (%)	96	97	91	96	98	96	95
ROC AUC (%)	97	99	89	99	99	99	98
TP	88	90	83	90	91	90	85
TN	46	45	41	43	47	43	47
FP	1	2	6	4	0	4	0
FN	6	4	11	4	3	4	9

Table S6 Scores for the classification outcomes and performance metrics found for different classifiers after retraining using the small feature set (CC_{anom} , $\Delta I/\sigma I$, m_{anom} , d_{max} , $\Delta F/F$, f''_{theor}).

	SVM linear	SVM rbf kernel	Decision tree	Decision tree with Bagging	Decision tree with AdaBoost	Random forest	Extreme randomiz ed forest
ACC (%)	91	92	91	94	95	94	89
Class Error (%)	9	8	9	6	5	6	11
Sensitivity (%)	94	96	91	95	96	95	95
Specificity (%)	85	85	89	91	94	91	79
FPR (%)	15	15	11	9	6	9	21
Precision (%)	93	93	95	96	97	96	90
F1 score (%)	93	94	93	95	96	95	92
ROC AUC (%)	98	98	93	99	99	99	97
TP	88	90	86	89	90	89	89
TN	40	40	42	43	44	43	37
FP	7	7	5	4	3	4	10
FN	6	4	8	5	4	5	5

Figure S1 Schema of how to train and assess a set of classifiers.

