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Note: the title should be concise and informative and not longer than 250 characters. Titles are often used in information-retrieval systems. Avoid abbreviations and formulae where possible.

Given-name Surname of the Author 1 (Arial font, 12 pts, one and a half-spaced)

Affiliation, Address, City and Postal Code, Country (Times New Roman font, 10 pts, Italics, one and a half-spaced)

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e-mail

Author's contribution (letter designation A, B,C, ... G)

Given-name Surname of the Author 2 (Arial font, 12 pts, one and a half-spaced)

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ORCID

e-mail

Author's contribution (letter designation A, B,C, ... G)

Given-name Surname of the Author 3 (Arial font, 12 pts, one and a half-spaced)

Affiliation, Address, City and Postal Code, Country (Times New Roman font, 10 pts, Italics, one and a half-spaced)

ORCID

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Author's contribution (letter designation A, B,C, ... G)

Corresponding author: Given-name Surname, e-mail, institution, street, number, city, zip code, country, telephone number)

Note: Please clearly indicate the given name(s) and family name(s) of each author and check that all names are accurately spelled. You can add your name between parentheses in your own script behind the English transliteration. Present the authors' affiliation addresses (where the actual work was done) below the names. Indicate all affiliations with a lowercase superscript letter immediately after the author's name and in front of the appropriate address. Provide the full postal address of each affiliation, including the country name.

For research articles with several authors, a short paragraph specifying their individual contributions must be provided. The following statements should be used: **A – preparation of the research project; B – assembly of data for the research; C – conducting of statistical analysis; D – interpretation of results; E – manuscript preparation; F – literature review; G – revising the manuscript.**

Clearly indicate who will handle correspondence at all stages of refereeing and publication, also post-publication. This responsibility includes answering any future queries about *Methodology and Materials*. Ensure that the e-mail address is given and that contact details are kept up to date by the corresponding author.

Abstract (Arial font, 14 pts, bolded, one and a half-spaced)

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Note: A concise and factual abstract is required. The abstract should state briefly the purpose of the research, the principal results and major conclusions. An abstract is often presented separately from the article, so it must be able to stand alone. For this reason, References should be avoided. The Abstract should not exceed 300 words and no abbreviations are allowed in the abstract.

KEYWORDS:

Key word 1, Key word 2, ... (Arial font, 12 pts, bolded, one and a half-spaced)

Note: The author can feel free to specify up to 30 key words, however only the first 5 key words will be included in the PDF version of the article. All the keywords specified by authors will be listed in the on-line version published on the journal website. Please, avoid general and plural terms and multiple concepts (avoid, for example, 'and', 'of'). Also, avoid using words that are already in the title. Be sparing with abbreviations: only abbreviations firmly established in the field may be eligible. These keywords will be used for indexing purposes.

Introduction (Arial font, 14 pts, bolded, one and a half-spaced)

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Note: The *Introduction*, as the name implies, should introduce the background to the work that has been carried out, effectively providing the scientific rationale. It should contain sufficient citations (in square brackets in line with the text) to the key literature to support this rationale and should lead to a clearly stated hypothesis or set of objectives. Authors should assume that the readership of the journal is well-informed and there is no need for any generic educational background. Do not insert figures, tables, formulas etc. in this section. The introduction should rarely be more than two manuscript pages long. It should not pre-empt the *Results and discussion* or *Conclusions*.

Materials and methods (Arial font, 14 pts, bolded, one and a half-spaced)

Type materials and methods here (Times New Roman font, 12 pts, one and a half-spaced)

Note: This section should specify exactly what was done experimentally, with sufficient detail for the reader to be able to repeat the experiments if he wishes. It is acceptable to refer to other publications if the methods have been used elsewhere, for example test is used very widely and it is unnecessary to repeat the details unless there has been a departure from standard practice. All of the experimental work discussed in the paper should be described in this section. Materials used in the work should be described in appropriate detail, including sources of commercial supply or synthetic routes, and all major equipment should be specified with the manufacturers name, reference number and location, for example, Perkin-Elmer 457 or Varian HA-100 spectrometers. The accuracy of primary measurements should be stated.

Subtitle 1 (Arial font, 12 pts, bolded, one and a half-spaced)

Type here (Times New Roman font, 12 pts, one and a half-spaced)

Subtitle 2 (Arial font, 12 pts, bolded, in italics, one and a half-spaced)

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Note: Using the ‘Object’ option and selecting the ‘**Microsoft Equation 3.0**’, you can create equations in the Word® equation plug-in editor, or if the MathType™ equation editor is installed on your computer, in the **MathType™** equation editor. Example equation:

$$\Delta G_{bind} = \Delta E_{MM} + \Delta G_{sol} + \Delta G_{SA} \quad (1)$$

All equations should be numbered, as above-mentioned.

Results and discussion (Arial font, 14 pts, bolded, one and a half-spaced)

Type here (Times New Roman font, 12 pts, one and a half-spaced)

Note: The section should, obviously, be factual and it is best to avoid any philosophy or speculation. Authors should consider very carefully how to present their data. It should not be presented in multiple formats (i.e. the same data should not appear in figures and tables). If the data is displayed very effectively in either a table or figure, it should not be necessary to explain results in great detail in the text, but rather to use the text as a medium for emphasizing the most significant data. It is occasionally acceptable not to provide actual evidence of the data, but this should not be done when the data is critical to interpretation. It should not be repetitive of the Introduction. It is entirely valid to suggest the potential implications of the work but without too much speculation. It is particularly important not to extend the discussion into areas that are not supported by the facts that are in evidence.

For **tabular summations** that do not deserve to be presented as a table, lists are often used. Lists may be either numbered or bulleted. Below you see examples of both.

1. The first entry in this list.
2. The second entry:
 - 2.1. A first subentry.
 - 2.2. A second subentry.
3. The last entry.

or

1. The first entry in this list:
 - a bulleted list item;
 - another bullet item.
2. The second entry.

Ensure that all **tables, figures and schemes** are cited in the text in numerical order. Trade names should have an initial capital letter, and trademark protection should be acknowledged in the standard fashion, using the superscripted characters for trademarks and registered trademarks respectively. All measurements and **data should be given in SI units** where possible, or other internationally accepted units. **Abbreviations** should be used consistently throughout the text, and all non-standard abbreviations should be defined on first usage. Below, the example table and figure with captions are attached.

Example of the table:

Table 1. General description of the used set of X-ray ligand–protein complexes with halogen bonding (XB)

Halogen ^a	No. of complexes	XB angle range [°]	XB distance range [Å]	Crystal resolution range [Å]
Cl	39	141–176	2.67–3.67	1.00–2.90
Br	32	159–176	2.34–3.69	1.10–2.92
I	35	148–178	2.83–3.76	1.25–2.90

^aThis is the format for table footnotes.

Note: All tables should be numbered with Arabic numerals. Headings should be placed above tables, centered. Only horizontal lines should be used within a table, to distinguish the column headings from the body of the table, and immediately above and below the table. Tables must be embedded into the text and not supplied separately.

Figure File Requirements:

- File format: TIFF or PNG.
- Resolution: 300 – 600 dpi.
- Text within Figures: Arial, Times font only in 8-12 points.
- Captions: in the manuscript, not in the figure file.

Please do not:

- Supply files that are optimized for screen use (e.g., GIF, BMP, PICT, WPG); the resolution is too low.
- Supply files that are too low in resolution.
- Submit graphics that are disproportionately large for the content.

Example of the figure:

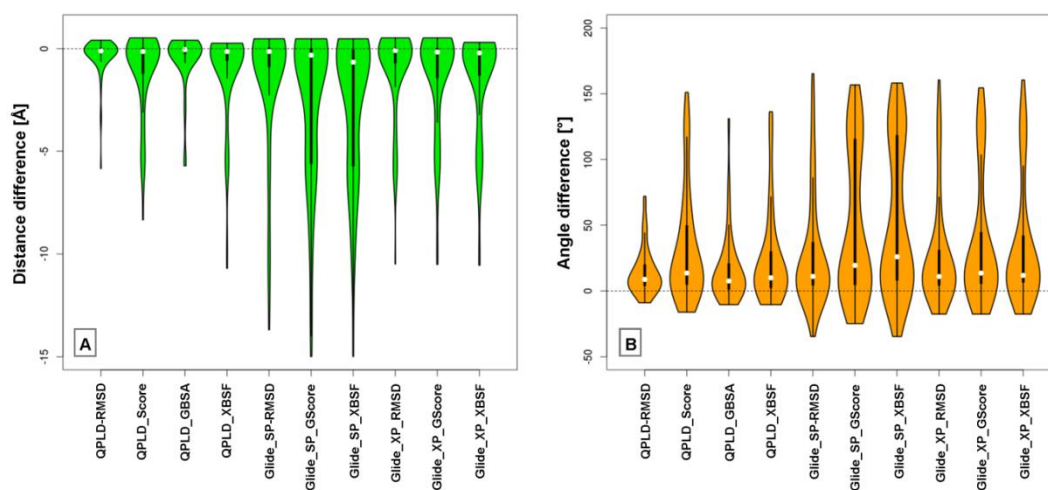


Figure 1. Violin plots showing the difference in halogen bonding distance (A) and σ -hole angle (B) calculated between the best pose predicted by the given scoring method and the crystallographic geometry

```
void Init_TIM3()
{
TIM3->CR1 = TIM_CR1_URS;
TIM3->CR2 = TIM_CR2_MMS_1;
TIM3->SMCR = TIM_SMCR_SMS &0x6;
TIM3->DIER = 0x0000; TIM3->CCMR1 |= TIM_CCMR1_OC1M_2| TIM_CCMR1_OC1M_1;
TIM3->CCMR1 |= TIM_CCMR1_OC1PE | TIM_CCMR1_OC2PE;
TIM3->CCMR2 = 0x0000;

TIM3->CCER = 0x0001;
TIM3->PSC = 0x0001;
TIM3->ARR = 0x007F; TIM3->CNT = 0x0000;
TIM3->CCR1 = 0x003F;
TIM3->CCR2 = 0x0000;
TIM3->CCR3 = 0x0000;
TIM3->CCR4 = 0x0000;
TIM3->DCR = 0x0000;

TIM3->DMAR = 0x0000;
TIM3->EGR = TIM_EGR_UG;
TIM3->CR1 |= TIM_CR1_ARPE | TIM_CR1_CEN;
}
```

Code 1. Code sections should be written in the table using Courier New font. Use indentations if necessary

Conclusions (Arial font, 14 pts, bolded, one and a half-spaced)

Type conclusions here (Times New Roman font, 12 pts, one and a half-spaced)

Note: many authors end the *Results and discussion* section with a paragraph on the conclusions. This is not the best way to draw the manuscript to an end, and we require that conclusions be separated into a distinct section. This should not be too long, nor should it be repetitive of the discussion, and especially should not bring new ideas into the paper. The conclusions have to be based on the facts in evidence and should be limited to reasonable speculation about the significance of the work. The editorial team are particularly vigilant over the use of unjustified, exaggerated language in the *Conclusions* section.

Acknowledgments (Arial font, 14 pts, bolded, one and a half-spaced)

Here you can put acknowledgments to people and institutions that contributed to the creation of the work, and are not its authors (Times New Roman font, 12 pts, one and a half-spaced)

Note: This section may be omitted from the manuscript.

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Note: All sources of funding for research and publication of the article (e.g. costs of translation, proofreading, statistical studies) should be disclosed. If the work was financed from a research grant, please provide the name of the institution and the grant number (e.g. The study was supported by the National Science Centre Grant

No DEC-2022...). If the work has not received funding, you can state, for example: *This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.*

Approval of ethics committee (Arial font, 14 pts, bolded, one and a half–spaced)

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Note: If studies were conducted with the participation of humans or animals, the name of the commission and the opinion/consent number should be provided. This section may be omitted.

References (Arial font, 14 pts, bolded, one and a half-spaced)

[1] Reference 1 (Times New Roman font, 12 pts, one and a half-spaced, dot et the end).

Note: Please use Vancouver Style as a citation and reference list format. The reference list should only include works that are cited in the text, ensure that every reference cited in the text is also present in the reference list (and vice versa). Unpublished results and personal communications are not recommended in the reference list, but may be mentioned in the text. Citation of a reference as 'in press' implies that the item has been accepted for publication.

General rules for references:

- Reference list should appear at the end of your assignment/report with the entries listed numerically and in the same order that they were cited in the text.
- It is very important to use the right punctuation and to check that the order of details in the reference is also correct.
- All authors must be listed in reference list; no use of & between author names.
- Journal titles must be given full name.
- Book and journal titles are not italicised or placed in quotation marks.
- Only first words of the article title and words that normally begin with a capital letter are capitalised.
- Abbreviate page numbers to p., for example p. 12–25.
- Place superscript reference number in square brackets before commas and full stops.
- Use the rule for ranges e.g. [1,2,3,4] becomes [1-4].
- For definition from encyclopaedia or dictionary please cite as a book with additional page of cited term.
- Use of DOI is highly encouraged if possible.

Examples of reference list style:

Article in journal

Hebels DG AJ, Carlier A, Coonen MLJ, Theunissen DH, de Boer J. cBiT: A transcriptomics database for innovative biomaterial engineering. *Biomaterials*. 2017;149:88–97. <https://doi.org/10.1016/j.biomaterials.2017.10.008>.

Book/book with different editions

Bibby C, Burgess N, Hill D, Mustoe S. Bird Census Techniques. Burlington: Elsevier; 2007.

Baken R, Orlikoff R. Clinical Measurement of Speech and Voice. 3rd ed. New York: Delmar Cengage Learning; 2010.

Book with editor/s

Kobayashi S, Müllen K, editors. Encyclopedia of polymeric nanomaterials. Berlin, Heidelberg: Springer Berlin Heidelberg; 2015.

Article or chapter in book

Kasoju N, Nguyen LTB, Padalhin AR, Dye JF, Cui Z, Ye H. Techniques for modifying biomaterials to improve hemocompatibility. In: Siedlecki C, editor. Hemocompatibility of Biomaterials for Clinical Applications. Oxford: Elsevier; 2018. p. 191–220.

Patent

Clarke J, Pines A, McDermott RF, Trabesinger AH, inventors. University of California, assignee. SQUID detected NMR and MRI at ultralow fields. European Patent 1474707. 2004-11-10.

Conference proceeding (the whole conference)

Bennett R, editor. New challenges for corporate and marketing communications. Proceedings of the Eighth International Conference on Corporate and Marketing Communications; 2003 Apr 7–8; London, UK. London: London Metropolitan University; 2003.

Article in press

Zane DM, Irwin JR, Reczek RW. Do less ethical consumers denigrate more ethical consumers? The effect of wilful ignorance on judgments of others. Journal of Consumer Psychology. In press 2015.

Supplementary information (Arial font, 14 pts, bolded, one and a half-spaced)

Note: supplementary material that may be helpful in the review process should be prepared and provided as have been shown below.

Figure S1. The comparison of atomic partial charges assigned by OPLS3 force field

File S1. The list of PDB ID codes including halogenated ligand–protein complexes used

Table S1. The comparison of median, 95% confidence interval (CI) and standard deviation (SD) calculated for differences between estimated halogen bonding geometry (XB distance and angle) by the given docking / scoring procedure and crystallographic structure

		XB distance [Å]			XB angle [°]		
		Median	95% CI	SD	Median	95% CI	SD
QPLD	RMSD	-0.11	-0.52; 0.11	-0.90	8.8	10.58; 18.68	17.84
	GScore	-0.14	-1.52; 0.63	1.96	13.63	23.39; 42.22	41.49
	GBSA	-0.05	-0.81; -0.20	1.35	7.58	10.55; 22.88	27.16
	XBSF	-0.13	-1.51; -0.52	2.19	9.99	16.91; 33.38	36.28
Glide_SP	RMSD	-0.14	-2.18; -0.76	3.13	11.06	18.89; 38.12	42.36
	GScore	-0.32	-3.38; -1.72	3.66	19.44	37.42; 62.51	55.27
	XBSF	-0.66	-3.46; -1.87	3.50	25.99	41.36; 66.74	55.89
Glide_XP	RMSD	-0.09	-1.50; -0.53	2.15	10.97	18.67; 36.94	40.23
	GScore	-0.21	-2.05; -0.91	2.51	13.59	26.32; 48.26	48.31
	XBSF	-0.17	-1.93; -0.82	2.45	11.81	24.01; 44.69	45.55