Towards a Pharmacophore for Amyloid

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Supporting Table S2

	KLVFFA/orange-G	VQIVYK/orange-G
PDB accession code	3OVJ	3OVL
Data Collection		
Beamline	APS 24-ID-E	APS 24-ID-E
Date	2008/11/15 and 2009/11/13	2008/11/17
Space group	P 1	C 2
Cell dimensions:		
a, b, c (Å)	9.54, 26.01, 25.80	55.06, 4.83, 22.13
α, β, γ (°)	62.3, 88.6, 88.5	90.0, 103.0, 90.0
Resolution range (Å) (*)	26.01 - 1.8 (1.9 - 1.8)	55.06 - 1.8 (1.9 - 1.8)
$\mathbf{R_{merge\ (square)}}$ **(%)**(*)(a)	18.9 (42.3)	17.9 (48.9)
I/σI(*)	4.38 (1.87)	3.55 (1.20)
Completeness (%) (*) (b)	91.5 (71.7)	87.6 (71.0)
Redundancy(*)	3.8 (1.7)	2.4 (1.4)
Unique Reflections	1870	587
Refinement		
Resolution range (Å) (*)	23.0 - 1.8 (2.0 - 1.8)	26.8 – 1.8 (2.0 - 1.8)
Unique Reflections	1692	525
$\mathbf{R_{work}}$**(%)**(*)(c)/ $\mathbf{R_{free}}$ **(%)**(*)(d) (e)	20.5 (28.9) / 22.0 (36.6)	25.9 (37.7) / 26.0 (44.8)
Completeness (%) (*)(b)	92.9 (79.9)	88.0 (76.4)
Observations/parameters ratio	1.6	1.5
Test set size [%], selection	9.2, random	10.4, random

Number of atoms in asymm. unit	273	88
Protein	208	53
Ligand	54	33
Water	11	2
Average B-factor (Å^2):		
Average B factor for main-chain atoms	12.0	12.4
Average B factor for side-chain atoms	16.1	14.7
Average B factor for ligands	23.3	27.1
Average B factor for water	25.4	28.4
R.m.s. deviations:		
r.m.s.d. bond length (Å)	0.01	0.01
r.m.s.d. bond angles (°)	1.69	1.22
R.m.s. B:		
R.m.s. B for main chain atoms	1.0	0.9
R.m.s. B for side-chain atoms	2.7	2.9
R.m.s. B for ligands	7.0	2.0

Table S2. Data collection and refinement statistics (molecular replacement).

(*) Values in brackets are for the highest resolution shells.

(a) $Rmerge(square) = \sum (I - I(mean))^2 / \sum I^2$, where I is the observed intensity of the reflection HKL and the sum is taken over all reflections HKL.

(b) The incompleteness (<80%) of the highest resolution shell is likely due to the rapid decay of the peptide crystals that are naturally susceptible to radiation decay due to their small size.

(c) $Rwork = \sum \| |F_o| - |F_c| \| / \sum |F_o|$.

(d) R_{free} as defined by [1].

(e) The statistical significance of R_{free} is limited in the case of peptide structures, where the small size of the unit cell leads to a paucity of reflections. In these cases, the R_{free} statistic has proven to be a useful, but less sensitive tool compared with R_{free} statistics reported from macromolecular structure.

Reference

1. Brunger AT (1992) Free R value: a novel statistical quantity for assessing the accuracy of crystal structures. Nature 355: 472-475.