

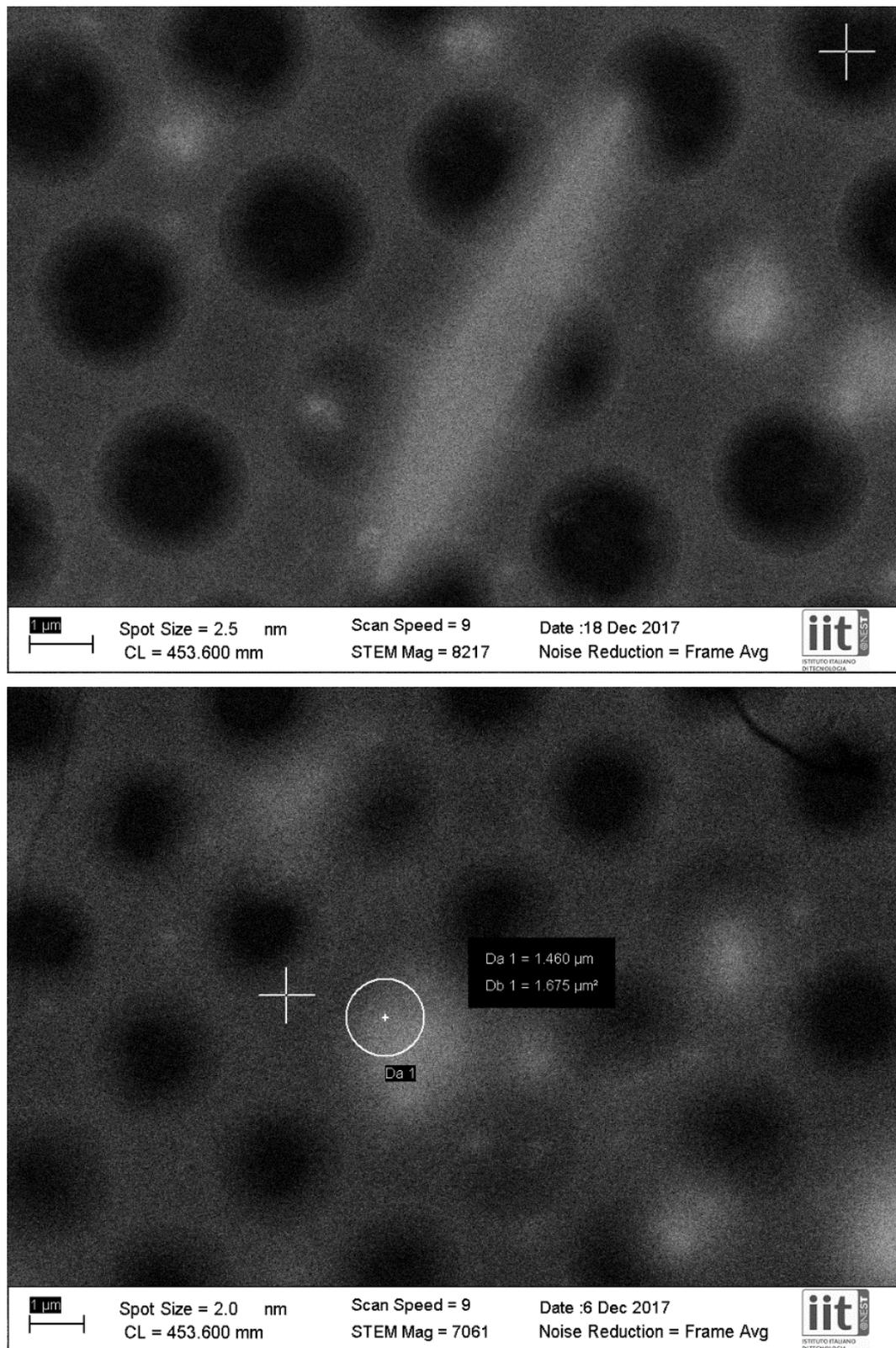
# IUCrJ

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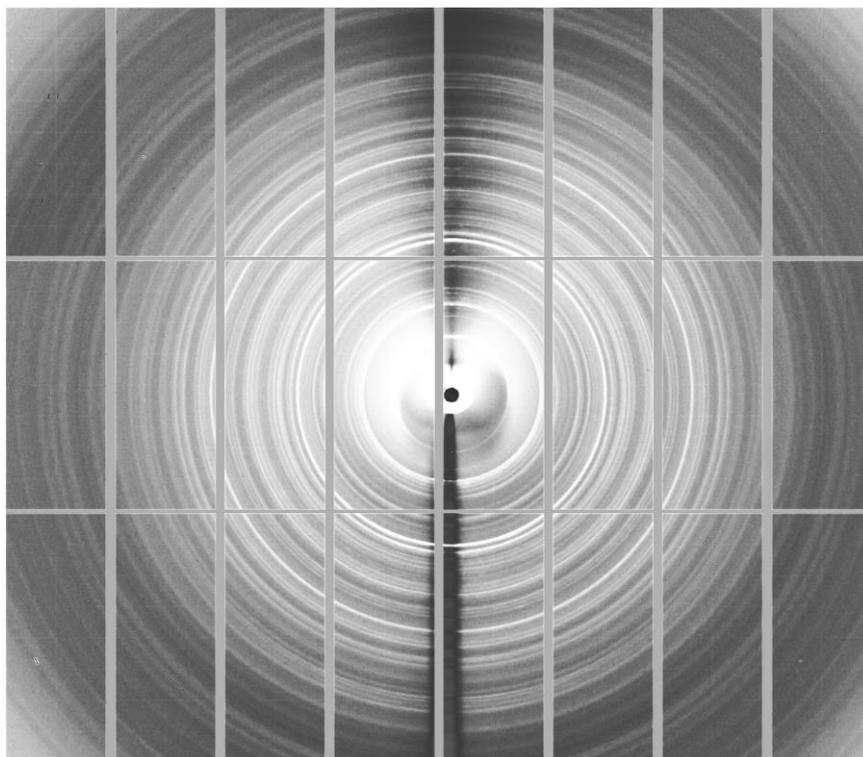
**Supporting information for article:**

**Nanobeam precession-assisted 3D electron diffraction reveals a new polymorph of hen egg-white lysozyme**

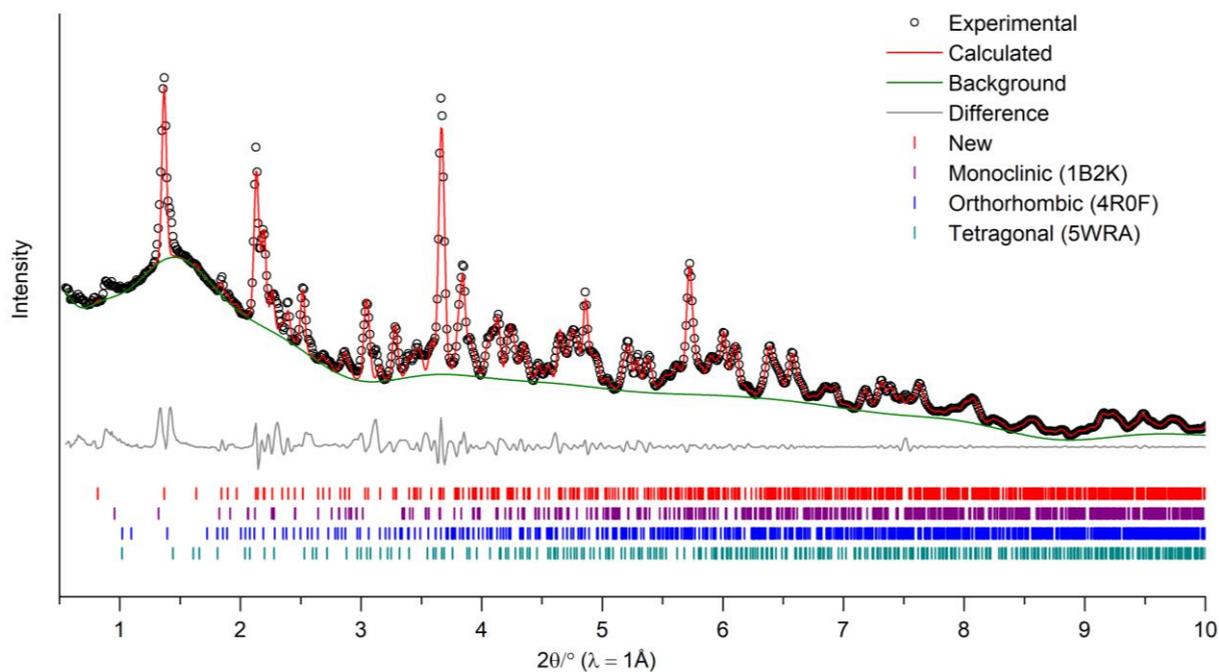
**Arianna Lanza, Eleonora Margheritis, Enrico Mugnaioli, Valentina Cappello, Gianpiero Garau and Mauro Gemmi**



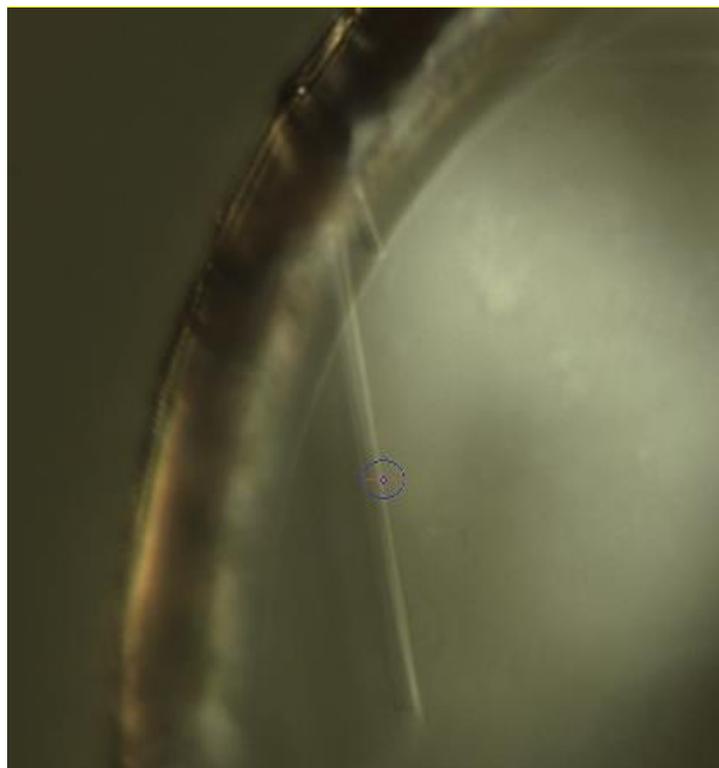
**Figure S1** STEM images of plunge-frozen HEWL samples. Typically some crystals preserving the acicular habitus can be found (top image), but in this study the best diffraction was obtained by one fragment of ca.  $1\mu\text{m} \times 1\mu\text{m} \times \leq 0.1\mu\text{m}$ , like the one in the bottom image. (Note: the white circle is not related with the size of the beam, it was only used to highlight the diffracting area exploited during the whole data collection.)



**Figure S2** High resolution powder diffraction image of the HEWL aggregate, collected at the XRD1 Beamline of ELETTRA synchrotron, with  $\lambda=1 \text{ \AA}$ .



**Figure S3** X-ray powder diffraction pattern obtained from the HEWL polycrystalline ensemble (black points), and the corresponding Pawley fit for the new  $P2_1$  cell parameters of HEWL (red, PDB 6HT2). For comparison, the peak positions of several known phases (see the PDB entries indicated in the legend) are shown.



**Figure S4** Single crystal used for the microfocus XRD experiment, mounted on a loop. The blue circle is ca. 4  $\mu\text{m}$  in diameter.

**Table S1** Summary of the potential interchain H-bonds for monoclinic, orthorhombic and tetragonal HEWL polymorphs, calculated with the program UCSF Chimera.

	mono 6HT2	mono 1B2K	ortho 4R0F	tetra 5WRA
interacting chains	8/6	12/12	10/9	8
possible H-bonds in the asymmetric unit	23	42	46	26
# per chain	11.5	21	23	26

**Table S2** List of the potential interchain H-bonds for monoclinic, orthorhombic and tetragonal HEWL polymorphs, calculated with the program UCSF Chimera.

Donor				Acceptor					Donor				Acceptor				
sym id	Residue type	Residue n. / chain	D atom	sym id	Residue type	Residue n. / chain	A atom	D...A /Å	sym id	Residue type	Residue n. / chain	D atom	sym id	Residue type	Residue n. / chain	A atom	D...A /Å
MONOCLINIC 6HT2									TETRAGONAL 5WRA								
#0	CYS	6.A	SG	#9	CYS	127.B	O	3.6	#0	LYS	13.A	NZ	#5	LEU	129.A	O	2.8
#0	ARG	21.A	NH1	#2	ASP	66.A	O	2.9	#0	ASN	39.A	ND2	#3	ASP	66.A	O	2.9
#0	ARG	21.A	NH2	#2	ASP	66.A	O	3.5	#0	GLN	41.A	NE2	#3	ASN	65.A	O	3.1
#0	ARG	68.A	NH1	#7	ARG	21.A	O	2.7	#0	THR	47.A	OG1	#8	GLY	126.A	O	2.7
#0	ARG	68.A	NH2	#7	ARG	21.A	O	3.2	#0	ARG	68.A	NH1	#3	THR	43.A	O	2.7
#0	ARG	73.A	NH1	#6	ARG	68.B	O	3.4	#0	ARG	68.A	NH2	#3	THR	43.A	O	3.1
#0	ARG	73.A	NH1	#8	GLY	102.B	O	3.3	#0	SER	81.A	N	#3	GLN	41.A	OE1	2.8
#0	ARG	112.A	NH2	#3	ASN	77.A	OD1	3.2	#0	SER	81.A	OG	#3	GLN	41.A	OE1	3.6
#0	ASN	113.A	ND2	#3	ASN	77.A	OD1	3.5	#0	ASN	106.A	ND2	#4	ASN	113.A	O	3.0
#0	ASN	19.B	ND2	#7	SER	81.B	O	2.7	#0	ARG	112.A	NH2	#6	GLY	102.A	O	3.1
#0	ARG	21.B	NH1	#7	ASP	66.B	O	2.9	#0	ASN	113.A	ND2	#6	GLY	102.A	O	3.0
#0	ARG	21.B	NH2	#7	ASP	66.B	O	3.5	#0	ARG	114.A	NH1	#6	GLY	22.A	O	2.9
#0	ARG	68.B	NH1	#2	ARG	21.B	O	3.2	#0	LYS	116.A	NZ	#4	ASN	113.A	O	3.0
#0	ARG	68.B	NH2	#2	ARG	21.B	O	3.1	#0	ARG	128.A	NE	#2	THR	47.A	O	3.2
#0	ARG	73.B	NH1	#3	ARG	68.A	O	2.7	#0	ARG	128.A	NH1	#5	ARG	14.A	O	3.2
#0	ASN	113.B	ND2	#0	ALA	122.A	O	2.7	#2	THR	47.A	OG1	#0	GLY	126.A	O	2.7
#8	ARG	73.B	NH1	#0	ARG	68.A	O	2.7	#3	ASN	39.A	ND2	#0	ASP	66.A	O	2.9
#2	ARG	68.A	NH1	#0	ARG	21.A	O	2.7	#3	GLN	41.A	NE2	#0	ASN	65.A	O	3.1
#2	ARG	68.A	NH2	#0	ARG	21.A	O	3.2	#3	ARG	68.A	NH1	#0	THR	43.A	O	2.7
#2	ASN	19.B	ND2	#0	SER	81.B	O	2.7	#3	ARG	68.A	NH2	#0	THR	43.A	O	3.1
#2	ARG	21.B	NH1	#0	ASP	66.B	O	2.9	#3	SER	81.A	N	#0	GLN	41.A	OE1	2.8
#2	ARG	21.B	NH2	#0	ASP	66.B	O	3.5	#3	SER	81.A	OG	#0	GLN	41.A	OE1	3.6
#3	ARG	73.A	NH1	#0	GLY	102.B	O	3.3	#4	ARG	112.A	NH2	#0	GLY	102.A	O	3.1
#4	ARG	73.A	NH1	#0	ARG	68.B	O	3.4	#4	ASN	113.A	ND2	#0	GLY	102.A	O	3.0
#5	CYS	6.A	SG	#0	CYS	127.B	O	3.6	#4	ARG	114.A	NH1	#0	GLY	22.A	O	2.9
#7	ARG	21.A	NH1	#0	ASP	66.A	O	2.9	#5	LYS	13.A	NZ	#0	LEU	129.A	O	2.8
#7	ARG	21.A	NH2	#0	ASP	66.A	O	3.5	#5	ARG	128.A	NH1	#0	ARG	14.A	O	3.2
#7	ARG	68.B	NH1	#0	ARG	21.B	O	3.2	#6	ASN	106.A	ND2	#0	ASN	113.A	O	3.0
#7	ARG	68.B	NH2	#0	ARG	21.B	O	3.1	#6	LYS	116.A	NZ	#0	ASN	113.A	O	3.0
#8	ARG	112.A	NH2	#0	ASN	77.A	OD1	3.2	#8	ARG	128.A	NE	#0	THR	47.A	O	3.2
#8	ASN	113.A	ND2	#0	ASN	77.A	OD1	3.5									

Donor				Acceptor					Donor				Acceptor				
sym id	Residue type	Residue n. / chain	D atom	sym id	Residue type	Residue n. / chain	A atom	D...A /Å	sym id	Residue type	Residue n. / chain	D atom	sym id	Residue type	Residue n. / chain	A atom	D...A /Å
ORTHORHOMBIC 4R0F									MONOCLINIC 1B2K								
#0	ARG	14.A	NH1	#0	ASN	37.B	O	3.1	#0	ARG	5.A	NH2	#13	ASP	101.A	O	2.9
#0	ASN	19.A	ND2	#4	SER	81.A	O	2.8	#0	ASN	39.A	ND2	#7	GLN	121.B	OE1	3.1
#0	ASN	19.A	ND2	#4	GLY	126.B	O	3.1	#0	ARG	73.A	NH2	#4	ASP	119.A	OD2	2.9
#0	ARG	61.A	NH1	#12	GLY	67.B	O	3.1	#0	LYS	97.A	NZ	#2	ARG	45.A	O	3.2
#0	ARG	61.A	NH2	#10	ASP	101.B	O	2.5	#0	ARG	112.A	NH1	#4	ARG	128.A	O	3.3
#0	ARG	68.A	NH1	#11	ARG	21.A	O	2.8	#0	ARG	112.A	NH2	#4	CYS	127.A	O	2.7
#0	ARG	68.A	NH2	#11	ARG	21.A	O	3.0	#0	ARG	112.A	NH2	#4	ARG	128.A	O	3.4
#0	ARG	73.A	NH2	#12	ARG	68.B	O	2.5	#0	ARG	114.A	NH1	#7	ASP	18.A	O	3.6
#0	ASN	77.A	ND2	#3	ASP	119.A	OD2	2.8	#0	ARG	125.A	NE	#13	ASP	101.A	OD2	2.9
#0	ASN	103.A	N	#12	GLY	71.B	O	2.8	#0	ARG	125.A	NH2	#13	ASP	101.A	OD1	3.1
#0	ARG	114.A	NE	#13	SER	86.B	OG	3.1	#0	ARG	128.A	NH2	#13	ASP	52.A	OD1	3.4
#0	GLN	121.A	NE2	#13	ASN	77.A	OD1	3.0	#0	LYS	1.B	NZ	#6	GLY	71.A	O	3.5
#0	ARG	125.A	NH2	#13	ARG	73.A	O	3.5	#0	VAL	2.B	N	#12	ASP	48.A	O	3.2
#0	ARG	125.A	NH2	#13	ASN	74.A	O	3.0	#0	ARG	5.B	N	#6	GLY	102.B	O	3.1
#0	ARG	128.A	N	#9	THR	47.B	O	2.9	#0	ARG	5.B	NE	#6	ASP	101.B	O	3.0
#0	ARG	128.A	NH1	#9	GLY	49.B	O	3.5	#0	ARG	5.B	NH2	#6	ASP	101.B	O	3.0
#0	ARG	128.A	NH2	#9	ASN	46.B	O	2.9	#0	CYS	6.B	N	#6	ASN	103.B	OD1	2.7
#0	ARG	128.A	NH2	#9	SER	50.B	O	2.9	#0	ARG	14.B	NH1	#6	PRO	70.A	O	2.6
#0	ARG	5.B	N	#0	ASP	87.A	OD2	3.3	#0	ARG	14.B	NH2	#6	PRO	70.A	O	3.0
#0	ASN	19.B	ND2	#11	SER	81.B	O	2.7	#0	ASN	19.B	ND2	#2	LEU	84.A	O	3.3
#0	ARG	68.B	NH1	#4	ARG	21.B	O	3.1	#0	ARG	68.B	NH1	#10	GLY	22.A	O	2.9
#0	ARG	68.B	NH2	#4	ARG	21.B	O	3.1	#0	SER	81.B	OG	#9	ASN	113.A	O	2.7
#0	ARG	73.B	NH1	#2	GLY	49.A	O	2.8	#0	ARG	114.B	NH1	#7	ARG	14.B	O	3.1
#0	ARG	73.B	NH1	#2	ARG	68.A	O	2.9	#0	LYS	116.B	NZ	#0	ASN	77.A	OD1	3.4
#0	SER	85.B	OG	#3	ASN	113.A	O	2.7	#0	ASP	119.B	N	#0	ASP	87.A	OD2	2.8
#0	THR	89.B	OG1	#3	LYS	116.A	O	2.8	#0	GLN	121.B	NE2	#2	ASN	39.A	OD1	3.6
#2	ARG	61.A	NH2	#0	ASP	101.B	O	2.5	#2	ASN	39.A	ND2	#0	GLN	121.B	OE1	3.1
#3	ARG	114.A	NE	#0	SER	86.B	OG	3.1	#2	ARG	114.A	NH1	#0	ASP	18.A	O	3.6
#3	GLN	121.A	NE2	#0	ASN	77.A	OD1	3.0	#2	ARG	114.B	NH1	#0	ARG	14.B	O	3.1
#3	ARG	125.A	NH2	#0	ARG	73.A	O	3.5	#3	VAL	2.B	N	#0	ASP	48.A	O	3.2
#3	ARG	125.A	NH2	#0	ASN	74.A	O	3.0	#4	ARG	5.A	NH2	#0	ASP	101.A	O	2.9
#4	ARG	68.A	NH1	#0	ARG	21.A	O	2.8	#4	ARG	125.A	NE	#0	ASP	101.A	OD2	2.9
#4	ARG	68.A	NH2	#0	ARG	21.A	O	3.0	#4	ARG	125.A	NH2	#0	ASP	101.A	OD1	3.1
#4	ASN	19.B	ND2	#0	SER	81.B	O	2.7	#4	ARG	128.A	NH2	#0	ASP	52.A	OD1	3.4
#5	ARG	61.A	NH1	#0	GLY	67.B	O	3.1	#5	LYS	1.B	NZ	#0	GLY	71.A	O	3.5
#5	ARG	73.A	NH2	#0	ARG	68.B	O	2.5	#5	ARG	5.B	N	#0	GLY	102.B	O	3.1
#5	ASN	103.A	N	#0	GLY	71.B	O	2.8	#5	ARG	5.B	NE	#0	ASP	101.B	O	3.0
#9	ARG	128.A	N	#0	THR	47.B	O	2.9	#5	ARG	5.B	NH2	#0	ASP	101.B	O	3.0
#9	ARG	128.A	NH1	#0	GLY	49.B	O	3.5	#5	CYS	6.B	N	#0	ASN	103.B	OD1	2.7
#9	ARG	128.A	NH2	#0	ASN	46.B	O	2.9	#5	ARG	14.B	NH1	#0	PRO	70.A	O	2.6
#9	ARG	128.A	NH2	#0	SER	50.B	O	2.9	#5	ARG	14.B	NH2	#0	PRO	70.A	O	3.0
#10	ARG	73.B	NH1	#0	GLY	49.A	O	2.8	#7	LYS	97.A	NZ	#0	ARG	45.A	O	3.2
#10	ARG	73.B	NH1	#0	ARG	68.A	O	2.9	#7	ASN	19.B	ND2	#0	LEU	84.A	O	3.3

#11	ASN	19.A	ND2	#0	SER	81.A	O	2.8	#7	GLN	121.B	NE2	#0	ASN	39.A	OD1	3.6
#11	ASN	19.A	ND2	#0	GLY	126.B	O	3.1	#8	SER	81.B	OG	#0	ASN	113.A	O	2.7
#11	ARG	68.B	NH1	#0	ARG	21.B	O	3.1	#11	ARG	68.B	NH1	#0	GLY	22.A	O	2.9
#11	ARG	68.B	NH2	#0	ARG	21.B	O	3.1	#13	ARG	73.A	NH2	#0	ASP	119.A	OD2	2.9
#13	ASN	77.A	ND2	#0	ASP	119.A	OD2	2.8	#13	ARG	112.A	NH1	#0	ARG	128.A	O	3.3
#13	SER	85.B	OG	#0	ASN	113.A	O	2.7	#13	ARG	112.A	NH2	#0	CYS	127.A	O	2.7
#13	THR	89.B	OG1	#0	LYS	116.A	O	2.8	#13	ARG	112.A	NH2	#0	ARG	128.A	O	3.4