A database of calculated solution parameters for the recently released AlphaFold predicted protein structures

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2 **protein structures.**

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Abstract

Recent spectacular advances by AI programs in 3D structure predictions from protein sequences have revolutionized the field in terms of accuracy and speed. The resulting "folding frenzy" has already produced predicted protein structure databases for the entire human and other organisms' proteomes. However, rapidly ascertaining a predicted structure's reliability based on measured properties in solution should be considered. Shape-sensitive hydrodynamic parameters such as the diffusion and sedimentation coefficients ($D_{t(20,w)}^0$, $s_{(20,w)}^0$) and the intrinsic viscosity ($[\eta]$) can provide a rapid assessment of the overall structure likeliness, and SAXS would yield the structure-related pair-wise distance distribution function $p(r)$ vs. r . Using the extensively validated UltraScan Solution MOdeler (US-SOMO) suite we have calculated from the AlphaFold structures the corresponding $D_{t(20,w)}^0$, $s_{(20,w)}^0$, $[\eta]$, $p(r)$ vs. r , and other parameters. Circular dichroism spectra were also computed. The resulting US-SOMO-AF database should aid in rapidly evaluating the consistency in solution of AlphaFold-predicted protein structures.

The Anfinsen dogma, that protein sequences dictates their three-dimensional (3D) structure, was postulated nearly fifty years ago¹. It set in motion a quest to find methods to reliably and accurately predict 3D protein structures from their sequence, which became even more important with the full sequencing of the human and other genomes (see <https://www.ncbi.nlm.nih.gov/genome>). Recent spectacular advances in the 3D structure prediction from protein sequences by Artificial Intelligence (AI) programs such as AlphaFold (AF) and RoseTTAfold appear to have revolutionized the field in terms of accuracy and speed^{2,3}. Boosted by their success in predicting structures to near (and sometimes even better than) crystallographic accuracy, the AlphaFold consortium (<https://alphafold.ebi.ac.uk>) has already made publicly available a series of databases of predicted protein structures for the entire human and several other organisms proteomes⁴. However, these AI programs have not tackled the folding issue from a thermodynamic/mechanistic approach, but rather by combining many different observations in a deep learning process⁵. Apart from simple cases of highly homologous sequences, or clearly recognized folding classes, to reasonably rapidly ascertain the degree of confidence of a predicted structure based on a few measured properties in solution we believe should become a necessary step. For instance, besides known occurrences of multi-chain proteins, determining a molecular mass M in solution can immediately verify the protein oligomerization state and prompt for the need of further modeling. On a different level, circular dichroism (CD) spectroscopy, possible on very small sample amounts⁶, would permit a rapid check of the actual secondary structure content of a predicted 3D structure. Particularly useful for known single-chain proteins in the AF databases, shape-sensitive hydrodynamic parameters such as the translational diffusion and sedimentation coefficients ($D_{t(20,w)}^0$, $s_{(20,w)}^0$) and the intrinsic viscosity ($[\eta]$), could provide a robust assessment of the overall fold likeliness. These measurements, requiring little material and with a reasonably quick turnaround, are usually accessible in most research endeavors, especially in core facilities where analytical ultracentrifugation^{7,8}, multi-angle static and dynamic light scattering (MALS and DLS) coupled to size-exclusion chromatography (SEC)^{9,10} or directly on plate readers¹¹, and SEC-coupled

differential viscosimetry^{12,13}, can often be found. On another level, small-angle X-ray scattering (SAXS) measurements can provide the rms radius of gyration R_g and the pair-wise distance distribution function $p(r)$ vs. r ^{14,15,16}. Notably, several synchrotron beamlines offer on-line SEC-SAXS (*e.g.*, Table 11.1 in¹⁷), some accepting mailed-in samples for this set-up (*e.g.*, <https://www.diamond.ac.uk/Users/Support-for-European-Access-to-Life-Sciences/Applications/Bio-SAXS.html>; <https://www.embl-hamburg.de/biosaxs/mailin.html>). Importantly, all these parameters and functions can be calculated, with varying degree of accuracy, from 3D structures. Among the CD spectra computational methods available, we have chosen SESCA, which appears to offer very accurate results for a wide variety of structures¹⁸. The computation of the hydrodynamic parameters from atomic level structures is a mature field, with several approaches and corresponding software available, and with an average accuracy comparable to that of the experimentally determined parameters, 2-4%^{19,20}. For the hydrodynamics and the $p(r)$ vs. r distribution calculations, we have employed the extensively validated UltraScan SOLUTION MOdeler (US-SOMO) public domain suite^{21,22,23}. This effort has allowed us to produce and make publicly available, from the AlphaFold released predicted protein structures databases, the comprehensive US-SOMO-AF database presented here, containing the corresponding calculated M , $D_{t(20,w)}^0$, $s_{(20,w)}^0$, $[\eta]$, $p(r)$ vs. r , CD spectra, and other ancillary information. Note that the AlphaFold databases (<https://alphafold.ebi.ac.uk>) were generated from the UniProt (<https://www.uniprot.org>) sequences without any curing. For instance, many proteins are synthesized with a signal peptide²⁴, which will be post-translationally removed. This will affect the calculated parameters in an inverse proportion to protein size. As the mature form will be nearly always purified and studied, we have removed the UniProt-identified signal peptide residues from the AlphaFold structures before performing the hydrodynamic, structural and spectroscopic calculations. Based on the calculated values, some analyses regarding the effectiveness of performing a screening of predicted structures against experimental parameters are presented. Advantages, drawbacks, and potential improvements are then discussed.

Results

Database generation and website implementation

The steps leading to the implementation of the US-SOMO-AF database are fully described in the Methods and Online Methods sections. Briefly, each entry in the entire AF database was first compared with the corresponding entry in the UniProt database to find the (putative) signal peptide regions, which were subsequently removed from the AF PDB files. Potential disulfides were identified (allowing a better evaluation of the partial specific volume $\bar{v}$ and of M) and written as SSBOND records in the cured PDBs, together with HELIX and SHEET information identified using the DSSP²⁵ implementation in UCSF Chimera²⁶. Batch-mode US-SOMO was used to calculate M , $\bar{v}$, $D_{t(20,w)}^0$, $s_{(20,w)}^0$, the derived Stokes' radius R_s , $[\eta]$, R_g , the maximum extensions along the principal X , Y and Z axes of the molecule, and the generation of the $p(r)$ vs. r distributions (normalized by the M of the structure). SESCA was used to generate 170-270 nm CD spectra.

US-SOMO Database	
US-SOMO-AF	
US-SOMO Hydrodynamic, Structural and SESCA CD Calculations on AlphaFold Predicted Structures	
UniProt accession	Q9Y5H4-F1
AlphaFold model name	AF-Q9Y5H4-F1-model_v1
Title	ALPHAFOLD V2.0 PREDICTION FOR PROTOCADHERIN GAMMA-A1 (Q9Y5H4)
Source	MOL_ID: 1 ORGANISM_SCIENTIFIC: HOMO SAPIENS ORGANISM_TAXID: 9606
Signal peptide removed	1-28
AlphaFold date	01-JUL-21
Mean confidence	75.64
Hydrodynamic, structural and CD calculations date	12-OCT-21
Molecular mass [Da]	98141.0
Partial specific volume $\bar{v}$ [cm ³ /g]	0.732
Translational diffusion coefficient $D_{20,w}^0$ [F]	3.26
Sedimentation coefficient $s_{20,w}^0$ [S]	3.54
Stokes radius R_s [nm]	6.56
Intrinsic viscosity $[\eta]$ [cm ³ /g]	23.3 +/- 0.37
Radius of gyration R_g [Å]	84.2
Maximum extension X [nm]	29.46
Maximum extension Y [nm]	10.86
Maximum extension Z [nm]	9.13
% Helix	9.2
% Sheet	25.5
External links	UniProt AlphaFold
Downloads	PDB mmCIF PDB-REDO CD CSV All zip'd All tgz'd

Figure 1 - A partial screenshot of the US-SOMO-AF webpage. See Fig. 2 for the bottom half containing graphs and a JSmol rendering of the structure.

In Fig. 1, a screenshot of the US-SOMO-AF webpage (<https://somo.genapp.rocks>) is shown, with the bottom containing the graphic output removed (see Fig. 2). The header contains hyperlinks to the US-SOMO, SESCO, and AlphaFold websites, and to ref.²². By hovering the mouse over entries, an explanation will appear below the corresponding field on the right column. A UniProt accession number, or some initial part of it, can be entered in the first field (typing just the initial part and clicking "Search" will provide a list of corresponding entries). In any case, if the code is present in the database, the corresponding entry will be shown in the "AlphaFold model name" field, followed by the "Title" and "Source" fields as retrieved from the PDB file. If a signal peptide was identified and its coordinates removed from the PDB file, the stretch of residues involved will be listed in the "Signal peptide removed" field, otherwise "n/a" will appear. The dates on which the AF predictions and US-SOMO/SESCA computations were performed appear in their corresponding fields, and in between the "Mean confidence" field reports the calculated mean % per-residue confidence, based on the values present in the AF-generated PDB file.

The following ten fields report the US-SOMO computed parameters. Since the hydrodynamic parameters were computed with the statistically-based ZENO method^{27,28,29} (see Methods), standard deviations (SD) can be generated. However, a SD is reported only for $[\eta]$, as they are tiny for all other parameters. Note that a calculated $\bar{v}$ is provided because besides being used to compute $s_{(20,w)}^0$ from $D_{t(20,w)}^0$ and M , it could also be used to compute an experimental M from SAXS data¹⁶. The bottom two entries report the per-residue % of α -helix and β -sheet as calculated from HELIX and SHEET fields in the cured PDB. They could be compared with CD-derived values, besides comparing experimental and calculated spectra (see below).

External links for the current entry to both UniProt and AlphaFold websites are placed after the parameters listings. Cured PDB- and mmCIF-formatted files for the entry can be retrieved from the provided hyperlinks, as well as text files with the $p(r)$ vs. r distribution and CD spectrum, and a csv-formatted file containing all the identifying information and the single-value parameters. All these files can be also retrieved as single compressed files (zip or tar.xz). Below these hyperlinks, the computed $p(r)$ vs. r distribution and CD spectrum graphs are presented, followed by a JSmol

(<https://sourceforge.net/projects/jsmol>) representation of the structure (see Fig. 2). Controls for the visualization and copying as an image of both graphs are provided. JSmol commands are also available to change the representation and export it. The default representation colors the structure according to the per-residue confidence level (red, lowest; blue, highest), but for a more in-depth analysis we refer the user to the original AF website. In the end, parameters for a total of 365,198 structures were generated from the AF databases (that include multiple predicted segments for certain sequences), and are stored in the freely accessible US-SOMO-AF database.

Figure 2 - The bottom part of the US-SOMO-AF website page showing the computed $p(r)$ vs. r distribution and CD spectrum plots, and the JSmol representation of the structure.

General data analyses

Although it is beyond the scope of this work to provide extensive data analyses and interpretations, some observations can be made. To this end, we have randomly selected from the 365,198 cured structures present in the US-SOMO-AF database, a subset containing 41,200 predicted structures with no counterparts in the RCSB PDB³⁰ database (<https://www.rcsb.org>), and we have analyzed their calculated properties (data provided as a spreadsheet, Supplementary Data 1).

Figure 3 - Plots of selected calculated parameters for 41,200 predicted structures with no corresponding entries in the solved structures PDB database, randomly-extracted from the 365,198 present in the US-SOMO-AF database. Panel **a**, R_s vs. M , log-log scale. Panel **b**, $[\eta]$ vs. M , log-log scale. Panel **c** $[\eta]$ vs. % decreasing mean confidence level, log-lin scale. Panel **d**, a 3D plot where M (log scale) is on the vertical Z-axis, and R_s and $[\eta]$ are on the horizontal X- and Y-axes, respectively (both linear scales).

The graphs in Fig. 3 allow for testing the discriminatory power of selected calculated parameters, by observing the spread of the R_s (Fig. 3a) and $[\eta]$ (Fig. 3b) values for a given M value (R_s was chosen as a proxy for either $s_{(20,w)}^0$ or $D_{t(20,w)}^0$, the experimentally determined parameters). It is evident that R_s alone (Fig. 3a) can already distinguish between structures, and its power, albeit somewhat limited, does not substantially change on increasing M in the interval 10^4 - 10^5 Da. A significantly larger discriminatory power is instead displayed by $[\eta]$, almost independently of M (Fig. 3b). $[\eta]$ is, however, more affected by potentially flexible regions not properly taken into account by the computations, sometimes leading to suspiciously very high values. Indeed, a correlation between increasing $[\eta]$ values vs. a decreasing % confidence level in the structure prediction can be seen in Fig. 3c, becoming, however, much less defined when the confidence level goes below 50%. Fig. 3d shows in 3D how combining two parameters, R_s and $[\eta]$, can effectively yield an increased discriminatory power. Another important parameter is R_g , but it can rarely be determined by MALS techniques, that have a lower detection limit of ~10-11 nm. While SAXS can

1 determine R_g , it can also be used to derive the $p(r)$ vs. r distribution¹⁶, which contains more
 2 information and can be directly compared with the one computed from structure. Note that the
 3 effect of not taking into account the hydration water in the computation of the $p(r)$ vs. r distribution
 4 is relatively minor, and its importance decreases as M increases. Therefore, plots involving R_g are
 5 not presented here, but could be easily generated from the Supplementary Data 1 spreadsheet.

6

7 *Some examples*

8 Table 1 - Some calculated parameters for a selection of AF-predicted structures with no RCSB PDB
 9 counterparts, ordered by decreasing molecular mass. The corresponding structures and calculated
 10 $p(r)$ vs. r distributions and CD spectra can be seen in Fig. 4.

UniProt Accession	Organism	Mean AF % conf.	Signal peptide	Molecular mass [Da]	R_g [nm]	R_s [nm]	$[\eta]$ [cm ³ /g]	Helix %	Sheet %
Q6PGP7 ^a	<i>H. Sapiens</i>	86.48	n/a	175,523	6.98	6.30	10.4	74.5	0.5
Q4DE01 ^b	<i>T. Cruzi</i>	65.88	n/a	102,098	3.99	5.74	12.0	6.5	23.2
Q9Y5H4 ^c	<i>H. Sapiens</i>	75.64	1-28	98,141	8.42	6.56	23.3	9.2	25.5
D3ZV97 ^d	<i>R. Norvegicus</i>	82.81	1-20	94,123	5.55	4.76	8.93	42.8	11.2
O88338 ^e	<i>M. Musculus</i>	84.24	1-21	87,414	8.69	5.87	21.2	5.7	32.5
Q9LMT9 ^f	<i>A. Thaliana</i>	78.02	1-26	82,090	5.16	4.66	8.96	25.4	15.2
IILDW0 ^g	<i>Glycine Max</i>	75.28	n/a	73,181	2.86	4.16	6.33	32.6	8.9
A4I8P1 ^h	<i>L. Infantum</i>	60.77	n/a	64,586	2.66	3.72	5.18	29.2	9.2
Q6PFT0 ⁱ	<i>Danio Rerio</i>	81.28	n/a	46,965	11.3	5.75	47.8	66.0	10.8
Q9VG48 ^j	<i>D. Melanog.</i>	88.50	1-18	44,673	2.04	2.89	3.44	38.0	9.0
A0A060D4L2 ^k	<i>Zea Mays</i>	68.46	n/a	30,921	3.90	4.06	15.7	32.2	10.4
Q8IJG3 ^l	<i>P. Falciparum</i>	69.83	n/a	19,460	2.05	2.57	5.66	26.4	11.9
P08372 ^m	<i>E. Coli</i>	82.28	n/a	12,010	2.89	2.48	10.5	44.3	21.7
O16446 ⁿ	<i>C. Elegans</i>	88.31	1-19	8,483	1.18	1.66	3.46	68.9	0.0

11 ^aTetratricopeptide repeat protein 37; ^bTrans-sialidase, putative; ^cProtocadherin gamma-a1;

12 ^dVomeroneural 2 receptor, 50; ^eCadherin-16; ^fPutative wall-associated receptor kinase-like 13;

13 ^gAminotran_5 domain-containing protein; ^hAdenosine deaminase-like protein; ⁱFlotillin; ^jLipase;

14 ^kBHLH transcription factor; ^lRNA-binding protein, putative; ^mPrepilin peptidase-dependent protein

15 C; ⁿUncharacterized protein.

In Table 1, we have listed 14 entries chosen from the 41,200 mentioned above. They were initially selected to represent intervals from 2.2 to 0.66 in the computed R_g/R_s ratio indicating deviation from globular shape ($R_g/R_s \sim 0.7$ for a sphere). A suitable range of $[\eta]$ values was also sought, as well as a good representation of the organisms present in the AF databases, the presence or absence of a signal peptide, and some spread in the mean % confidence. M , R_g , R_s , and $[\eta]$ were chosen as the calculated parameters, and the entries are ordered by decreasing M . Connected to Table 1 is Fig. 4, that displays snapshots of the 3D structures for each entry colored according to the per-residue confidence level, followed by the $p(r)$ vs. r and CD plots.

Figure 4 - JSmol snapshots of the structures for the entries reported in Table 1, together with the calculated $p(r)$ vs. r and CD plots.

Table 1 and Fig. 4 provide an insightful glimpse on the great variety of predicted structures and their associated calculated parameters, suggesting that performing some of these checks can indeed boost, or question, their reliability. As expected, CD spectra display differences between most

structures, and they are a robust check on the predicted secondary structure content. The variability in $[\eta]$ values in Table 1 appears to confirm its discriminating power above that of R_s , but clearly it is the $p(r)$ vs. r distribution that would provide the best test, although it is the least rapidly experimentally accessible parameter among those considered.

To provide an additional measure of the predictive power of the hydrodynamic parameters and of the $p(r)$ vs. r distribution, we have selected the O88338 Cadherin-16 from *M. Musculus* structure (see Table 1 and Fig. 4) that contains a number of independently folded domains connected by linkers, and we have run a Discrete Molecular Dynamics (DMD)^{31,32} simulation to expand its conformational space (see Online Methods for details), followed by hydrodynamic and $p(r)$ vs. r calculations on 100 produced structures. As can be seen in the Supplementary Video 1, sufficiently different alternative conformations were generated within an overall frame, allowing an evaluation of the spread in the predicted parameters and their potential discriminating power. For instance, the R_s spread, 5.88-6.16 nm (a ~4.5% change) would be barely above experimental error in distinguishing between the most different conformations in this set, while the spread in $[\eta]$, 20.8-23.8 cm³/g (a ~12.6% change), would clearly allow distinguishing between many conformations (all this set's individual data are in Supplementary Data 2 spreadsheet, and the R_s and $[\eta]$ are reported in each video frame, along with the $p(r)$ vs. r distributions). Even more striking is the variation in the $p(r)$ vs. r distributions that are also collectively reported in Fig. 5.

Figure 5 - Calculated $p(r)$ vs. r distributions for all the conformations generated in the DMD run on the AF-predicted O88338 structure.

Thus, even for such a restricted structural variation, comparing experimental and calculated parameters can provide reliable tests of the predicted structures.

Discussion

We have presented here a new database stemming from the AlphaFold predicted protein structures database. It contains calculated hydrodynamic and structural parameters whose experimental determination should be within the reach of scientists working with a particular protein for which a "hard" structure is either currently unavailable or in the making. Indeed, it is interesting to note that crystallographers and cryo-electron microscopists are already suggesting using AF-predicted structures to solve experimental structures by molecular replacement methods³³. Performing some rapid tests and comparing the results with those we provide in the US-SOMO-AF database could save them valuable time and perhaps hint at twists that should be applied to a predicted structure to better fit the X-ray, cryo-EM, and NMR data. In this respect, we would like to point out a tool present in the US-SOMO program that allows one to color-code a visualized structure based on the contribution of residues to a particular set of distances in a $p(r)$ vs. r distribution³⁴. For instance, this could provide an easier identification of domains that under- or over-contribute to that set of distances. This is another reason why we chose to produce $p(r)$ vs. r distributions instead of simulated SAXS intensity vs. scattering vector curves, for which a wide variety of methods, often quite computationally intensive, exist³⁵. More in-depth analyses could be subsequently performed on case-by-case basis.

For a more general use, assessing the reliability of a predicted structure could lead to better designed function/structure relationship experiments. The availability of the US-SOMO-AF database has the distinctive advantage of allowing a quick comparison without the need to master the expertise necessary to soundly calculate the relevant solution parameters.

There are, of course, a series of drawbacks associated with these computations. First and foremost, all the AF predicted structures consider all proteins as single chain entities. Efforts are apparently underway (see⁵) to cope with this issue by allowing multi-chain predictions, and when an evolution in that sense appears in the AF database, we can re-calculate all parameters for a new set. A second evident drawback resides in the post-translational modifications that many proteins undergo. None were considered by the AF team, and we have just scratched the surface by removing the signal

1 peptides. The most important modification, affecting the calculated parameters, is glycosylation
2 (*e.g.*, see Table 1 in³⁶). While UniProt provides a list of potential glycosylation sites for entries, and
3 publications describing them when available, there is no direct way to have the composition of each
4 carbohydrate associated with a particular site. This is a pity, as methods for building complex
5 carbohydrates are already available and/or under development (see³⁷), and it should be relatively
6 straightforward to automatically add them at the appropriate sites. Indeed, this has just been
7 independently advocated in a very recent letter to this journal³⁸. Even in absence of time-consuming
8 molecular dynamics minimization steps, this simple addition could increase the reliability of
9 calculated hydrodynamic and structural parameters. While we hope that such an important step will
10 be taken at the UniProt database level, users that need to refine the calculations on a predicted
11 structure after having manually added any prosthetic group can easily do so by using one of the
12 downloadable (<http://somo.aucsolutions.com>) US-SOMO versions.

13 The third drawback is the handling of flexibility, especially if large unstructured parts are predicted.
14 Here the US-SOMO-AF database can only raise red flags, such as very high predicted $[\eta]$ values
15 associated with visualized extended, unstructured parts. Dealing with these issues requires much
16 longer calculations involving either Monte Carlo methods or Brownian dynamics simulations
17 (see³⁹), that would require a major effort to be applied systematically on >365,000 structures.
18 All considered, we believe that the publicly available (<https://somo.genapp.rocks>) US-SOMO-AF
19 database described here will become a useful tool allowing the research community, by comparing
20 one or more experimentally-determined parameters with the corresponding computed ones, to
21 quickly evaluate the compatibility in solution of an AlphaFold-predicted protein structure.

22 **Methods**

23 Production of the results presented in this paper required five major steps: collect the AlphaFold
24 entries and additional metadata; prepare the structures for hydrodynamic, structural and CD
25 calculations; compute the hydrodynamic, structural and CD properties; build a database containing
26 the hydrodynamic properties and additional metadata; and finally build a website allowing users
27

1 convenient access to the database.

2 After downloading the AlphaFold database, we prepared the structures by removing the signal
3 peptide regions, where present, identified from the UniProt website. We utilized US-SOMO^{21,22,23}
4 to compute hydrodynamic and structural properties. The US-SOMO suite uses a bead modeling
5 strategy which takes into account the theoretical amount of bound hydration water, and the ZENO
6 computational algorithm^{27,28,29} was employed to calculate the hydrodynamic parameters in a rigid-
7 body frame. US-SOMO was also used to compute the $p(r)$ vs. r distribution on not-hydrated
8 structures, using SAXS-related parameters. To compute the CD spectra, we used SESCA¹⁸.

9 All the computed results were collected and inserted into a database.

10 Full descriptions for all these steps can be found in the Supplementary Methods section.

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23 **Authors contributions**

24 MR conceived the outline of the work, analyzed results, and wrote the paper. EB contributed to
25 define the work, developed all software, performed all computational and website implementation
26 tasks, and wrote the paper.

Competing Financial Interests

The Authors declare no competing financial interests.

Data Availability Statement

The datasets generated during and/or analyzed during the current study are available in the US-SOMO-AF website, <https://somo.genapp.rocks>.

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1 **Figures Legends**

2 Figure 1 - A partial screenshot of the US-SOMO-AF webpage. See Fig. 2 for the bottom half
3 containing graphs and a JSmol rendering of the structure.

4 Figure 2 - The bottom part of the US-SOMO-AF website page showing the computed $p(r)$ vs. r
5 distribution and CD spectrum graphs, and the JSmol representation of the structure.

6 Figure 3 - Plots of selected calculated parameters for 41,200 predicted structures with no
7 corresponding entries in the solved structures PDB database, randomly-extracted from the 365,198
8 present in the US-SOMO-AF database. Panel **a**, R_s vs. M , log-log scale. Panel **b**, $[\eta]$ vs. M , log-log
9 scale. Panel **c** $[\eta]$ vs. % decreasing mean confidence level, log-lin scale. Panel **d**, a 3D plot where M
10 (log scale) is on the vertical Z -axis, and R_s and $[\eta]$ are on the horizontal X - and Y -axes, respectively
11 (both linear scales).

12 Figure 4 - JSmol snapshots of the structures for the entries reported in Table 1, together with the
13 calculated $p(r)$ vs. r and CD plots.

14 Figure 5 - Calculated $p(r)$ vs. r distributions for all the conformations generated in the DMD run on
15 the AF-predicted O88338 structure.

16

Supplementary Files

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