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Table S1 Isotropic atomic *B*-factors present in the PDB subset.

Atomic *B*-factor [Å²]	Number of atoms	Percentage of atoms
$B < 0$	3	<0.01 %
$B = 0$	4,610	0.05 %
$0 < B < 80$	10,143,262	99.65 %
$B \geq 80$	31,338	0.31 %

Atoms with negative atomic *B*-factors were found in PDB structure entry 3cls.

Table S2 Occupancy values present in the PDB subset.

Occupancy *occ*	Number of atoms	Percentage of atoms
$occ < 0$	5	<0.01 %
$occ = 0$	9,177	0.09 %
$0 < occ < 0.5$	68,511	0.67 %
$occ = 0.5$	234,192	2.30 %
$0.5 < occ < 1$	72,020	0.71 %
$occ = 1$	9,795,303	96.23 %
$occ > 1$	5	<0.01 %

Some PDB structures contain occupancy values outside the valid probability range: the structure entries 1ie0 and 1wul report occupancies above 1, and the structure 3hkw reports occupancies below 0.

Table S3 Packing densities of protein secondary structure.

Density metric, radius	Secondary structure	Min	Mean	Max	Variance	Secondary structure	Min	Mean	Max	Variance
Ooi, 8 Å	b	4	11.5	21	6.1	H	4	10.5	22	5.5
	C	1	9.7	22	8.5	I	4	12.4	20	6.9
	E	4	12.0	23	5.1	T	8	9.6	22	8.1
	G	4	9.5	21	7.1					
Ooi, 13 Å	b	10	43.4	72	89.5	H	8	42.9	80	103.6
	C	3	39.7	78	106.2	I	22	48.8	71	136.1
	E	11	47.0	84	93.6	T	5	38.6	82	106.8
	G	8	39.6	75	104.2					
Ooi, 14 Å	b	11	53.1	90	132.1	H	8	52.6	100	148.6
	C	3	48.9	95	153.9	I	29	59.9	82	211.8
	E	12	58.0	102	141.3	T	5	47.8	96	154.3
	G	9	49.1	96	150.4					
ACN, 8 Å	b	13	92.3	141	333.9	H	8	89.2	147	360.8
	C	0	81.1	145	444.8	I	22	98.8	141	337.2
	E	8	96.5	145	294.2	T	8	79.9	144	447.6
	G	8	82.2	141	424.6					
ACN, 13 Å	b	72	340.6	531	5,245.9	H	46	336.2	542	5,757.5
	C	11	313.7	541	6,032.7	I	158	385.7	517	7,705.1
	E	46	366.8	547	5,191.2	T	35	306.7	540	6,229.6
	G	48	314.5	539	6,074.3					
ACN, 13.5 Å	b	74	376.7	589	6,416.0	H	50	372.4	600	6,973.5
	C	14	348.1	597	7,293.6	I	173	428.4	570	9,721.7
	E	53	405.5	601	6,377.9	T	37	340.8	597	7,541.5
	G	51	349.3	602	7,341.6					
ACN, 14 Å	b	80	415.3	654	7,790.0	H	52	410.9	666	8,366.2
	C	16	385.1	658	8,757.2	I	190	474.0	633	12,043.5
	E	56	446.8	668	7,762.1	T	38	377.4	666	9,056.6
	G	57	386.4	659	8,809.8					

Range, mean and variance of different packing density metrics applied to the 2,704 selected PDB structures. Both ACN and Ooi metrics are counts, so minimum and maximum values are integers. Mean and variance are given to 1 dp. The seven secondary structure labels are: alpha helix (H; n=3,323,956), 3-10 helix (G; n=428,747), π-helix (I; n=1,515), extended conformation (E; n=2,351,831), isolated bridge (b; n=120,856), turn (T; n=1,859,115) and coil (C; n=1,679,478) (Frishman & Argos, 1995).

Table S4 List of the 2,704 selected PDB structures

1A3A 1A3C 1A4I 1A7D 1AKY 1AL3 1ATZ 1B2L 1B2P 1B4V 1B4Z 1B5E 1B6A 1B8O 1BQC 1BRT 1BW9 1BX4 1C7S 1CJW 1CQX 1CZF 1D2N 1D8W 1DBW 1DEO 1DGW 1DJ0
1DJE 1DK8 1DLW 1DPS 1DQG 1DQZ 1DWK 1DYP 1DYQ 1E19 1E2R 1E2W 1E30 1E42 1E4C 1E5M 1E6Y 1E71 1E7R 1EDG 1EEX 1EJD 1ELK 1ELW 1EOK 1EQM 1EWF 1EYE
1EYH 1EZW 1F0L 1F46 1F5V 1F60 1F74 1F7L 1FCQ 1FJ2 1FJJ 1FN9 1FNL 1FO9 1FQT 1FT5 1FTR 1FXO 1G2Q 1G58 1G60 1G6S 1G8M 1GD0 1GGZ 1GKB 1GKK 1GNY
1GP6 1GTJ 1GTK 1GU7 1GUQ 1GV2 1GVG 1GXN 1GXY 1GZJ 1H03 1H14 1H16 1H2B 1H41 1H4C 1H4R 1H4Y 1H6L 1H72 1H9M 1HBZ 1HD5 1HFE 1HH8 1HT6 1HTW 1HW1
1HX6 1HXI 1I0S 1I1N 1I2H 1I3K 1I86 1IAB 1ID0 1IE0 1IIB 1IJB 1IJT 1ILK 1INL 1IOM 1IQQ 1IV2 1J1M 1J1Y 1J27 1J2W 1J7G 1J83 1J8B 1J8U 1J97 1JA9
1JB3 1JG9 1JH6 1JNE 1JNR 1JP4 1JQ5 1JQC 1JSR 1JWQ 1JY1 1JYH 1K1E 1K20 1K4N 1K4V 1K6X 1K75 1K77 1K92 1K9Z 1KAP 1KDG 1KG6 1KGS 1KI0 1KIC 1KLL
1KM4 1KOE 1KP4 1KPT 1KSC 1KTG 1KUI 1L0G 1L2H 1L6P 1L7A 1L9X 1LC8 1LJ8 1LK9 1LMI 1LN4 1LO7 1LOV 1LQV 1LV7 1M0W 1M2A 1M2X 1M4I 1M5T 1M65 1M6K
1M6S 1M7J 1M8U 1MG4 1MIX 1MPG 1MR7 1MSK 1MTY 1MXI 1N45 1N57 1N5Q 1N5W 1N7H 1N8U 1N93 1N9E 1NBC 1NBU 1NC5 1NEP 1NF9 1NH8 1NKG 1NLN 1NN5 1NNH
1NOG 1NPY 1NQD 1NR0 1NS5 1NSZ 1NTH 1NTY 1NU0 1NU3 1NVK 1NWA 1NXC 1NYT 1NZJ 1O1Y 1O1Z 1O3Y 1O4R 1O6V 1O9G 1OA1 1OA4 1OAD 1OC6 1OCY 1OD6 1OF8
1OFL 1OFN 1OFZ 1OGO 1OGQ 1OI2 1OJK 1ONW 1OOE 1OQ1 1OQ5 1ORR 1ORU 1OSY 1OW4 1OWL 1OXS 1OYG 1OYW 1OZ2 1P0Z 1P1J 1P3C 1P3D 1P5D 1P5Z 1P7S 1P90
1P9H 1PB1 1PBY 1PDO 1PG4 1PKK 1PM4 1PMJ 1PMY 1POA 1PU6 1PV5 1PVM 1PX5 1PXV 1PZ3 1Q0G 1Q11 1Q1A 1Q1F 1Q4U 1Q5Z 1Q7E 1Q8D 1Q9U 1QAZ 1QCZ 1QD1
1QF8 1QG8 1QGI 1QH8 1QJP 1QMG 1QNS 1QQ9 1QQJ 1QSA 1QTO 1QTP 1QVY 1QWD 1QWG 1QWO 1QWR 1QZ0 1R0U 1R2R 1R3S 1R4P 1R5L 1R5M 1R7A 1R8M 1R9L 1R9Y
1RCV 1RKI 1RLI 1ROC 1RU4 1RV9 1RW7 1RWG 1RWR 1RXQ 1S0I 1S1D 1S1Z 1S5A 1S99 1S9R 1SBX 1SDI 1SFX 1SG6 1SH8 1SHU 1SK2 1SNG 1ST9 1SYY 1T0B 1T0T
1T1U 1T2W 1T3I 1T61 1T6C 1T6E 1T92 1TAG 1TCA 1TE2 1THG 1TJ6 1TJP 1TLU 1TOA 1TP6 1TP9 1TR0 1TU7 1TWD 1TXG 1TY9 1TZW 1U0K 1U14 1U5D 1U60 1U69
1U6K 1U6R 1U8V 1UAQ 1UAS 1UEK 1UFO 1UGX 1UH4 1UI0 1UJ2 1UKK 1UO9 1UPG 1URR 1US5 1USG 1UT1 1UUQ 1UUX 1UV7 1UX7 1UXL 1UXO 1UZA 1V0T 1V2B 1V3H
1V5D 1V5V 1V7W 1V9F 1VCL 1VDK 1VHF 1VHN 1VIA 1VJF 1VJV 1VK5 1VKA 1VKE 1VKF 1VKN 1VL1 1VL7 1VLA 1VLJ 1VM0 1VMB 1VMJ 1VPB 1VPD 1VPR 1VRM 1VSR
1VYB 1VYI 1W0H 1W1D 1W2W 1W2Y 1W3E 1W4S 1W4W 1W5P 1W6G 1W9I 1WAB 1WBH 1WCU 1WDV 1WEH 1WHI 1WKU 1WLG 1WNY 1WO8 1WOL 1WS8 1WTA 1WTJ 1WUL 1WV3
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1XTE 1XTT 1XV5 1XY7 1Y07 1Y0B 1Y0H 1Y0K 1Y0P 1Y21 1Y27 1Y7B 1Y7R 1YAC 1YB6 1YBI 1YGT 1YJ7 1YKI 1YLE 1YLL 1YN9 1YO3 1YOC 1YQH 1YRK 1YRW 1YS2
1YSQ 1YT3 1YTL 1YU0 1YUM 1YV1 1YWF 1YX1 1Z0B 1Z3E 1Z3X 1Z6N 1Z7A 1Z9N 1ZBF 1ZD7 1ZHS 1ZI9 1ZJC 1ZLD 1ZMT 1ZRS 1ZVT 1ZW6 1ZXU 1ZY7 1ZZ1 1ZZW
2A0B 2A14 2A2K 2A32 2A35 2A3M 2A4D 2A4O 2A5L 2A65 2A6B 2A6V 2A7B 2A94 2A9D 2A9I 2A9S 2AAL 2ABW 2AD6 2AEX 2AFW 2AG4 2AH5 2AHF 2AII 2AJ6 2AJ7
2AL1 2AML 2APJ 2AR1 2ARC 2ASF 2ATF 2AUO 2AVD 2AXC 2AXQ 2B0P 2B0V 2B2H 2B3L 2B4V 2B5H 2B5W 2B61 2B65 2B7U 2B8M 2BBA 2BDR 2BEK 2BEM 2BHY 2BJF
2BJN 2BJQ 2BJV 2BKM 2BKV 2BMW 2BNM 2BP6 2BRJ 2BSY 2BT6 2BUE 2BV9 2BWR 2BZ1 2C0H 2C2I 2C2P 2C2T 2C54 2C61 2C6Q 2C6U 2C79 2C8B 2C92 2C9Q 2CBO
2CBZ 2CCM 2CD7 2CDO 2CF7 2CFE 2CHC 2CI3 2CIH 2CIS 2CIU 2CJ2 2CJ4 2CJS 2CKI 2CMW 2CO3 2CWL 2CWR 2CX1 2CXA 2CXH 2CXY 2CYJ 2CZ6 2CZL 2D1G 2D1R
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2F1F 2F1K 2F1N 2F24 2F2B 2F4Q 2F57 2F5X 2F62 2F6D 2F6R 2F7V 2F8A 2F9F 2F9H 2FA1 2FC3 2FCT 2FDV 2FEX 2FGR 2FH1 2FHP 2FI9 2FLU 2FNU 2FOM 2FOZ
2FP1 2FQX 2FR2 2FSR 2FSU 2FSX 2FTN 2FUL 2FUR 2FW0 2FY7 2FYF 2FYG 2FZB 2G0W 2G1U 2G2C 2G40 2G50 2G62 2G82 2G8S 2GA8 2GAI 2GEY 2GFF 2GHS 2GI3
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2I7A 2I7G 2I8D 2I8E 2I9W 2IA1 2IBA 2IBD 2ICA 2ICG 2ICU 2IDL 2IEQ 2IF6 2IG7 2IGI 2IGP 2IIH 2IJA 2IK9 2IKB 2IKK 2IM9 2IMD 2IMH 2IMJ 2IML 2IMZ
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3L1W 3L34 3L3X 3L40 3L4A 3L4E 3L4H 3L4N 3L51 3L6B 3L8Q 3LAT 3LB4 3LCC 3LD7 3LEW 3LFJ 3LFR 3LFU 3LGB 3LGI 3LHE 3LHO 3LI3 3LID 3LIM 3LIO 3LKM
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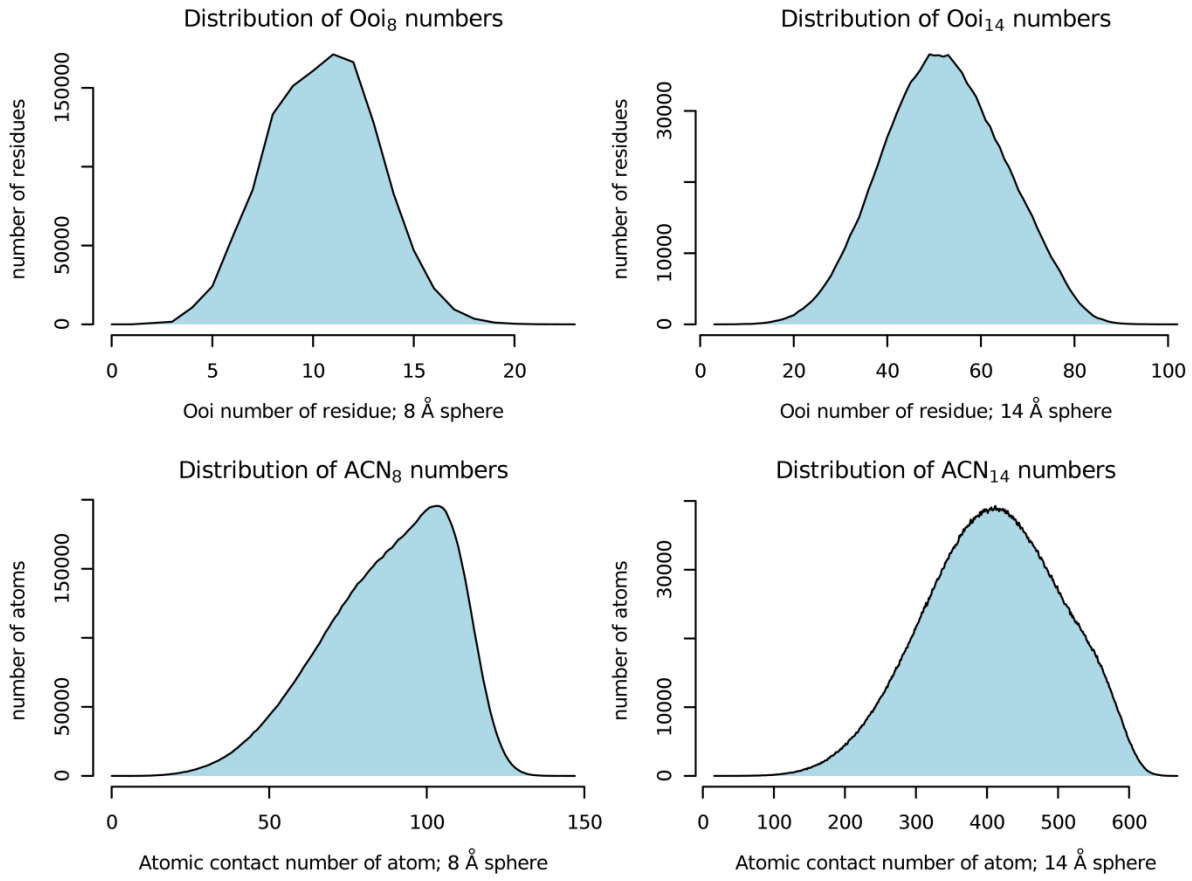

Figure S1 Distribution of Ooi numbers and atomic contact numbers (ACN) for radii of 8 Å and 14 Å for the 2,704 selected PDB structures. Note that both Ooi numbers and ACNs are discrete metrics; they can only take integer values.

1. Let the variable a denote a single atom.

2. Let the set A describe the set of all non-hydrogen protein atoms within the same PDB structure.

3. Choose a packing density function $P\colon A \to \mathbb{R}$ mapping every atom to a packing density. For this paper P was defined using atomic contact numbers with a range of 14 Å.

4. Let $B\colon A \to \mathbb{R}$ map every atom to its atomic B factor (atomic displacement parameter).

5. The function of average B factors returns the arithmetic mean of the atomic B factors of a set of atoms $X \subseteq A$:

$$\bar{B}(X) := \frac{\sum_{a \in X} B(a)}{|X|}$$

6. Define the packing density environments $E_n := \{a \in A \mid P(a) = n\}$ as sets, that contain all atoms with the packing density n as determined by P. The set of all nonempty E_n is a partition of A.

7. Similar packing density environments S_m are defined as sets of all atoms with a packing density *similar* to $m \in \mathbb{R}$:

$$S_m := \bigcup_{n \in sim(m)} E_n$$

8. Similarity can be defined by range, e.g. $sim(m) := \{x \in \mathbb{R} \,|m - \varepsilon \leq x \leq m + \varepsilon\}$, $\varepsilon \geq 0$ or by binning, e.g. $sim(m) := \left\{x \in \mathbb{R} \,\middle|\, \left\lfloor \frac{x}{z} \right\rfloor = \left\lfloor \frac{m}{z} \right\rfloor \right\}$ with a bin size $z > 0$. Here the latter definition was used with $z = 10$.

9. Define B_{Damage} of an atom a as the atomic B factor divided by the average B factor of all non-hydrogen protein atoms within the same PDB structure and with a similar packing density as a:

$$B_{Damage}(a) := \frac{B(a)}{\bar{B}\left(S_{P(a)}\right)}$$

Figure S2 Mathematical description of B_{Damage} calculation.

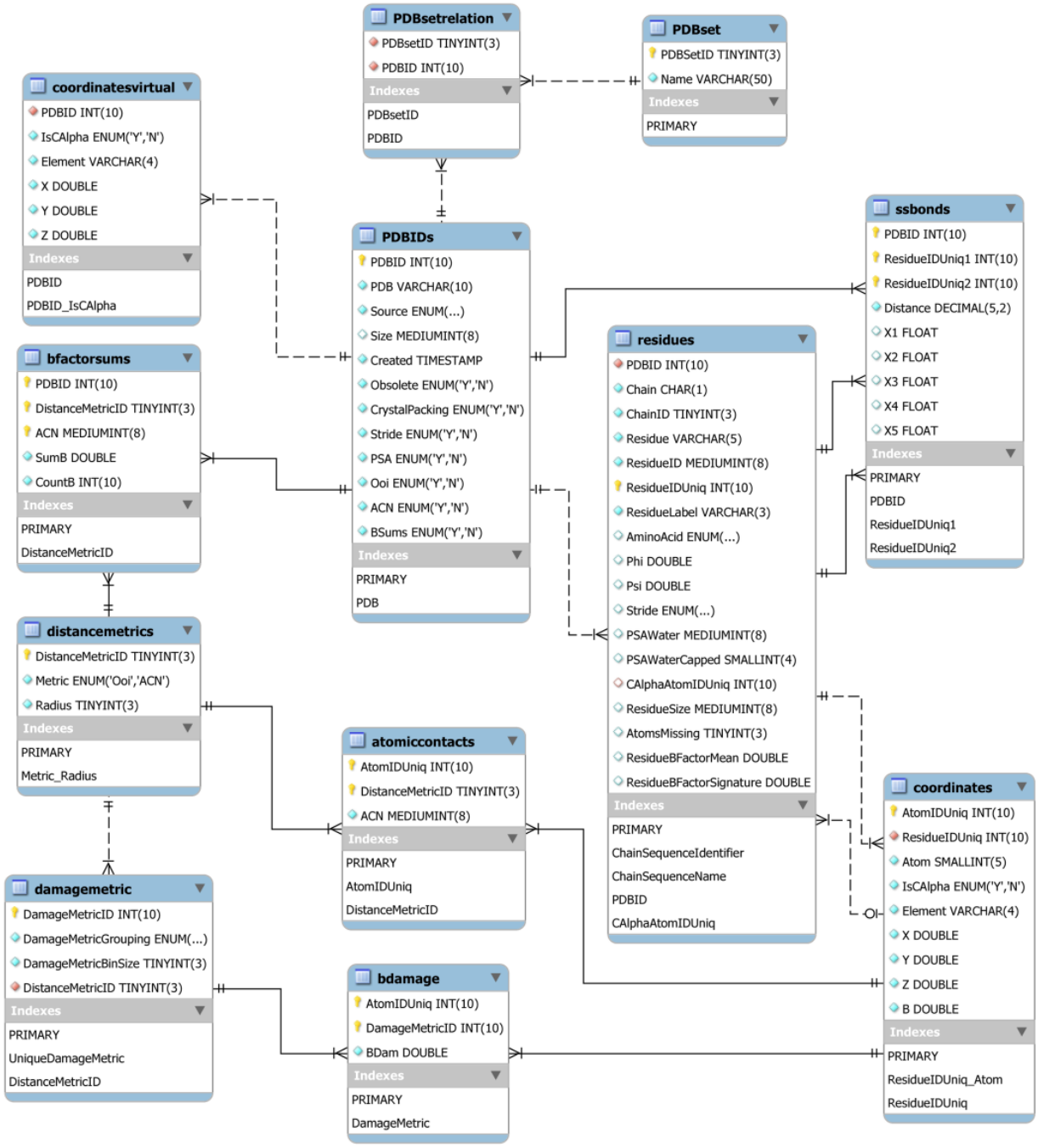

Figure S3 Entity-Relationship diagram of the relational database used for this investigation. Diagram prepared using MySQL Workbench 6.0 (http://mysqlworkbench.org/).

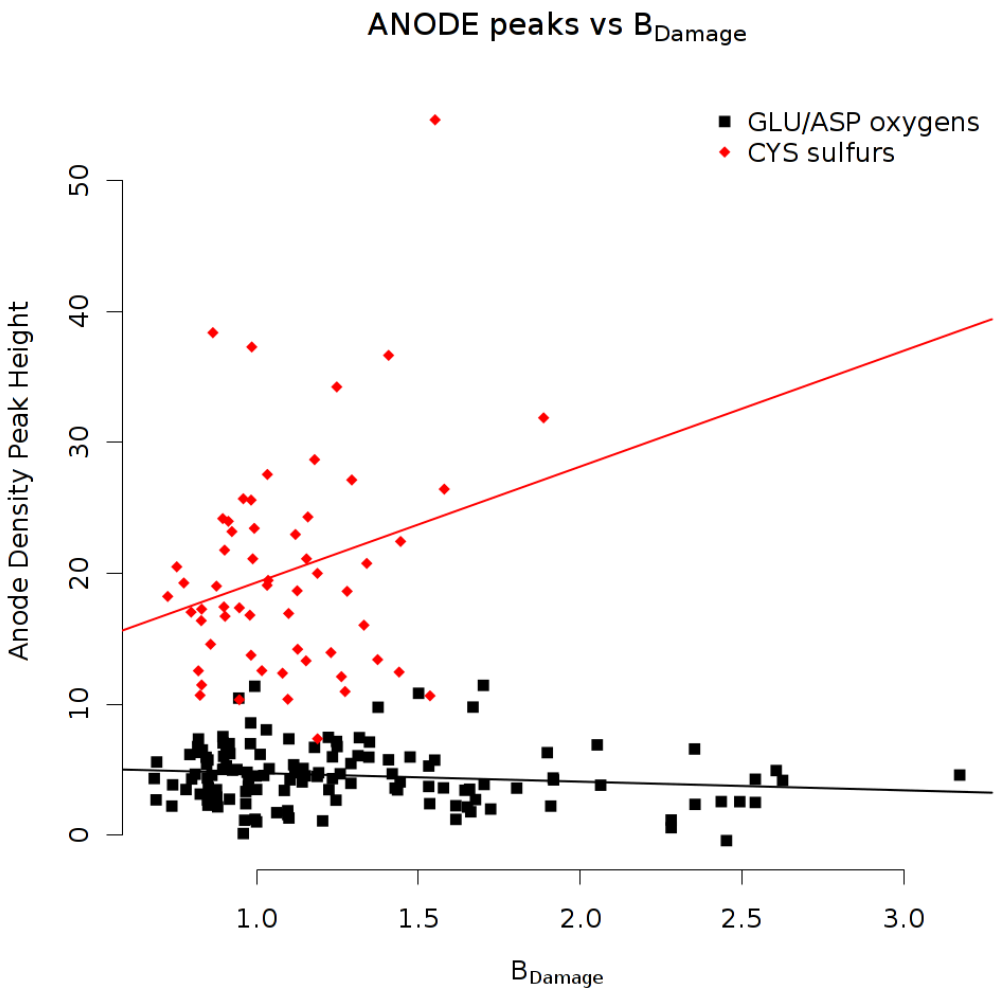

Figure S4 Peak heights of electron density difference maps around the cysteine sulfurs (red) and the terminal oxygens of glutamic and aspartic acids (black) plotted against their B_{Damage} values for the six Nanao protein datasets. Lines show least squares fits to the points. Peak heights were calculated using SHELXC (Sheldrick, 2010) and ANODE (Thorn & Sheldrick, 2011). B_{Damage} values were calculated for the relevant high-dose dataset.

There is some evidence for a correlation of high B_{Damage} values and strong electron density peak differences for cysteine sulfurs (CC=0.25, p=0.05). The apparent inverse correlation for GLU/ASP oxygens is not statistically significant (CC=-0.15, p=0.09).

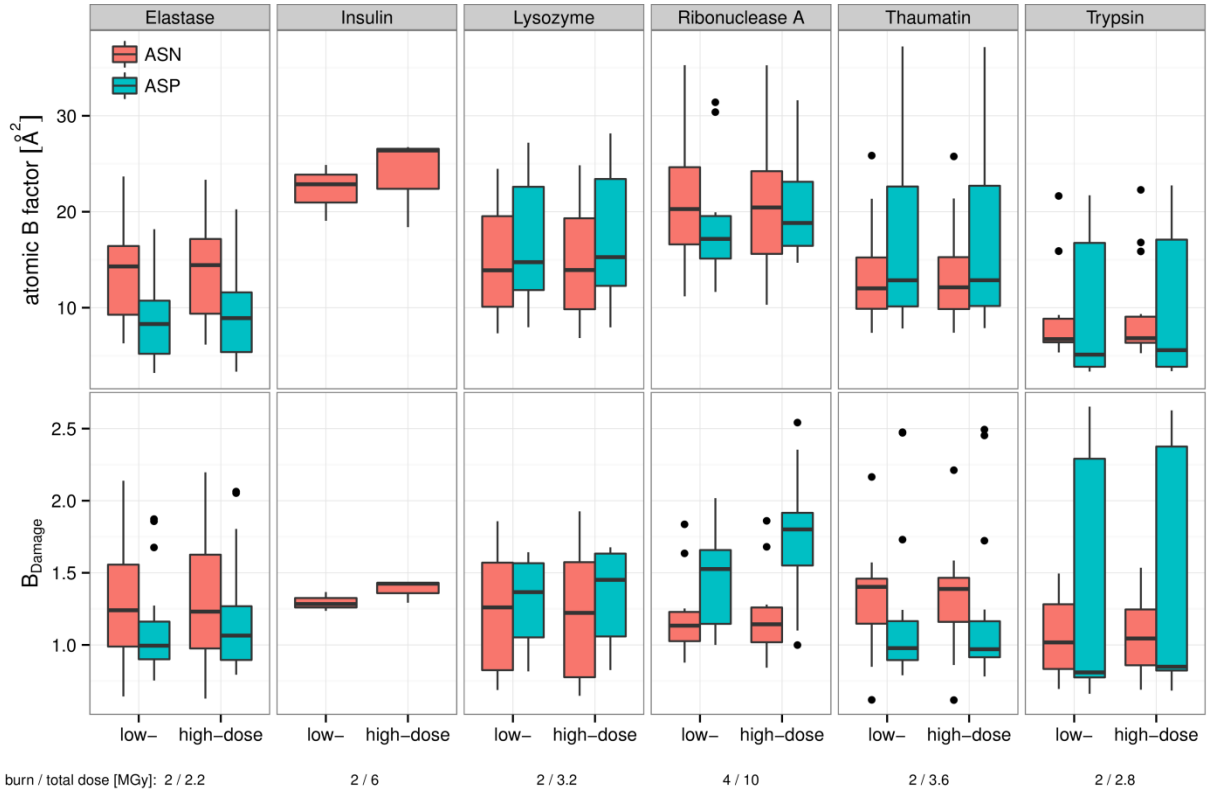

Figure S5 *B*-factor (**above**) and B_{Damage} (**below**) of ASP and ASN Oδ atoms of the six Nanao *et al.* (2005) proteins in two different dose states. The deterioration of the ASP side chain termini of ribonuclease A cannot be observed from the *B*-factor alone, but is clearly indicated by B_{Damage}. The ASN oxygens remain unaffected.

References

Sheldrick, G. M. (2010). Acta Cryst. D66, 479–485.

Thorn, A. & Sheldrick, G. M. (2011). J. Appl. Cryst. 44, 1285–1287.