

## Supporting Information

**Table S1.** Real space correlation coefficients for ligands involved in the region QM refinement.

PDB	LIG ID	Year	Resolution	CC Original	CC QM Refined
low					
3IX1	NFM	2009	2.4	0.82	0.84
2VTS	LZC	2008	1.9	0.87	0.86
2YHD	TES	2011	2.2	0.91	0.92
3QYI	PG4	2011	2.18	0.75	0.76
3NC9	TR3	2010	2.4	0.90	0.92
3BEA	IXH	2007	2.02	0.91	0.91
3RDP	NMF	2011	2.8	0.82	0.82
3SUV	NOK	2011	1.6	0.83	0.83
2VWW	7X2	2008	1.9	0.78	0.91
2Q3Y	1CA	2007	2.4	0.89	0.89
medium					
3NYX	TZ1	2010	2.5	0.90	0.91
3VKJ	FNR	2011	1.7	0.88	0.88
3R22	D37	2011	2.9	0.89	0.89
3O50	LJE	2010	2.0	0.87	0.88
4DQC	017	2012	1.94	0.86	0.85
3L5E	BDW	2009	1.53	0.87	0.89
2XK4	OL2	2010	2.1	0.88	0.88
3OTU	BI4	2010	2.1	0.89	0.89
3GUS	N11	2009	1.53	0.75	0.76
3OWJ	1EL	2010	1.85	0.83	0.84
high					
<b>2ZL9</b>	<b>VDA</b>	<b>2008</b>	<b>1.9</b>	<b>0.88</b>	<b>0.88</b>
2Y68	T04	2011	1.49	0.86	0.87

3II4	3II	2009	2.42	0.84	0.88
3H2O	B63	2009	2.7	0.80	0.81
3V7Y	A3N	2011	1.97	0.82	0.82
3DRR	R8E	2008	2.89	0.09	0.12
<b>2WUE</b>	<b>KEK</b>	<b>2009</b>	<b>1.8</b>	<b>0.59</b>	<b>0.59</b>
2XNP	WCX	2010	1.98	0.92	0.93
3FE9	CMJ	2008	1.75	0.84	0.85
2OGA	PGU	2007	2.05	0.85	0.86

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metal

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2OF1	THP: Ca	2007	1.92	0.90	0.90
3OVS	CTP: Ca	2010	2.8	0.86	0.86
3MTW	M3R: Zn	2010	1.7	0.87	0.88
3SPZ	UPC: Ca	2011	2.43	0.82	0.82
2WO9	68: Zn	2009	1.7	0.64	0.64
3OIM	VZ5: Zn	2010	1.45	0.59	0.60
2PJC	343: Zn	2007	1.74	0.76	0.78
3ZYF	147: Ca	2011	1.94	0.75	0.76
<b>2X7T</b>	<b>WZB: Zn</b>	<b>2010</b>	<b>1.89</b>	<b>0.65</b>	<b>0.65</b>
3QIY	QI1: Zn	2011	2.3	0.46	0.46

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bound

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<b>3NCK</b>	<b>NFF</b>	<b>2010</b>	<b>2.8</b>	<b>0.80</b>	<b>0.82</b>
3UME	HC4	2011	1.8	0.72	0.72
3LXS	4MC	2010	1.5	0.82	0.82
2WZZ	ZX1	2009	1.57	0.83	0.83
2WJ1	S99	2009	1.84	0.81	0.81
3FA6	LSR	2008	1.54	0.83	0.83
2UZJ	E64	2008	1.55	0.62	0.62
2VK7	FSI	2007	1.2	0.81	0.81
2V6N	XP1	2007	1.98	0.72	0.73
3IXH	PCZ	2009	2.3	0.77	0.77

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