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Studies on an acetylcholine binding protein identify a basic residue in loop G on the β1-strand as a new structural determinant of neonicotinoid actions

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Abbreviations: ACh, acetylcholine; nAChR, nicotinic acetylcholine receptor; *Ls*-AChBP, *Lymnaea stagnalis*-acetylcholine binding protein; IMI, imidacloprid; CTD, clothianidin, THI, thiacloprid; CH-IMI, nitromethylene imidacloprid analogue, DN-IMI, desnitro-imidacloprid; HEPES, 4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid; SOS, standard oocyte saline; EC_{50}, half maximal effective concentration; I_{max}, normalized maximal response

Abstract

Neonicotinoid insecticides target insect nicotinic acetylcholine receptors (nAChRs). Their widespread use and possible risks to pollinators make it extremely urgent to understand the mechanisms underlying their actions on insect nAChRs. We therefore elucidated X-ray crystal structures of the *Lymnaea stagnalis* acetylcholine binding protein (*Ls*-AChBP) and its Gln55Arg mutant, more closely resembling insect nAChRs, in complex with a nitromethylene imidacloprid analogue (CH-IMI) and desnitro imidacloprid metabolite (DN-IMI) as well as commercial neonicotinoids, imidacloprid, clothianidin and thiacloprid. Unlike imidacloprid, clothianidin and CH-IMI, thiacloprid did not stack with Tyr185 in the wild-type *Ls*-AChBP, but did in the Gln55Arg mutant, interacting electrostatically with Arg55. In contrast, DN-IMI lacking the NO_2 group was directed away from Lys34 and Arg55 to form hydrogen bonds with Tyr89 in loop A and the main chain carbonyl of Trp143 in loop B. Unexpectedly, we found that several neonicotinoids interacted with Lys34 in loop G on the β1 strand in the crystal structure of the Gln55Arg mutant. Basic residues introduced into the α7 nAChR at positions equivalent to AChBP Lys34 and Arg55 enhanced agonist actions of neonicotinoids, while reducing the actions of acetylcholine, (-)-nicotine and DN-IMI. Thus, not only the basic residues in loop D, but also those in loop G determine the actions of neonicotinoids. These novel findings provide new insights into the modes of action of neonicotinoids and emerging derivatives.

Introduction

Nicotinic acetylcholine receptors (nAChRs) are members of the Cys-loop superfamily of ligand-gated ion-channels (LGICs), and neuronal nAChRs play a central role in fast cholinergic neurotransmission in both vertebrates and invertebrates (Changeux, 2012; Hurst et al., 2013). nAChRs are composed of five subunit protein, and form pentagonal assembly. Subunit proteins consist of an extracellular ligand-binding domain (LBD) and four transmembrane regions (TMs), the second of which (TM2) lines an integral ion channel. Agonists binding sites are formed at the subunit interfaces of the LBD, where historically regions involved in agonist binding are named loops A, B, C, D, E and F (Corringer et al., 2000). The binding of acetylcholine (ACh) to nAChRs triggers gating of the integral cation channel to mediate cholinergic neurotransmissions (Unwin and Fujiyoshi, 2012).

Imidacloprid and several insecticidal imidacloprid analogues (Fig. 1A) have been developed since 1990s and these neonicotinoids made up 20.8% of global insecticide sales of US$15.045 billion/annum in 2012 (PhillipsMcDougall, 2013). Normally neonicotinoids act as nAChR agonists (Casida and Durkin, 2013; Ihara et al., 2003; Ihara et al., 2004; Matsuda et al., 2001; Matsuda et al., 2009; Matsuda et al., 2005; Tomizawa and Casida, 2003; Tomizawa and Casida, 2005), however imidacloprid can also act as an antagonist depending on targeted nAChR subtypes (Ihara et al., 2006; Ihara et al., 2003; Salgado and Saar, 2004). Site-directed mutagenesis, electrophysiology and molecular modeling have pointed to basic residues in loop D together with non-acidic residues in loop C as potential determinants of the selectivity of neonicotinoids for insect over vertebrate nAChRs (Matsuda et al., 2009; Shimomura et al., 2002; Shimomura et al., 2006; Toshima et al., 2009) (Fig. 1B). However, neonicotinoids show no particular selectivity among insect species. Indeed, they may even play a role in “colony collapse disorder (CCD)” of honey bees (Gill et al., 2012; Maus et al., 2003). Also a possible contribution of neonicotinoids to the declines of insectivorous birds has been reported (Hallmann et al., 2014). Thus, understanding the molecular mechanism of neonicotinoid actions is of considerable importance.

Since AChBP has been widely recognized as a surrogate for the LBD of nAChRs (Rucktooa et al., 2009), we previously elucidated the X-ray crystal structures of the *Lymnaea stagnalis* acetylcholine binding protein (*Ls*-AChBP) (Brejc et al., 2001) in complex with imidacloprid and clothianidin (Ihara et al., 2008). Crystal structures of *Aplysia californica* AChBP (*Ac*-AChBP) in complex with imidacloprid and thiacloprid were also reported (Talley et al., 2008). Both studies agree in two important respects. First, the guanidine moiety of imidacloprid stacks with the tyrosine residue (Tyr185 in *Ls*-AChBP and the equivalent residue Tyr188 in *Ac*-AChBP) in loop C. Secondly, the NO_2 group of imidacloprid forms a hydrogen bond with the glutamine residue (Gln55 for *Ls*-AChBP and Gln57 for *Ac*-AChBP), which is equivalent to the basic residues frequently observed in loop D of insect nAChRs (Fig. 1B, C; see Supplementary Fig. 1 for entire amino acid sequences), accounting, at least in part, for the role of loop D in selective insecticidal actions of neonicotinoids. However, structural and functional studies of more neonicotinoid family members are needed to help build an improved picture of key target-site determinants.

We therefore generated a Gln55Arg *Ls*-AChBP mutant that mimics more closely loop D of the insect nAChR LBD (Fig. 1C), and elucidated the crystal structures of both wild-type and Gln55Arg mutant of *Ls*-AChBPs complexed with desnitro-imidacloprid (DN-IMI) lacking the NO_2 group as well as with several neonicotinoids (Fig. 1A). We also investigated the actions of these same compounds on the homo pentameric avian α7 nAChR (Couturier et al., 1990). This study enhances our understanding of neonicotinoid–target interactions and highlights a role for basic residues in loop G on the β1 strand as well as in loop D on the β2 strand.

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Materials and Methods

Chemicals

Imidacloprid, thiacloprid and nitromethylene imidacloprid analogue (CH-IMI) were donated by Bayer CropScience, whereas clothianidin was a gift of Sumitomo Chemical. DN-IMI was synthesized *de novo* as described (Latli et al., 1996). ACh and (-)-nicotine were purchased from Sigma-Aldrich (St. Louis, MO, USA) and used without further purification. Bromine-substituted clothianidin analogue (Br-Clothianidin) was prepared as reported previously (Ihara et al., 2008).

Expression constructs

A *Pichia pastoris* expression system (Life Technologies, Carlsbad, CA, USA) was used for the preparation of the recombinant *Ls*-AChBPs as described previously (Ihara *et al.*, 2008). The *Ls*-AChBP gene was cloned in the pPICZα B vector (Life Technologies, Carlsbad, CA, USA). In this process, the leucine at position 1 was mutated to alanine to adapt the sequence to the Pst I restriction site. The cDNA encoding the chicken α7 nAChR, kindly donated by Prof. Mark Ballivet of Geneva University, was cloned into pcDNA3.1 (+) vector (Ihara et al., 2008). Any mutations to expression constructs were introduced using a QuikChange kit (Agilent Technologies, CA, USA), and all DNA sequences were confirmed using a 3100 Genetic analyzer (Life Technologies).

Protein preparation

Both wild-type and the Gln55Arg mutant of *Ls*-AChBP were expressed in *P. pastoris* X-33 and purified as described previously (Ihara et al., 2008). In brief, proteins secreted by *P. pastoris* X-33 were purified using a Q-Sepharose column (GE Healthcare, Piscataway, NJ, USA) and

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subsequently deglycosylated with peptide-*N*-glycosidase F (Wako Pure Chemical Industries, Osaka, Japan) at a concentration of 50 U/mg protein at 37˚C for 24 h. The protein samples were further purified using Mono Q and Superdex 200 columns (GE Healthcare). Purified *Ls*-AChBPs were confirmed by mass spectrometry and N-terminal analysis.

Evaluation of binding of neonicotinoids by Isothermal Titration Calorimetry

Isothermal Titration Calorimetry (ITC) was recorded by an iTC$_{200}$ (GE Healthcare) using 10 μM *Ls*-AChBP and 125 or 250 μM ligands in 25 mM sodium phosphate buffer (pH 8.0) containing 100 mM NaCl at 25ºC. The titration curve was fitted using the manufacturer's software.

Crystallization and X-ray data collection

Purified *Ls*-AChBPs (6.0 mg/mL) were incubated with 0.5 mM neonicotinoids at 4°C for 1 h prior to crystallization. Crystals of *Ls*-AChBP–neonicotinoid complexes were obtained by the vapor diffusion method at 20°C with 1:1 ratio of protein to reservoir solution containing 0.2 M Na citrate pH 5.7, 15-22% PEG3350, and about 0.5 mM of either imidacloprid, clothianidin, Br-clothianidin, thiacloprid, or CH-IMI; 1.5 M Na acetate, 0.05 M $CdSO_4$, 0.1 M HEPES-Na, pH 7.5, and about 0.5 mM of DN-IMI for wild-type complex; 24-27% PEG4000, 0.1-0.3 M Li_2SO_4, 0.1 M Tris-HCl, pH 8.5, and about 0.5 mM DN-IMI for the Gln55Arg mutant complex. The crystals were flash-cooled in liquid nitrogen after soaking in the cryo-protectant solutions containing the reservoir solution comprising 10% higher concentration of the precipitant, supplemented with 20% glycerol and 0.5 mM of each neonicotinoid. X-ray diffraction data sets were collected at 90 or 100 K using either Bruker AXS DIP6040 detector at BL44XU (Yoshimura et al., 2007), ADSC QUANTUM 210 detector at BL44B2 (Adachi et al., 2001), Jupitor210 at BL26B1, or Mar225 at BL26B2 (Ueno et al., 2006) beamlines in SPring-8, and processed with Mosflm (Leslie, 1992) or HKL2000 (Otwinowski and Minor, 1997). In addition, anomalous data from Br-clothianidin bound to the Gln55Arg mutant *Ls*-AChBP were collected at a wavelength of 0.919 Å to identify the position of the chlorine atom in clothianidin, while those from thiacloprid bound to the wild-type and Gln55Arg mutant *Ls*-AChBP were collected at a wavelength of 1.75 Å to identify the position of the sulfur atom in thiacloprid.

Phase determination and refinement

The structure of wild-type *Ls*-AChBP complexed with DN-IMI was solved by molecular replacement with PHASER (McCoy, 2007) using the coordinate of *Ls*-AChBP–imidacloprid complex (PDB entry: 2ZJU) whose ligands and waters were removed. For the Gln55Arg mutant complexed with DN-IMI, the structure was solved by molecular replacement using MOLREP (Vagin and Teplyakov, 1997) with the coordinate 2ZJU whose waters but not the ligand were removed. For the other neonicotinoids, crystal parameters were quite similar to those of the *Ls*-AChBP–imidacloprid complex (2ZJU), thus initial models were obtained by rigid body refinement with CNS version 1.2 (Brünger et al., 1998) using the coordinates of 2ZJU whose ligands and waters were removed. Subsequently, the initial models were refined with either CNS version 1.2, CCP4 Program version 6.4 (Winn et al., 2011) or PHENIX version 1.9-1691 (Adams et al., 2010). Manual model building was performed on the basis of $2F_o$-F_c, F_o-F_c, and omit maps with Coot (Emsley and Cowtan, 2004). The neonicotinoids and the mutated residue were introduced to the model after the initial refinement. The geometries of all the ligands were validated using Mogul (Bruno et al., 2004). The NCS restraints were initially applied for the refinements and removed at later steps. The details of data collection and refinement statistics are provided in Table 1. Simulated annealing omit maps of bound ligands were calculated using PHENIX. The binding orientations of thiacloprid in the crystals were verified by the sulfur atom position in the anomalous map, while those of clothianidin were deduced from the bromine atom position in the anomalous map for the bound Br-clothianidin. Figures are generated by PyMOL (Schrödinger, New York, NY, USA) and each interface of five interfaces in crystals was named according to the chain names in the coordinates.

Functional expression of α7 nAChR and electrophysiology

Xenopus laevis oocytes at stage V or VI were used for expression of the avian α7 nAChR (Couturier et al., 1990). Functional expression was achieved by injecting cDNA encoding nAChR gene as previously described (Ihara et al., 2003; Shimomura et al., 2002). Robust currents were obtained without the need to co-express the RIC-3 (Miller et al., 1996; Nguyen et al., 1995) with α7 nAChR. *Xenopus* oocytes were perfused extracellularly with a standard oocyte saline containing 100 mM NaCl, 2 mM KCl, 1.8 mM $CaCl_2$, 1 mM $MgCl_2$ and 5 mM HEPES 5.0 (pH 7.6). Atropine (0.5 μM) was added to SOS to suppress any muscarinic response of oocytes. Membrane currents evoked by agonist application were recorded using a GeneClamp 500B amplifier and Digidata 1200 digitizer with pClamp 8 software (Molecular Devices, Sunnyvale, CA, USA). The peak current amplitude of the response of wild-type and mutant α7 to ligands tested was normalized to that of the ACh-induced response at concentrations where concentration-response curves reached a maximum. Data was processed using pClamp 9 software (Molecular Devices) and analyzed by non-linear regression analysis using Prism 4 (GraphPad Software, La Jolla, CA, USA) to obtain half maximal concentration EC_{50} (M) and normalized maximal response I_{max} (Ihara et al., 2003; Shimomura et al., 2002).

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Results

Structures of AChBP complexed with neonicotinoids and analogues

We co-crystallized the wild-type and Gln55Arg mutant *Ls*-AChBPs with commercial neonicotinoids (imidacloprid, clothianidin and thiacloprid) and a nitromethylene imidacloprid analogue CH-IMI (Fig. 1A) excluding only the wild-type *Ls*-AChBPs in complex with imidacloprid and clothianidin which were reported earlier (Ihara et al., 2008). These crystals in complex with commercial neonicotinoids and CH-IMI belong to the same space group, $P6_5$. We also co-crystallized wild-type and Gln55Arg mutant *Ls*-AChBPs with the denitrated imidacloprid metabolite DN-IMI, and obtained crystals belonging to space group $P2_12_12_1$. The crystal structures were solved and refined at 2.09–2.68Å resolution (Table 1). Common to other AChBP structures reported, a pentameric ring structure with a center aperture was obtained for all complexes (Fig. 1D). Electron density of ligand-omit maps (Fig. 2) indicated that all five LBDs were occupied by a single ligand, and no empty binding site was observed. The model for clothianidin interacting with the binding site was confirmed with anomalous peaks observed at the bromine atom from Br-clothianidin complexed with the Gln55Arg mutant of the *Ls*-AChBP in the X-ray diffraction data collected at 0.919 Å (Fig. 2B and Table 1), as in the wild-type protein (Ihara et al., 2008), allowing unequivocal determination of the ring orientation, because the ring structure of clothianidin with its substituent groups is asymmetric. In the case for thiacloprid modeling, anomalous peaks observed in the X-ray diffraction data, which were collected at 1.75 Å for the wild-type and mutant *Ls*-AChBP complexes (Table 1), indicated the sulfur and chlorine atom positions in thiacloprid along with the sulfur atom position in Met114 (Fig. 2C), and thus permit unambiguous determination of the thiacloprid binding mode. The stereochemical geometries for all the bound ligands were verified by Mogul (Bruno et al., 2004) (Table 1 and Supplementary Tables 1–10).

There were no large structural differences observed at the aromatic ring system of the neonicotinoids and the surrounding amino acid residues in the *Ls*-AChBP between the wild-type and Gln55Arg, as well as among all the tested neonicotinoids (Figs. 2, 3 and Supplementary Fig. 2). The aromatic ring moiety of thiacloprid formed a hydrogen bond at the nitrogen atom via a single water molecule associated with the main chain amide (both NH and C=O) of Met114 and the main chain carbonyl of Leu102 in loop E (Supplementary Fig. 2A), as also seen in imidacloprid, clothianidin (Ihara et al., 2008; Talley et al., 2008), CH-IMI (Supplementary Fig. 2B) and DN-IMI (Supplementary Fig. 2C).

Interactions of the guanidine and related moieties with wild-type AChBP

We previously reported that the guanidine moiety of imidacloprid and clothianidin stacked with Tyr185 in loop C, while the hydrogen atoms of the ethylene bridge of imidacloprid and the *N*-methyl group of clothianidin underwent CH-π interactions (Nishio, 2006) with the aromatic ring of Trp143 in loop B in the wild-type *Ls*-AChBP (Fig. 3A, D) (Ihara et al., 2008). In addition, we showed that the NO_2 group of imidacloprid (Fig. 3A), but not of clothianidin (Fig. 3D), formed a hydrogen bond with Gln55 (Ihara et al., 2008). Here we provide evidence that thiacloprid does not stack with Tyr185 in the wild-type protein, but instead interacts with Tyr89 in loop A, Trp143 in loop B, Tyr192 in loop C and Trp53 in loop D, while forming a hydrogen bond between the CN group and the main chain amide of Tyr185 (Fig. 3G). In a similar way to imidacloprid, the nitromethylene imidacloprid analogue CH-IMI stacked with Tyr185, while forming a hydrogen bond at the NO_2 group with Gln55 (Fig. 3J). In addition, CH-IMI interacted with Lys34 on the β1 strand (not shown in Fig. 3J. See below for details).

We also investigated the binding characteristics of neonicotinoids by isothermal titration calorimetry (ITC, see Supplementary Fig. 3 for titration curves). CH-IMI showed the highest affinity (K_d = 92 nM) of all the neonicotinoids tested. Thiacloprid bound to the wild-type protein more strongly (K_d = 297 nM) than imidacloprid (K_d = 530 nM) and clothianidin (K_d = 1.79 μM) (Table 2). Entropy for thiacloprid was positive, while that for imidacloprid, clothianidin, and CH-IMI was negative (Table 2), consistent with distinct binding characteristics of thiacloprid from those of the other neonicotinoids.

Effects of the Gln55Arg mutation on AChBP–neonicotinoid interactions

We investigated the impact of the Gln55Arg mutation on AChBP–neonicotinoid interactions based on X-ray crystal structures of the ligand complexes. The Gln55Arg mutation had no major impact on the stacking with Tyr185 of the guanidine moiety of imidacloprid, clothianidin and CH-IMI. However, not only the NO_2 group of imidacloprid (Fig. 3B, C) and CH-IMI (Fig. 3K, L), but also of clothianidin (Fig. 3E, F) which had no contact with loop D in the wild-type protein, interacted electrostatically with the side chain of Arg55 in loop D. The most striking impact of the Gln55Arg mutation was observed in its interactions with thiacloprid. Although thiacloprid did not stack with Tyr185 in the wild-type protein (Fig. 3G)), it did stack with Tyr185, orienting the CN group toward Arg55 (Fig. 3H, I).

In response to the Gln55Arg mutation, neonicotinoid affinity was slightly enhanced or at least retained, whereas the affinity of (-)-nicotine (Table 2) was markedly reduced. Interestingly, the Gln55Arg mutation enhanced enthalpy and reduced entropy for thiacloprid, whereas the reverse was the case for clothianidin (Table 2).

Unique binding of DN-IMI to *Ls*-AChBP

DN-IMI is an imidacloprid metabolite lacking the negatively charged NO_2 group, which is an important structural feature of neonicotinoids. The removal of the NO_2 group results in a positively charged guanidine group (Fig. 1A). DN-IMI interacted with the wild-type and Gln55Arg mutant of *Ls*-AChBPs in a completely different manner from the other neonicotinoids (Fig. 4). In the wild-type protein, DN-IMI stacked with Tyr185, yet directed its guanidine away from Gln55 (Fig. 4A), forming a hydrogen bond with Tyr89 in loop A and the main chain of Trp143 in loop B (Fig. 4A). The Gln55Arg mutation further induced a change of the stacking partner of DN-IMI from Tyr185 to Tyr192, retaining the hydrogen bond with Tyr89 and Trp143 (Fig. 4B, C) with increased entropy (Table 2).

Ligand interactions with a basic residue on the β1 strand

In addition to the anticipated interactions with loops A–F, we found for the first time that the NO_2 group in clothianidin (Fig. 5A) and the CN group in thiacloprid (Fig. 5B) interacted with Lys34, which corresponds to Ile44 in loop G on the β1 strand of the mouse serotonin 5-HT_3 receptor (Hassaine et al., 2014), in the Gln55Arg mutant. CH-IMI also interacted with Lys34 in the Gln55Arg mutant (Fig. 5C) as in the wild-type protein with the highest affinity (Table 2).

The effects of mutations of Ser55 and Gln79 to basic amino acids on the α7 nAChR responses to neonicotinoids, DN-IMI, (-)-nicotine and ACh

To clarify whether basic residues on the β1 strand, as well as the basic residues in loop D, play a key role in neonicotinoid actions on nAChRs, we employed the avian α7 nAChR because 1) it shows higher similarity than heteropentameric nAChRs to the *Ls*-AChBP in its amino acid sequence of the extracellular domain (for the avian α7, 26%; for the human α7, 24%) as well as in its ability to form a homopentamer (Brejc et al., 2001) and 2) higher neonicotinoid sensitivity than vertebrate heteropentameric nAChRs (Ihara et al., 2003) and thus has been used extensively in characterizing neonicotinoid actions (Ihara et al., 2003; Shimomura et al., 2002;

Shimomura et al., 2003). We mutated to basic residues Ser58 and Gln79 corresponding Lys34 and Gln55, respectively of the *Ls*-AChBP and investigated the effects of such mutations on agonist action of the ligands studied. All the ligands induced inward currents in oocytes expressing the wild-type and mutant α7 nAChRs (Fig. 6). Imidacloprid, clothianidin and thiacloprid were partial agonists, while CH-IMI, DN-IMI and (-)-nicotine were full or nearly full agonists (Fig. 7A). The Ser58Lys mutation selectively enhanced the efficacy in terms of I_{max} of neonicotinoids (Fig. 7B). Notably, imidacloprid, thiacloprid and CH-IMI showed greater I_{max} than ACh for the Ser58Lys mutant. In contrast, the Ser58Lys mutation reduced the affinity in pEC_{50} of ACh, (-)-nicotine and DN-IMI ($p < 0.05$, one way ANOVA, Dunnett's test). Similarly, the Gln79Arg mutation corresponding to the Gln55Arg mutation in the *Ls*-AChBP (Figure 7C) enhanced the efficacy of neonicotinoids, while reducing the affinity of ACh, (-)-nicotine and DN-IMI (Table 3).

When both Ser58 and Gln79 were mutated to basic residues, the pEC_{50} value of imidacloprid was significantly increased ($p < 0.05$, one way ANOVA, Dunnett's test) (Fig. 7D, Table 3). Also, the Ser58Lys;Gln79Arg double mutation resulted in enhanced I_{max} values of all the neonicotinoids tested compared to those obtained for wild-type α7, while significantly reducing the pEC_{50} values of ACh, (-)-nicotine and DN-IMI as well as the I_{max} values of (-)-nicotine and DN-IMI ($p < 0.05$, one way ANOVA, Dunnett's test). No significant effect of the mutations was observed on the decay time constant for the agonist-induced currents in *Xenopus* oocytes expressing α7 (data not shown).

Discussion

In this study, we employed the *Ls*-AChBP as a surrogate for the nAChR LBD, and co-crystallized with neonicotinoids both wild *Ls*-AChBP and its Gln55Arg mutant – the arginine residue at this loop D position being found in many insect nAChR LBDs (Fig. 1C). The resolution (2.09-2.68 Å) of these X-ray crystal structures are sufficient to model ligands and side chains/main chains involved in ligand binding. Such resolution also permits identification of water molecules including those involved in the aromatic ring nitrogen–loop E interactions (Supplementary Fig. 2) (Ihara et al., 2008), although such interactions with loop E would not directly contribute to the selective actions of neonicotinoids on insect nAChRs because similar interactions are also observed for (-)-nicotine (Celie et al., 2004) and epibatidine (Hansen et al., 2005).

We examined whether neonicotinoids generally stack with the tyrosine residue in loop C and interact electrostatically with the basic residue in loop D. Novel crystal structures of the wild-type and Gln55Arg mutant of the *Ls*-AChBP complexed with DN-IMI helped address whether the NO_2 group, so important in the actions of imidacloprid, is a key determinant of the interactions with loop D. Although thiacloprid did not stack with Tyr185 in loop C of the wild-type *Ls*-AChBP (Fig. 3G), it did stack with Tyr185 in the Gln55Arg mutant (Fig. 3H) as was the case for other neonicotinoids (Fig. 3B, E, K). The NO_2 group of clothianidin (Fig. 3D) and the CN group of thiacloprid (Fig. 3G) had no contact with Gln55 in the wild-type *Ls*-AChBP, apparently undermining the generalization that neonicotinoids interact with loop D. However, the Gln55Arg mutant induced stacking of both clothianidin and thiacloprid with Tyr185 in loop C. The Gln55Arg mutation also lead to electrostatic interactions of the clothianidin NO_2 group with the inserted basic residue, while breaking another hydrogen bond between the guanidine NH and the backbone carbonyl (Fig. 3E). In addition, this mutation changed the orientation of the thiacloprid CN group from the main chain of loop C to Arg55 in loop D, demonstrating that the basic residue generally determines the binding mode of neonicotinoids at LBD. Nevertheless, the interactions with loop C cannot be ignored in the neonicotinoid actions because a glutamate residue in this loop of vertebrate nAChR α subunits (Fig. 1C) was shown to play a role in the low neonicotinoid sensitivity (Shimomura et al., 2004).

To investigate such Gln55Arg mutation-induced changes of the binding mode in another way, we measured the thermodynamic parameters by ITC for interactions of all the ligands studied with the wild-type and Gln55Arg mutant *Ls*-AChBPs. In the case of clothianidin, enthalpy was reduced, while entropy was increased in response to the Gln55Arg mutation, which may result from a break of the hydrogen bond with the main chain of Trp143 in loop B. On the other hand, the wild-type *Ls*-AChBP–thiacloprid interactions resulted in positive entropy, possibly reflecting dehydration of the functional group as a consequence of hydrogen bond formation with the main chain of loop C. The Gln55Arg mutation induced thiacloprid stacking with Tyr185, resulting in reduced mobility of the compound (Table 2), which may, at least in part, account for the reduced entropy.

In contrast with the effects on neonicotinoids, the Gln55Arg mutation reduced the affinity of (-)-nicotine (Table 2), suggesting a gate-keeper role for the basic residue that repels positively charged agonists. In the wild-type and the Gln55Arg mutant of *Ls*-AChBP, the positively charged guanidine of DN-IMI was oriented away from loop D (Fig. 4), supporting the critical role for neutral to negatively charged “nitro-” and “cyano-” groups of neonicotinoids.

Bass *et al*. (2011) found that the Arg81Thr mutation in loop D of the β1 subunit (Fig. 1C) conferred strong neonicotinoid resistance in the peach aphid *Myzus persicae* (Bass et al., 2011). The weakest impact of the Gln79Arg mutation on thiacloprid actions on α7 (Fig. 7C) is in accord with the weakest electrostatic interactions between the CN group in thiacloprid and Arg55 in the Gln55Arg mutant *Ls*-AChBP (Fig. 3H). We therefore suggest that thiacloprid actions are less profoundly affected by this mutation than the actions of other neonicotinoids.

Unexpectedly, we found that Lys34 on the β1 strand in the complementary side contributes to the interactions of clothianidin, thiacloprid and CH-IMI with LBD (Fig. 5). We presumed that such a basic residue in loop G could also play a role in the selective actions of neonicotinoids and thus investigated agonist actions of neonicotinoids, DN-IMI, (-)-nicotine and ACh on the avian α7 nAChR mutagenized to yield basic residues at the equivalent position of Lys34. This resulted in significant impact on efficacy (Fig. 7, Table 3). No previous study has shown that any mutation of Ser58 and equivalent amino acids in loop G affects the selectivity and diversity of agonist actions on Cys-loop ligand-gated ion channels. CH-IMI contacted most strongly with Lys34 (Fig. 5C), accounting for the highest impact of the Ser58Lys mutation on its agonist actions on α7 (Fig. 7B) (Fig. 3). When combined with Arg79 (Fig. 7C), Lys58 exerted even more striking effect than the single mutation, not only on the affinity of imidacloprid, but also on the efficacy of all the ligands studied (Fig. 7D, Table 3). Presumably, similar results would also be observed with human α7, as it shares high similarity with the avian α7 (93.8% in the extracellular agonist binding regions; overall similarity, 89.9%). In future, it will be of interest to examine by a double mutant cycle analysis (Horovitz, 1996) whether there is any possible cooperativity of the two basic residues. Also, in future it will be necessary to examine whether the agonist profile of α7 concurs with that of robustly expressed insect nAChRs. Nevertheless, not only the interactions at the α–non-α subunit interface, but also those at the α–α subunit interface, may well underlie the neonicotinoid actions because the basic residue in loop G in the complementary side of the *Ls*-AChBP interacted with neonicotinoids and significantly enhanced the agonist actions of neonicotinoids on α7. In addition, we predict that neonicotinoid resistance may occur in pest insect species by a mutation of the basic residue to serine in loop G (Fig. 1C) as in the case of the R81T mutation in loop D (Bass et al., 2011).

Honey bees (*Apis mellifera*) also possess the “canonical” two basic residues in both loops D and G of nAChRs other than those consisting of α5–α7 subunits (Fig. 1**C**), thereby showing some sensitivity to the commercial neonicotinoids. Thus it appears difficult to design pest-species-selective chemicals acting on the neonicotinoid-binding pocket in nAChRs. Nevertheless, the pocket in honey bee nAChRs has distinct size, electrostatic potentials and hydrogen-bond capability from that in pest insect species (Matsuda et al., 2009). Thus the structural data generated in this study may help in the design of compounds that are safer to mammals and beneficial insects.

In conclusion, we have identified structural determinants defining the interactions of neonicotinoids and DN-IMI with the wild-type and Gln55Arg mutant of *Ls*-AChBP. In addition to the basic residue in loop D, we newly found that Lys34 in loop G on the β1 strand also interacted with neonicotinoids in the *Ls*-AChBP and noted significant impact of the equivalent residue on the agonist actions of both neonicotinoids and other agonists on the homopentameric α7 nAChR. Thus we show that both loop D and loop G basic residues strengthen the nAChR–neonicotinoid interactions.

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Authorship contribution

Participated in research design: Ihara, Yamashita, Okajima, Sattelle, Matsuda

Conducted experiments: Ihara, Yamashita, Okajima, Oda, Matsui, Asano, Matsuda

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FOOTNOTES

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Figure legends

Figure 1. Chemical structures of acetylcholine, (-)-nicotine and neonicotinoids; sequence alignments of *Lymnaea stagnalis* (*Ls*)-AChBP and LBD of α7; alignments of loop D and β1 strand of AChBPs and nAChRs; whole view of Gln55Arg mutant of *Ls*-AChBP in complex with imidacloprid. (A) Chemical structures of acetylcholine (ACh), (-)-nicotine, neonicotinoids [Imidacloprid (IMI), clothianidin (CTD), thiacloprid (THI) and a nitromethylene imidacloprid analogue (CH-IMI)] and desnitro-imidacloprid (DN-IMI). (B) Pairwise alignment of *Lymnaea stagnalis* (*Ls*)-AChBP and chicken α7 nAChR. The secondary structures are illustrated above the primary structures. Positions of the binding site “loops A–F” are shown by horizontal bold lines. Residues Gln55 (corresponding to Gln79 of α7 nAChR) and Lys34 (Ser58 of α7) are colored red and arrowed. (C) Multiple sequence alignment of loop D and loop G of insect and vertebrate nAChR subunits alongside *Ls*-AChBP. Numbers indicate the position counted from the N-terminal Met1 of each nAChR subunit sequence, whereas those of *Ls*-AChBP indicate the position from the mature N-terminal. (D) The whole structure of Gln55Arg mutant of *Ls*-AChBP in complex with CH-IMI. CH-IMI, Lys34 (in sky blue) and Arg55 (in magenta) are drawn by space-fill models. Carbons, nitrogen, oxygen and chlorine atoms of CH-IMI are colored bright grey, blue, red and green, respectively.

Figure 2. F_o-F_c omit maps for bound neonicotinoids in the Gln55Arg mutant of *Ls*-AChBP. The simulated annealing F_o-F_c omit maps (blue) for imidacloprid (A), clothianidin (B), thiacloprid (C), CH-IMI (D) and DN-IMI (E) bound to the Gln55Arg mutant of *Ls*-AChBP are drawn with the final model. The omit maps for imidacloprid, thiacloprid, CH-IMI and DN-IMI are contoured at 3 σ, while that for clothianidin is contoured at 3.5 σ. In (B), an anomalous map of bromine atom contoured at 5.0 σ from an isomorphous crystal of the Gln55Arg mutant of the *Ls*-AChBP complexed with Br-clothianidin was overlaid. In (C), the anomalous maps

(orange) of sulfur and chlorine atoms contoured at 3.0 σ are overlaid. In each ligand, carbon, chlorine, nitrogen, oxygen and sulfur atoms are colored bright grey, green, blue, red and yellow, respectively.

Figure 3. Ligand binding domain of wild-type and Gln55Arg mutant of *Ls*-AChBP in complex with neonicotinoids. (A) Wild-type *Ls*-AChBP–imidacloprid complex, (B) Gln55Arg *Ls*-AChBP mutant–imidacloprid complex, (D) wild-type *Ls*-AChBP–clothianidin complex, (E) Gln55Arg *Ls*-AChBP mutant–clothianidin complex, (G) wild-type *Ls*-AChBP–thiacloprid complex, (H) Gln55Arg *Ls*-AChBP mutant–thiacloprid complex, (J) wild-type *Ls*-AChBP–nitromethylene imidacloprid analogue (CH-IMI) complex and (K) Gln55Arg *Ls*-AChBP mutant–CH-IMI complex. Abbreviations: Imidacloprid, IMI; clothianidin, CTD; thiacloprid, THI; nitromethylene imidacloprid analogue, CH-IMI. Carbon, chlorine, nitrogen, oxygen and sulfur atoms of the ligands are colored bright grey, green, blue, red and yellow, respectively. The binding site of imidacloprid (A, B) is represented by the subunit AB interface. The clothianidin-binding site of the wild-type (D) and Gln55Arg mutant (E) are represented by the subunit EA and CD interfaces, respectively. The binding sites of thiacloprid (G, H) and CH-IMI (J, K) are represented by the subunit EA and CD interfaces, respectively. The carbon atoms of the principal chains are colored bright pink, whereas those of the complementary chain are colored cyan. Panels A and D were generated using PDB data (PDB entry codes: 2ZJU, 2ZJV, respectively) reported in previous study (Ihara et al., 2008). The binding sites of the wild-type (light green) are superimposed on those of the Gln55Arg mutant (violet) in imidacloprid (C), clothianidin (F), thiacloprid (I) and CH-IMI (L) complexes. The coordinate data of the principal chain is used for superposition of the binding sites of the wild-type and Gln55Arg mutant *Ls*-AChBP. Bright blue and orange broken lines depict hydrogen bonds and electrostatic interactions, respectively.

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Figure 4. Crystal structures of wild-type and Gln55Arg mutant *Ls*-AChBP in complex with desnitro-imidacloprid (DN-IMI). The binding sites of wild-type (A) and the Gln55Arg mutant (B) *Ls*-AChBPs are represented by the subunit AB interface. The carbon atoms of the principal chain are colored bright pink, whereas those of the complementary chain are colored cyan. The binding sites of the wild-type (light green) are superimposed on those of the Gln55Arg mutant (magenta) (C). In DN-IMI, chlorine, nitrogen and oxygen atoms are colored green, blue and red, respectively, whereas the carbon atoms are colored bright grey. Bright blue broken lines depict hydrogen bonds. For Gln55Arg mutant, three among the five ligand binding sites exhibit the same ligand binding configuration shown in the figure.

Figure 5. Expanded view of neonicotinoid-binding sites of the Gln55Arg mutant of *Ls*-AChBP. The binding sites of clothianidin (A), thiacloprid (B), and the nitromethylene imidacloprid analogue (CH-IMI) (C) on the Gln55Arg mutant of *Ls*-AChBP. The subunit BC interface is shown and interactions of the neonicotinoids with loop C, Arg55 in loop D on the β2 strand and Lys34 in loop G on the β1 strand are highlighted. Three (for clothianidin), four (for thiacloprid), and three (for CH-IMI) among the five ligand binding sites exhibited the distinct salt bridge formation with the distances less than 4 Å, as shown in the figures. The carbon atoms of the principal chains are colored bright pink, whereas those of the complementary chain are colored cyan. In the bound neonicotinoids, carbon, chlorine, nitrogen, oxygen and sulfur atoms are colored bright grey, green, blue, red and yellow, respectively. Orange broken lines depict hydrogen bonds/electrostatic interactions. See Supplementary Fig. 4 for electron-density map and the distribution of the B-factor for the Gln55Arg mutant–clothianidin complex.

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Figure 6. Current responses to ACh, imidacloprid, clothianidin, thiacloprid, CH-IMI, DN-IMI and (-)-nicotine of wild-type and mutant (Ser58Lys, Gln79Arg and Ser58Lys;Gln79Arg) α7 nAChRs expressed in *Xenopus laevis* oocytes. Typical responses to the applied ligands are indicated.

Figure 7. Concentration-response curves showing agonist actions of acetylcholine, neonicotinoids [imidacloprid, clothianidin, thiacloprid, nitromethylene imidacloprid analogue (CH-IMI)], desnitro-imidacloprid (DN-IMI) and (-)-nicotine on wild-type and mutant α7 nicotinic acetylcholine receptors (α7 nAChRs) expressed in *Xenopus laevis* oocytes. Examples of the responses of α7 are shown in Fig. 7). Normalized peak current amplitude of the responses of α7 nAChRs were plotted against concentrations of the ligands tested. Each plot represents mean ± stand error of the mean of repeated experiments (n = 4–6). (A) Wild-type, (B) Ser58Lys mutant, (C) Gln79Arg mutant, (D) Ser58Lys;Gln79Arg double mutant. Ser58 and Gln79 correspond to Lys34 and Gln55 of *Ls*-AChBP, respectively. Note that the Ser58Lys (B) and Ser58Lys;Gln79Arg mutants (D) of α7 nAChR correspond to the wild-type and Gln55Arg mutant of *Ls*-AChBP. See Table 3 for affinity (pEC_{50}) and efficacy (I_{max}) of ligands obtained by fitting the concentration-response curves.

Table 1. X-ray diffraction data collection and refinement statistics for *L*-AChBP-neonicotinoid[a] complexes

	Gln55Arg mutant Imidacloprid	Gln55Arg mutant Clothianidin	Wild-type Thiacloprid	Gln55Arg mutant Thiacloprid	Wild-type CH-IMI	Gln55Arg mutant CH-IMI	Wild-type DN-IMI	Gln55Arg mutant DN-IMI	Gln55Arg mutant Br-Clothianidin (Br ano)[h]	Wild-type Thiacloprid (S ano)[h]	Gln55Arg mutant Thiacloprid (S ano)[h]
Data collection											
Beamline[b]	BL44XU	BL44XU	BL44B2	BL44XU	BL44B2	BL44XU	BL44B2	BL26B2	BL44B2	BL44B2	BL44B2
Wavelength (Å)	0.9	0.9	0.919	0.9	0.919	0.9	0.9	0.9	0.919	1.75	1.75
Space group	$P6_5$	$P6_5$	$P6_5$	$P6_5$	$P6_5$	$P6_5$	$P2_12_12_1$	$P2_12_12_1$	$P6_5$	$P6_5$	$P6_5$
Cell dimensions *a*, *b*, *c* (Å)	74.6, 74.6, 350.7	74.1, 74.1, 351.6	74.5, 74.5, 351.0	74.5, 74.5, 350.8	75.0, 75.0, 351.0	74.8, 74.8, 351.4	77.0, 118.4, 243.6	73.1, 120.7, 139.3	74.8 74.8 351.8	74.6, 74.6, 351.2	74.6, 74.6, 350.9
Resolution (Å)	18.1-2.52	39.6-2.67	47.5-2.24	39.6-2.68	47.6-2.30	18.0-2.48	50.0-2.09	50.0-2.25	50-3.2	50.0-2.90	50.0-3.0
R_{sym} (%)[c, d]	8.7 (40.0)	9.4 (40.2)	9.1(43.8)	8.4 (40.3)	7.7 (41.4)	9.9 (37.5)	7.4 (46.3)	7.6 (44.9)	13.8 (36.2)	10.3 (30.8)	8.9(34.0)
I/σ^{χ}	8.4 (1.9)	6.9 (1.8)	37.2 (5.20)	7.8 (1.8)	24.9 (2.42)	6.4 (2.0)	24.7 (2.30)	38.5 (4.44)	19.4 (8.4)	64.7 (16.5)	47.8(11.5)
Completeness	99.7 (100)	99.6 (99.9)	99.9 (100)	98.9 (99.9)	99.0 (91.1)	99.5 (99.5)	99.2 (93.7)	99.8 (99.7)	100 (100)	99.8 (99.6)	95.3(97.4)
Redundancy[b]	5.1 (5.1)	3.4 (3.4)	11.2 (10.3)	2.6 (2.6)	10.9 (7.9)	5.2 (5.2)	7.1 (6.4)	7.3 (7.0)	14.6 (14.8)	22.1 (22.0)	22.8(23.2)
Refinement											
Resolution (Å)	18.1-2.54	39.6-2.68	47.5-2.24	39.6-2.69	47.6-2.30	18.0-2.48	47.8-2.09	20.8-2.25			
No. reflections	35965	30443	52420	30084	48471	37741	131114	58862			
R/R_{free} (%)[e]	19.7/27.1	19.3/26.0	22.2/26.6	20.0/27.4	21.0/26.5	20.3/26.2	21.3/26.2	21.5/26.2			
Bond length (Å)/angles (deg)[f] Protein (ligands)	0.008/1.3 (0.004/0.29)	0.007/1.3 (0.001/0.16)	0.007/1.3 (0.004/0.25)	0.008/1.3 (0.004/0.31)	0.006/1.3 (0.003/0.15)	0.008/1.6 (0.003/0.14)	0.006/1.3 (0.003/0.16)	0.007/1.4 (0.004/0.25)			
B factor Protein (ligands)	38.9 (39.0)	48.0 (50.1)	38.2 (41.1)	46.9 (4837)	40.7 (32.0)	37.3 (28.6)	38.5 (31.1)	43.8 (29.8)			
PDB code[g]	3WTH	3WTI	3WTJ	3WTK	3WTL	3WTM	3WTN	3WTO			

[a] See text for abbreviations of the neonicotinoid names.

[b] All data sets were collected at SPring-8.

[c] Values in parentheses refer to data in the highest resolution shells.

[d] $R_{sym} = \Sigma|I - \langle I \rangle|/\Sigma I$, where *I* is the observed intensity and <*I*> is the average intensity from multiple observations of the symmetry related reflections.

[e] $R = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$. R_{free} is an *R* factor of the CNS refinement evaluated for 5% of reflections that were excluded from the refinement.

[f] R.m.s. deviations from ideal values were calculated using either CNS, CCP4, or PHENIX for the protein parts, and Mogul for the ligand parts.

[g] The atomic coordinates and structure factors have been deposited in the Protein Data Bank.

[h] Data sets for detection of anomalous peaks at sulfur, bromine and chlorine atoms.

Table 2. K_d, ΔH and ΔS as determined by isothermal titration calorimetry

Compounds	K_d (µM)		ΔH (kcal/mol)		ΔS (cal/mol/K)	
	Wild-type	Gln55Arg mutant	Wild type	Gln55Arg mutant	Wild-type	Gln55Arg mutant
Imidacloprid	0.530 ± 0.023[a]	0.514 ± 0.053	-10.33 ± 0.11	-10.50 ± 0.21	-5.93 ± 0.39	-6.38 ± 0.89
Clothianidin	1.79 ± 0.05	1.27 ± 0.15	-9.85 ± 0.09	-6.28 ± 0.41	-6.74 ± 0.33	+5.97 ± 1.61
Thiacloprid	0.297 ± 0.012	0.294 ± 0.015	-6.87 ± 0.09	-11.49 ± 0.06	+6.84 ± 0.37	-8.62 ± 0.24
CH-IMI	0.092 ± 0.004	0.100 ± 0.003	-12.93 ± 0.92	-13.28 ± 0.46	-7.45 ± 0.61	-15.00 ± 1.47
DN-IMI	0.091 ± 0.004	0.119 ± 0.003	-12.84 ± 0.22	-10.74 ± 0.30	-10.78 ± 0.69	-4.32 ± 1.05
(-)-Nicotine	0.114 ± 0.017	0.609 ± 0.012	-15.07 ± 0.07	-14.45 ± 0.19	-18.97 ± 0.26	-20.03 ± 0.64

[a] Data are represented as means ± standard error of means from three replicates.

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Table 3. pEC_{50} and I_{max} values of neonicotinoids and DN-IMI for the wild-type and mutant chicken α7 nicotinic acetylcholine receptors expressed in *Xenopus laevis* oocytes

Ligands	Wild-type		Ser58Lys mutant	
	pEC_{50}[a]	I_{max}[a]	pEC_{50}	I_{max}
Acetylcholine	3.82 ± 0.07	1.22 ± 0.05	1.82 ± 0.17	2.41 ± 0.39
Imidacloprid	3.67 ± 0.08	0.51 ± 0.03	ND[b]	23.1 ± 1.5[c]
Clothianidin	3.42 ± 0.18	0.16 ± 0.03	3.44 ± 1.37	1.72 ± 0.16
Thiacloprid	4.38 ± 0.17	0.49 ± 0.05	4.11 ± 0.10	3.15 ± 0.20
CH-IMI	4.42 ± 0.16	1.43 ± 0.12	4.67 ± 0.10	24.7 ± 1.2
DN-IMI	5.46 ± 0.09	1.00 ± 0.04	4.02 ± 0.03	2.45 ± 0.07
(-)-Nicotine	4.93 ± 0.03	0.88 ± 0.02	3.69 ± 0.05	0.15 ± 0.01
Ligands	Gln79Arg mutant		Ser58Lys;Gln79Arg mutant	
	pEC_{50}	I_{max}	pEC_{50}	I_{max}
Acetylcholine	2.63 ± 0.05	1.11 ± 0.03	2.14 ± 0.04	1.62 ± 0.06
Imidacloprid	4.02 ± 0.10	1.48 ± 0.11	4.16 ± 0.16	4.48 ± 0.45
Clothianidin	3.55 ± 0.05	1.04 ± 0.05	3.70 ± 0.09	2.84 ± 0.19
Thiacloprid	3.89 ± 0.06	0.30 ± 0.01	4.36 ± 0.17	5.53 ± 0.52
CH-IMI	4.89 ± 0.16	3.13 ± 0.21	5.02 ± 0.28	8.72 ± 0.95
DN-IMI	4.39 ± 0.05	0.67 ± 0.02	3.99 ± 0.02	0.69 ± 0.02
(-)-Nicotine	3.71 ± 0.07	0.35 ± 0.02	3.58 ± 0.14	0.10 ± 0.01

[a] All the data were newly measured. pEC_{50} is -log EC_{50} (Half maximal effective concentration (M)), whereas I_{max} is normalized maximal response. Data are represented as means ± standard error of 4–6 replicates.

[b] Could not be determined because the concentration-response curve did not reach a maximum.

[c] I_{max} was determined at 3 mM.

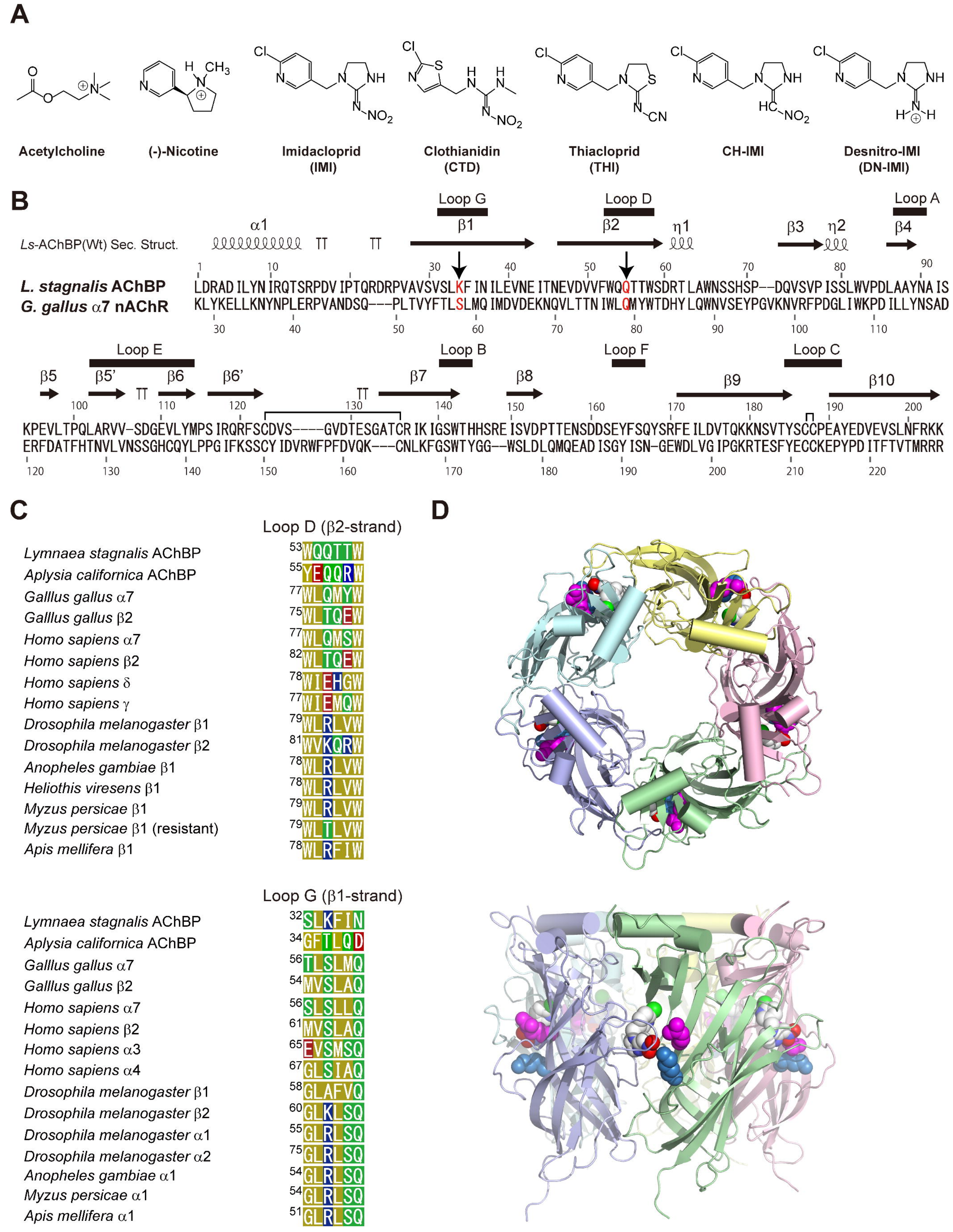

A
Cl
N
O
Acetylcholine
(-)-Nicotine
Imidacloprid
(IMI)
Clothianidin
(CTD)
Thiacloprid
(THI)
CH-IMI
Desnitro-IMI
(DN-IMI)
B
Loop G
Loop D
Loop A
α1
β1
β2
η1
β3
η2
β4
Ls-AChBP(Wt) Sec. Struct.
L. stagnalis AChBP
G. gallus α7 nAChR
LDRADILYNIRQTSRPDVIPTQRDRPVAVSVSLKFINILEVNEITNEVDVVFWQQTTWSDRTLAWNSSHSP--DQVSVPISSLWVPDLAAYNAIS
KLYKELLKNYNPLERPVANDSQ---PLTVYFTLSLMQIMDVDEKNQVLTTNIWLQMYWTDHYLQWNVSEYPGVKNVRFPDGLIWKPDILLYNSAD
Loop E
Loop B
Loop F
Loop C
β5
β5'
β6
β6'
β7
β8
β9
β10
KPEVLTPQLARVV-SDGEVLYMPSIRQRFSCDVS----GVDTESGATCRIKIGSWTHHSREISVDPTTENSDDSEYFSQYSRFEILDVTQKKNSVTYSCCPEAYEDVEVSLNFRKK
ERFDATFHTNVLVNSSGHCQYLPPGIFKSSCYIDVRWFPFDVQK---CNLKFGSWTYGG--WSLDLQMQEADISGYISN-GEWDLVGIPGKRTESFYECCKEPYPDITFTVTMRRR
C
Loop D (β2-strand)
Lymnaea stagnalis AChBP 53 WQQTTW
Aplysia californica AChBP 55 YEQQRW
Gallus gallus α7 77 WLQMYW
Gallus gallus β2 75 WLTQEW
Homo sapiens α7 77 WLQMSW
Homo sapiens β2 82 WLTQEW
Homo sapiens δ 78 WIEHGW
Homo sapiens γ 77 WIEMQW
Drosophila melanogaster β1 79 WLRLVW
Drosophila melanogaster β2 81 WVKQRW
Anopheles gambiae β1 78 WLRLVW
Heliothis viresens β1 78 WLRLVW
Myzus persicae β1 79 WLRLVW
Myzus persicae β1 (resistant) 79 WLTLVW
Apis mellifera β1 78 WLRFIW
Loop G (β1-strand)
Lymnaea stagnalis AChBP 32 SLKFIN
Aplysia californica AChBP 34 GFTLQD
Gallus gallus α7 56 TLSLMQ
Gallus gallus β2 54 MVSLAQ
Homo sapiens α7 56 SLSLLQ
Homo sapiens β2 61 MVSLAQ
Homo sapiens α3 65 EVSMSQ
Homo sapiens α4 67 GLSIAQ
Drosophila melanogaster β1 58 GLAFVQ
Drosophila melanogaster β2 60 GLKLSQ
Drosophila melanogaster α1 55 GLRLSQ
Drosophila melanogaster α2 75 GLRLSQ
Anopheles gambiae α1 54 GLRLSQ
Myzus persicae α1 54 GLRLSQ
Apis mellifera α1 51 GLRLSQ
D

Figure 1

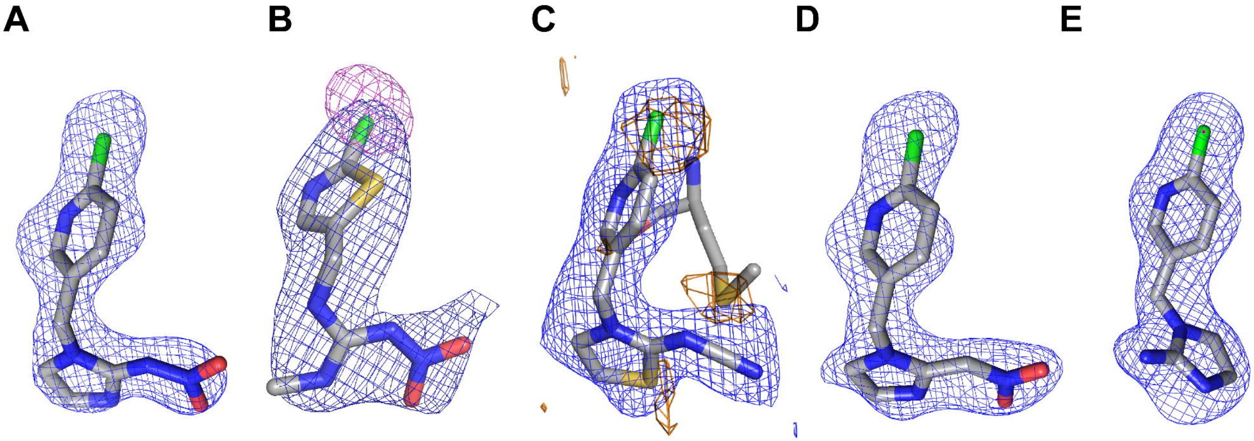


Figure 2

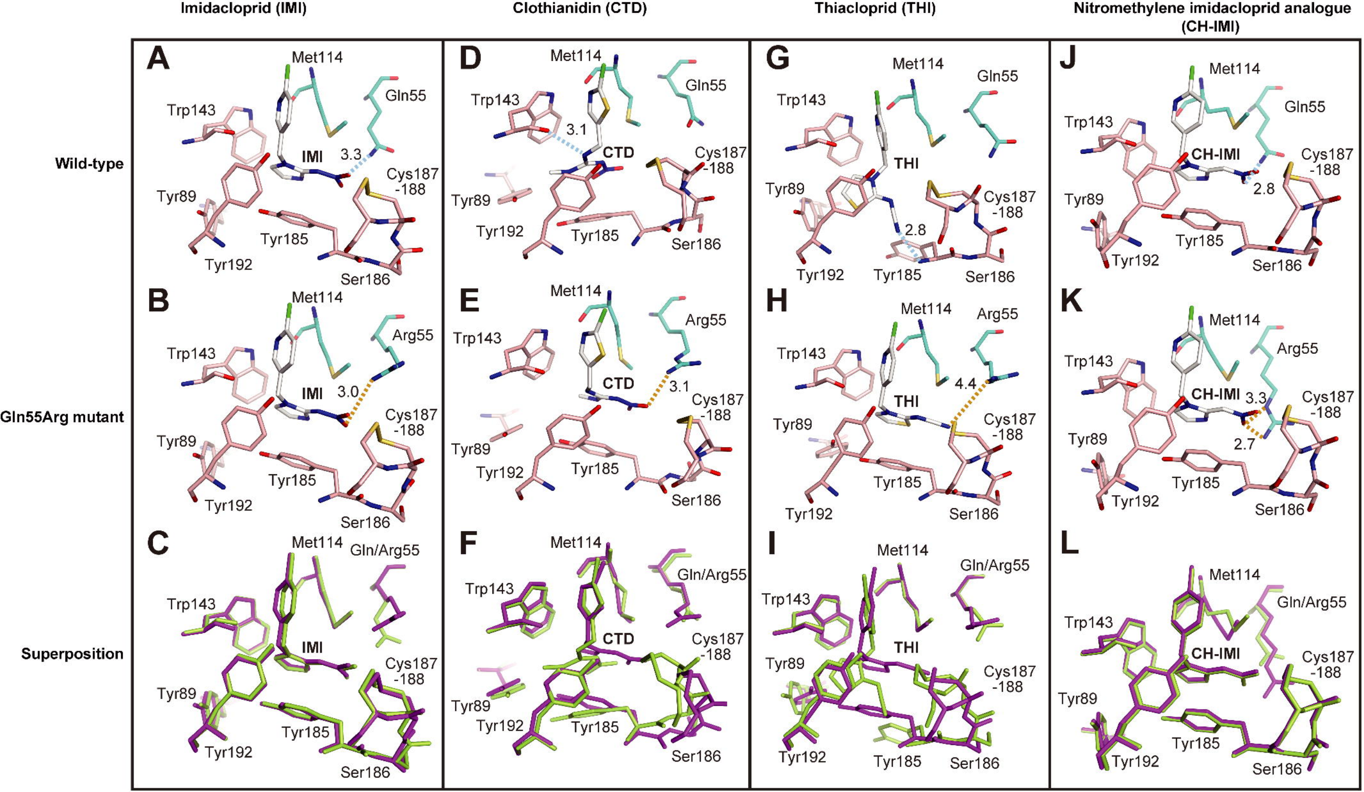

Imidacloprid (IMI)
Clothianidin (CTD)
Thiacloprid (THI)
Nitromethylene imidacloprid analogue (CH-IMI)
Wild-type
Gln55Arg mutant
Superposition
A
Met114
Gln55
Trp143
IMI
3.3
Cys187 -188
Tyr89
Tyr185
Tyr192
Ser186
B
Met114
Arg55
Trp143
IMI
3.0
Cys187 -188
Tyr89
Tyr185
Tyr192
Ser186
C
Met114
Gln/Arg55
Trp143
IMI
Cys187 -188
Tyr89
Tyr185
Tyr192
Ser186
D
Met114
Gln55
Trp143
3.1
CTD
Cys187 -188
Tyr89
Tyr192
Tyr185
Ser186
E
Met114
Arg55
Trp143
CTD
3.1
Cys187 -188
Tyr89
Tyr192
Tyr185
Ser186
F
Met114
Gln/Arg55
Trp143
CTD
Cys187 -188
Tyr89
Tyr192
Tyr185
Ser186
G
Met114
Gln55
Trp143
THI
Tyr89
Cys187 -188
2.8
Tyr192
Tyr185
Ser186
H
Met114
Arg55
Trp143
4.4
THI
Tyr89
Cys187 -188
Tyr185
Tyr192
Ser186
I
Met114
Gln/Arg55
Trp143
THI
Tyr89
Cys187 -188
Tyr192
Tyr185
Ser186
J
Met114
Gln55
Trp143
CH-IMI
Cys187 -188
2.8
Tyr89
Tyr185
Tyr192
Ser186
K
Met114
Arg55
Trp143
CH-IMI
3.3
Cys187 -188
Tyr89
2.7
Tyr185
Tyr192
Ser186
L
Met114
Gln/Arg55
Trp143
CH-IMI
Cys187 -188
Tyr89
Tyr185
Tyr192
Ser186

Figure 3

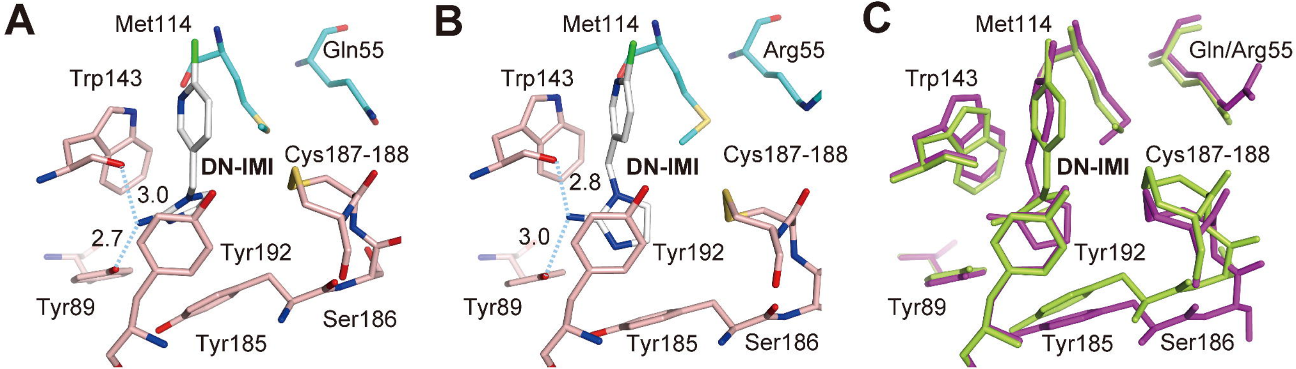

A
Met114
Gln55
Trp143
DN-IMI
Cys187-188
3.0
2.7
Tyr192
Tyr89
Ser186
Tyr185
B
Met114
Arg55
Trp143
DN-IMI
Cys187-188
2.8
3.0
Tyr192
Tyr89
Tyr185
Ser186
C
Met114
Gln/Arg55
Trp143
DN-IMI
Cys187-188
Tyr192
Tyr89
Tyr185
Ser186

Figure 4

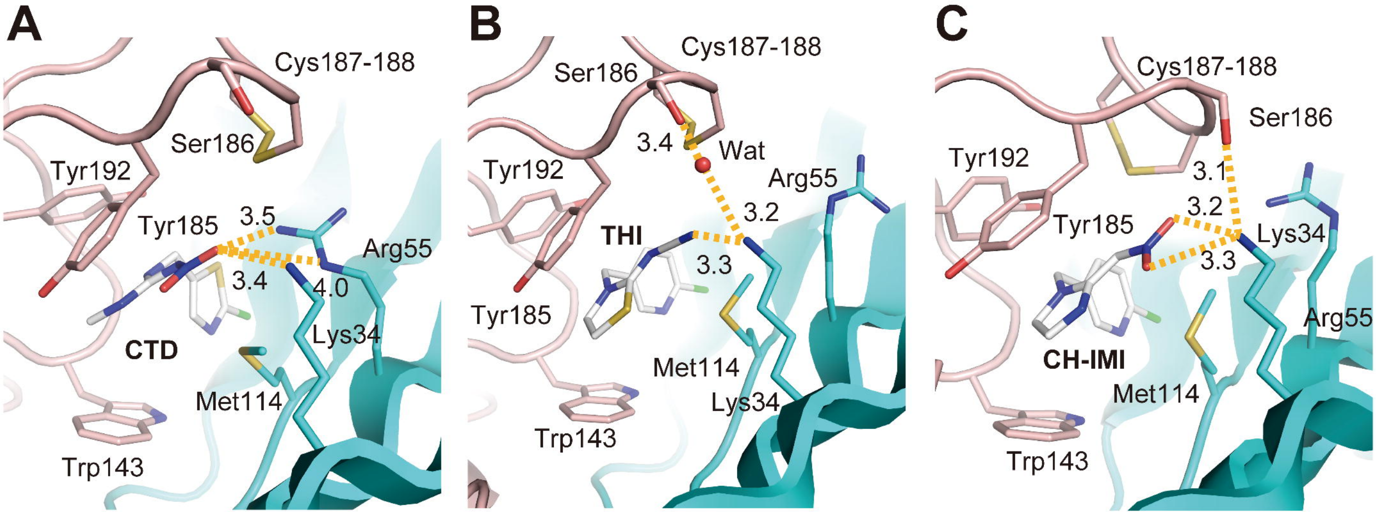

A
Cys187-188
Ser186
Tyr192
Tyr185
3.5
3.4
4.0
Arg55
Lys34
CTD
Met114
Trp143
B
Cys187-188
Ser186
3.4
Wat
Tyr192
Arg55
3.2
THI
3.3
Tyr185
Met114
Lys34
Trp143
C
Cys187-188
Ser186
Tyr192
3.1
3.2
Tyr185
Lys34
3.3
Arg55
CH-IMI
Met114
Trp143

Figure 5

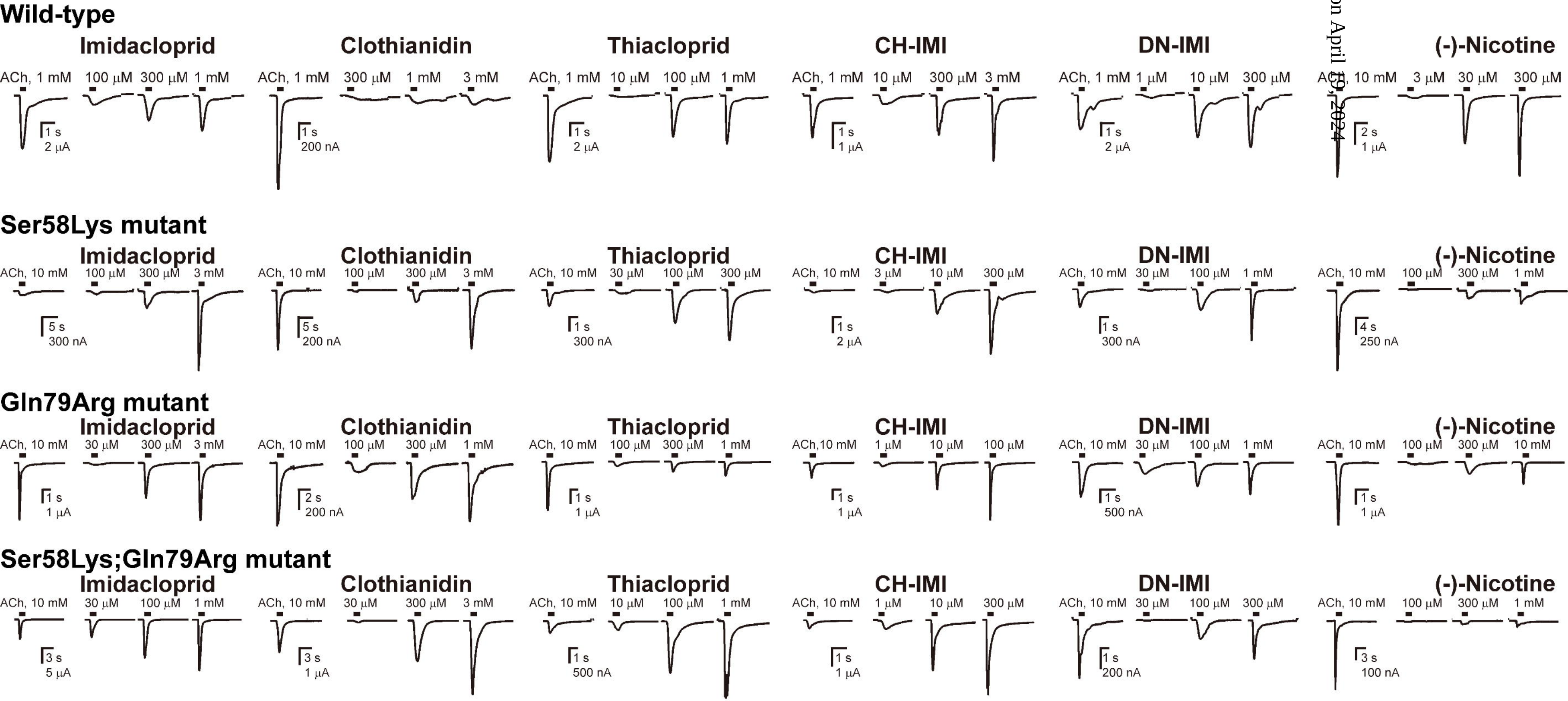

Wild-type
Imidacloprid
ACh, 1 mM
100 µM
300 µM
1 mM
1 s
2 µA
Clothianidin
ACh, 1 mM
300 µM
1 mM
3 mM
1 s
200 nA
Thiacloprid
ACh, 1 mM
10 µM
100 µM
1 mM
1 s
2 µA
CH-IMI
ACh, 1 mM
10 µM
300 µM
3 mM
1 s
1 µA
DN-IMI
ACh, 1 mM
1 µM
10 µM
300 µM
1 s
2 µA
(-)-Nicotine
ACh, 10 mM
3 µM
30 µM
300 µM
2 s
1 µA
Ser58Lys mutant
Imidacloprid
ACh, 10 mM
100 µM
300 µM
3 mM
5 s
300 nA
Clothianidin
ACh, 10 mM
100 µM
300 µM
3 mM
5 s
200 nA
Thiacloprid
ACh, 10 mM
30 µM
100 µM
300 µM
1 s
300 nA
CH-IMI
ACh, 10 mM
3 µM
10 µM
300 µM
1 s
2 µA
DN-IMI
ACh, 10 mM
30 µM
100 µM
1 mM
1 s
300 nA
(-)-Nicotine
ACh, 10 mM
100 µM
300 µM
1 mM
4 s
250 nA
Gln79Arg mutant
Imidacloprid
ACh, 10 mM
30 µM
300 µM
3 mM
1 s
1 µA
Clothianidin
ACh, 10 mM
100 µM
300 µM
1 mM
2 s
200 nA
Thiacloprid
ACh, 10 mM
100 µM
300 µM
1 mM
1 s
1 µA
CH-IMI
ACh,10 mM
1 µM
10 µM
100 µM
1 s
1 µA
DN-IMI
ACh, 10 mM
30 µM
100 µM
1 mM
1 s
500 nA
(-)-Nicotine
ACh, 10 mM
100 µM
300 µM
10 mM
1 s
1 µA
Ser58Lys;Gln79Arg mutant
Imidacloprid
ACh, 10 mM
30 µM
100 µM
1 mM
3 s
5 µA
Clothianidin
ACh, 10 mM
30 µM
300 µM
3 mM
3 s
1 µA
Thiacloprid
ACh, 10 mM
10 µM
100 µM
1 mM
1 s
500 nA
CH-IMI
ACh, 10 mM
1 µM
10 µM
300 µM
1 s
1 µA
DN-IMI
ACh, 10 mM
30 µM
100 µM
300 µM
1 s
200 nA
(-)-Nicotine
ACh, 10 mM
100 µM
300 µM
1 mM
3 s
100 nA

Figure 6

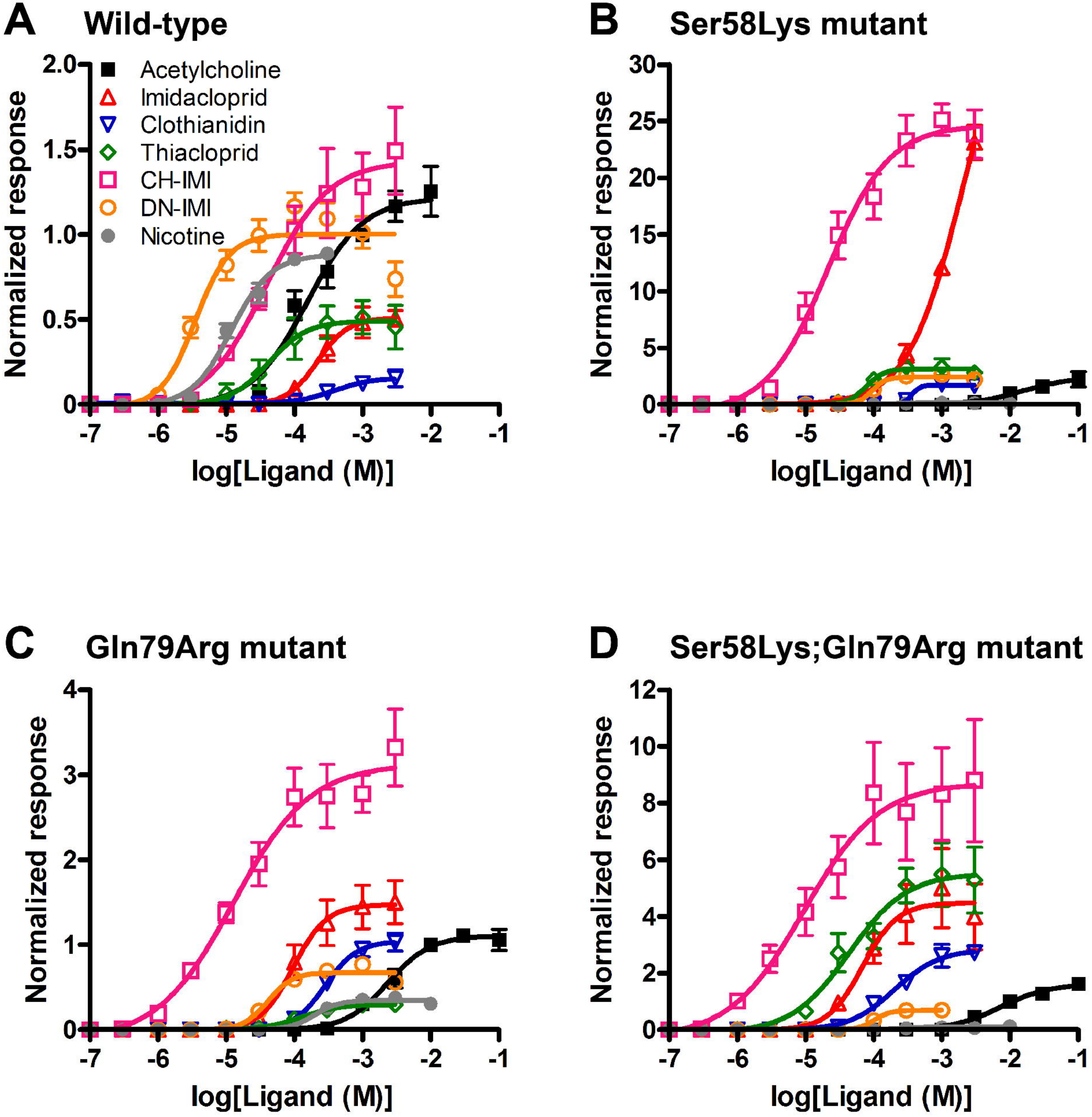

A
Wild-type
Normalized response
0
0.5
1.0
1.5
2.0
Acetylcholine
Imidacloprid
Clothianidin
Thiacloprid
CH-IMI
DN-IMI
Nicotine
-7
-6
-5
-4
-3
-2
-1
log[Ligand (M)]
B
Ser58Lys mutant
Normalized response
0
5
10
15
20
25
30
-7
-6
-5
-4
-3
-2
-1
log[Ligand (M)]
C
Gln79Arg mutant
Normalized response
0
1
2
3
4
-7
-6
-5
-4
-3
-2
-1
log[Ligand (M)]
D
Ser58Lys;Gln79Arg mutant
Normalized response
0
2
4
6
8
10
12
-7
-6
-5
-4
-3
-2
-1
log[Ligand (M)]

Figure 7

Supplemental Data

Molecular Pharmacology

Studies on an acetylcholine binding protein identify a basic residue in loop G on the β1-strand as a new structural determinant of neonicotinoid actions

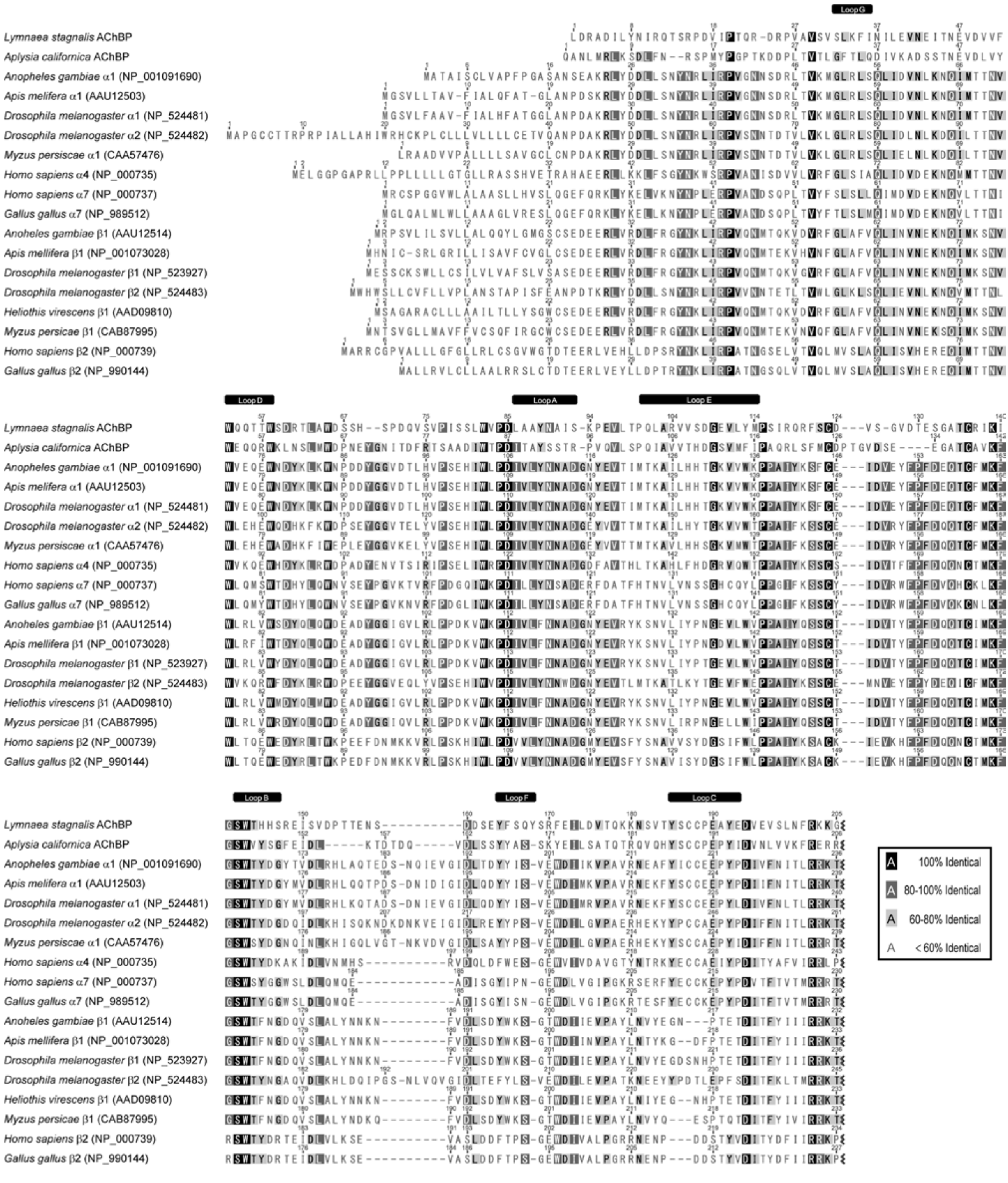
Makoto Ihara, Toshihide Okajima, Atsuko Yamashita, Takuma Oda, Takuya Asano, Mikana Matsui, David B. Sattelle and Kazuhiko Matsuda

Department of Applied Biological Chemistry, Faculty of Agriculture, Kinki University, 3327-204 Naka-machi, Nara 631-8505, Japan (M.I., T.O., T.A., M.M., K.M.)

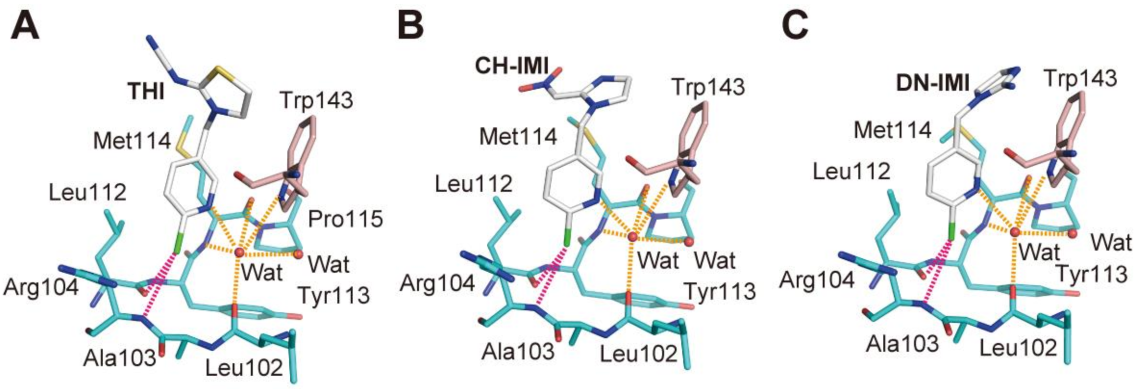
Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan (T.O.)

Graduate School of Medicine, Dentistry and Pharmaceutical Sciences, Okayama University, 1-1-1 Tsushima-naka, Kita-ku, Okayama 700-8530, Japan (A.Y.)

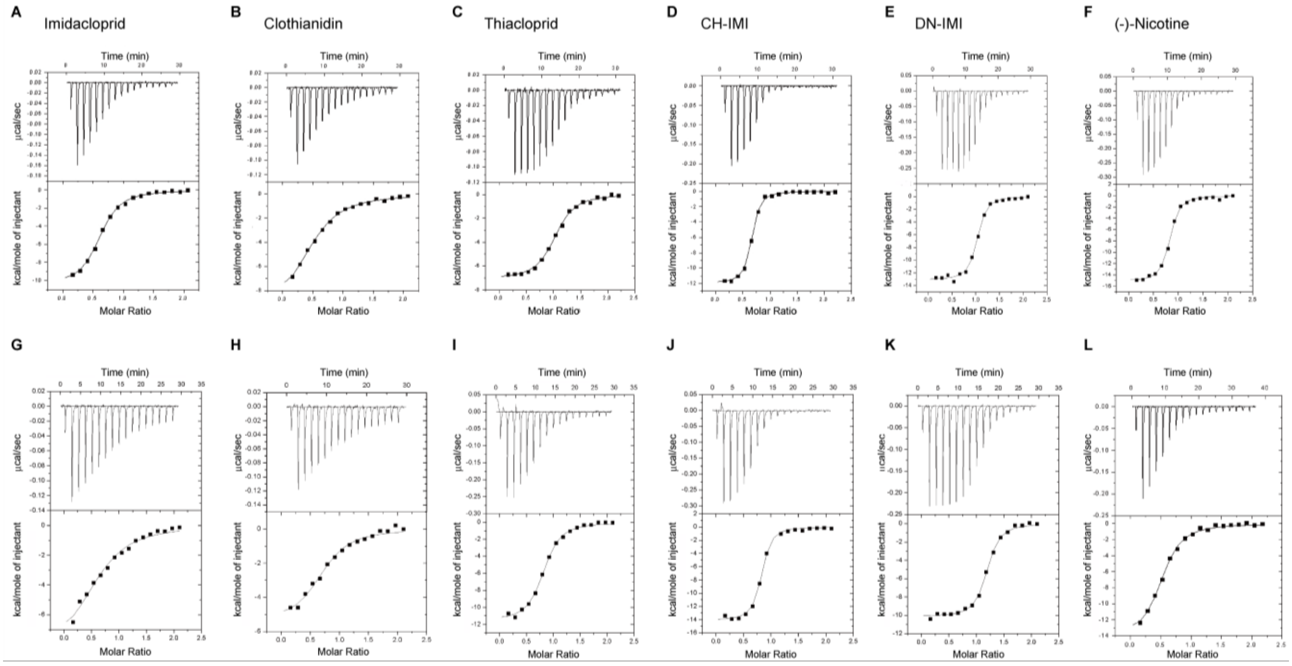
The Wolfson Institute for Biomedical Research, Department of Medicine, Cruciform Building, University College London, Gower Street, London, WC1E 6BT, United Kingdom (D.B.S.)



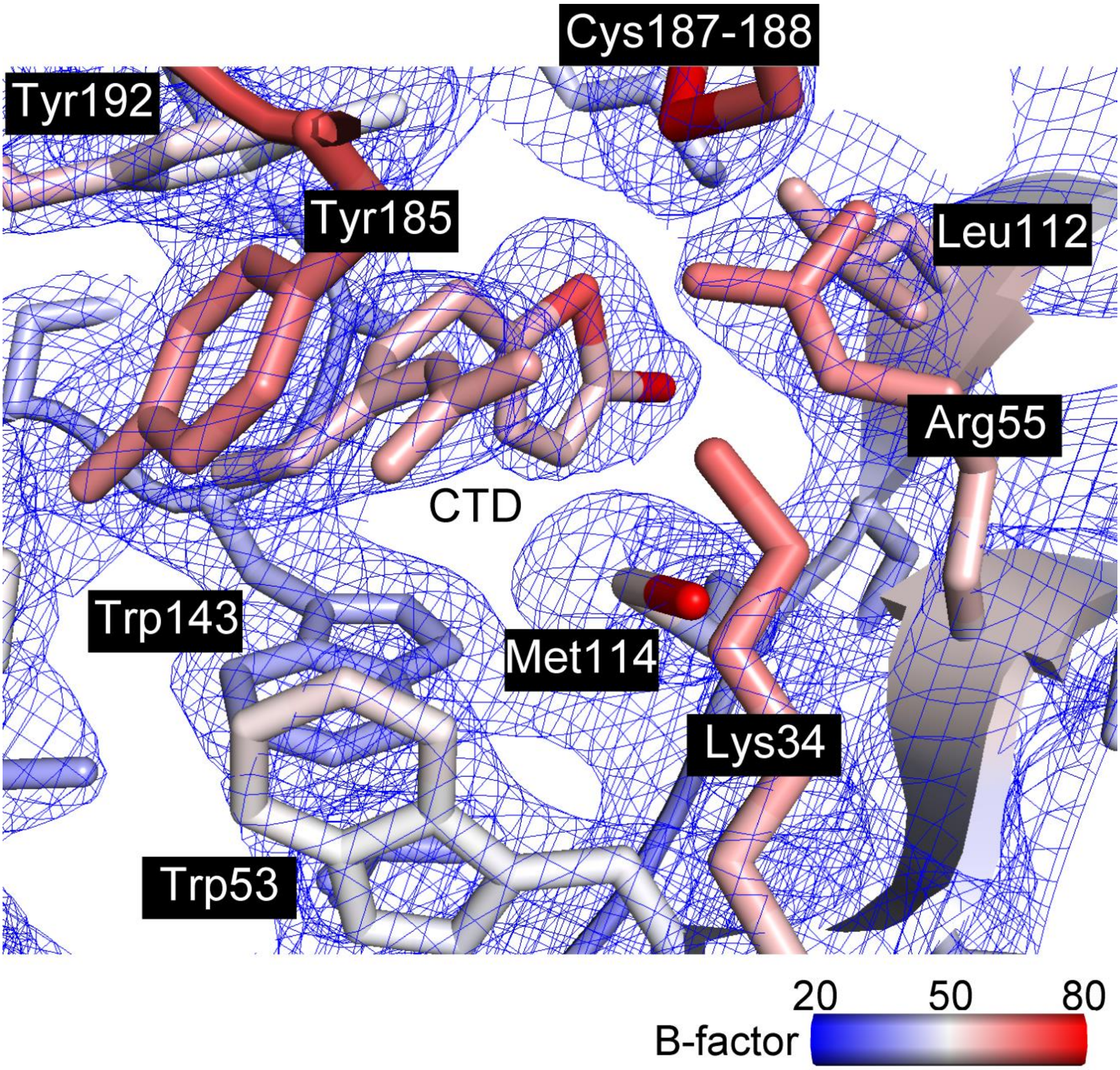
Supplementary Figure 1. Multiple sequence alignment of ligand binding domain (LBD) of nicotinic acetylcholine receptor subunits. Accession numbers are given in parenthesis. Amino acids of the *Ls*-AChBP were numbered from the N-terminal of the mature protein, whereas those for the other nAChRs were from the initial methionine.



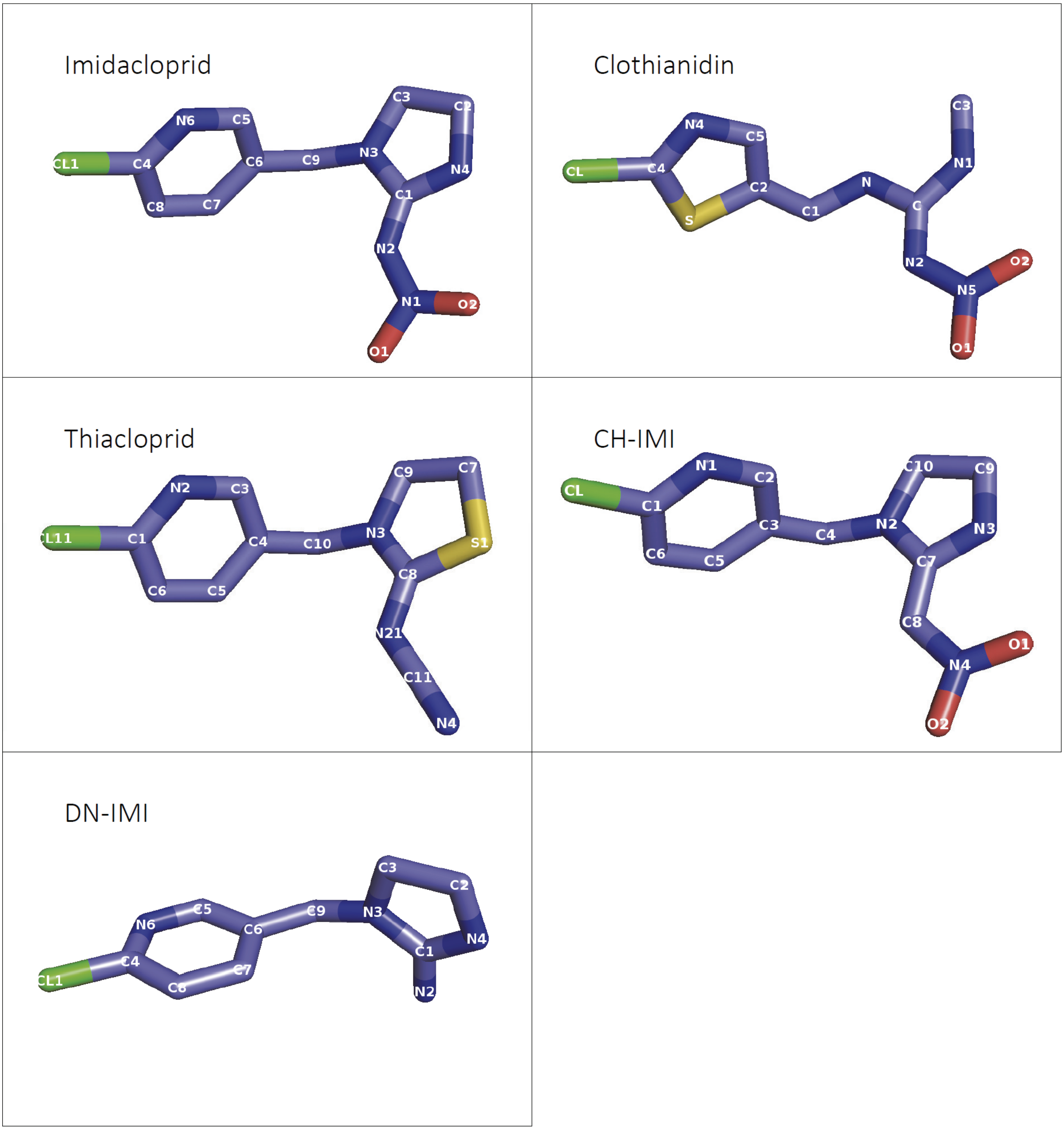
Supplementary Figure 2. The interactions of thiacloprid (**A**), CH-IMI (**B**) and DN-IMI (**C**) with loop E via a water molecule in the wild-type *Ls*-AChBP. Hydrogen bonds are indicated by a dotted orange line, while halogen bonds are indicated by a dotted magenta line. Trp143 belongs to the principal side, while the other residues to the complementary side. In each ligand, carbon, chlorine, nitrogen, oxygen and sulfur atoms are colored bright grey, green, blue, red and yellow, respectively. Water (Wat) is indicated by a red ball.



Supplementary Figure 3. Binding of neonicotinoids and their derivatives to *Ls*-AChBP as evaluated by isothermal titration calorimetry (ITC). The peak amplitude of the heat generation by each injection was plotted against molar ratio (ligand/protein). (A–F) ITC data for the wild type *Ls*-AChBP; (G–L) ITC data for the Q55R mutant *Ls*-AChBP. (A, G) Imidacloprid, (B, H) clothianidin, (C, I) thiacloprid, (D, J) CH-IMI, (E, K) DN-IMI, (F, L) (-)-nicotine.



Supplementary Figure 4. Expanded view of the ligand binding domain in the Gln55Arg mutant of *Ls*-AChBP in complex with clothianidin at the BC interface. The model was colored according to the B-factor of each atom. The B-factor was refined over the “weighted nearest-neighbor restraints” using PHENIX. A $2F_o$-F_c electron density map contoured at $\sigma = 1.0$ was overlaid.


Imidacloprid

Clothianidin

Thiacloprid

CH-IMI

DN-IMI

Figures for Tables 1–10.

Table 1. Geometry Analysis by Mogul of Imidacloprid in Complex with Wild-Type *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	|z-score|	|x - mean|	Minimum	Maximum	Median	|d(min)|	Local density
bond	00000001_1	N2 N1	Not unusual (enough hits	218	1.376	1.342	0.035	0.977	0.034	1.286	1.462	1.336	0.004	
bond	00000001_1	C3 N3	Not unusual (enough hits	1978	1.472	1.468	0.023	0.182	0.004	1.336	1.699	1.468	0	
bond	00000001_1	C9 N3	Not unusual (enough hits	931	1.477	1.465	0.015	0.799	0.012	1.386	1.561	1.465	0	
bond	00000001_1	C2 N4	Not unusual (enough hits	1745	1.463	1.457	0.022	0.261	0.006	1.204	1.687	1.458	0	
bond	00000001_1	C3 C2	Not unusual (enough hits	252	1.543	1.521	0.02	1.124	0.022	1.452	1.629	1.52	0.001	
bond	00000001_1	C4 CL1	Not unusual (enough hits	743	1.739	1.738	0.019	0.053	0.001	1.561	1.806	1.74	0	
bond	00000001_1	C4 N6	Not unusual (enough hits	245	1.34	1.321	0.025	0.736	0.018	1.254	1.422	1.317	0.001	
bond	00000001_1	C5 N6	Not unusual (enough hits	2818	1.345	1.34	0.022	0.235	0.005	1.05	1.584	1.337	0	
bond	00000001_1	C7 C6	Not unusual (enough hits	14050	1.422	1.384	0.022	1.75	0.038	0.618	1.8	1.386	0	
bond	00000001_1	C9 C6	Not unusual (enough hits	10549	1.539	1.51	0.019	1.54	0.029	1.278	1.842	1.51	0	
bond	00000001_1	C8 C7	Not unusual (enough hits	20000	1.419	1.383	0.019	1.911	0.035	0.882	1.685	1.383	0	
bond	00000001_1	O1 N1	Unusual (enough hits)	476	1.286	1.241	0.019	2.371	0.045	1.169	1.356	1.241	0.001	
bond	00000001_1	O2 N1	Unusual (enough hits)	476	1.302	1.241	0.019	3.21	0.061	1.169	1.356	1.241	0.005	
bond	00000001_1	C1 N2	Unusual (enough hits)	38	1.285	1.345	0.012	5.109	0.06	1.322	1.369	1.343	0.037	
bond	00000001_1	C1 N3	Unusual (enough hits)	23	1.432	1.351	0.021	3.802	0.081	1.327	1.394	1.344	0.038	
bond	00000001_1	C1 N4	Unusual (enough hits)	56	1.413	1.335	0.02	3.852	0.078	1.304	1.41	1.331	0.003	
bond	00000001_1	C8 C4	Unusual (enough hits)	479	1.421	1.373	0.022	2.224	0.049	1.267	1.455	1.373	0.002	
bond	00000001_1	C5 C6	Unusual (enough hits)	560	1.437	1.381	0.017	3.311	0.056	1.279	1.497	1.382	0.002	
bond	00000001_2	N2 N1	Not unusual (enough hits	218	1.373	1.342	0.035	0.88	0.031	1.286	1.462	1.336	0.001	
bond	00000001_2	C3 N3	Not unusual (enough hits	1978	1.466	1.468	0.023	0.101	0.002	1.336	1.699	1.468	0	
bond	00000001_2	C9 N3	Not unusual (enough hits	931	1.476	1.465	0.015	0.719	0.011	1.386	1.561	1.465	0	
bond	00000001_2	C2 N4	Not unusual (enough hits	1745	1.457	1.457	0.022	0.009	0	1.204	1.687	1.458	0	
bond	00000001_2	C3 C2	Not unusual (enough hits	252	1.535	1.521	0.02	0.732	0.014	1.452	1.629	1.52	0	
bond	00000001_2	C4 CL1	Not unusual (enough hits	743	1.735	1.738	0.019	0.181	0.003	1.561	1.806	1.74	0	
bond	00000001_2	C4 N6	Not unusual (enough hits	245	1.35	1.321	0.025	1.122	0.028	1.254	1.422	1.317	0.002	
bond	00000001_2	C5 N6	Not unusual (enough hits	2818	1.35	1.34	0.022	0.45	0.01	1.05	1.584	1.337	0	
bond	00000001_2	C7 C6	Not unusual (enough hits	14050	1.427	1.384	0.022	1.964	0.043	0.618	1.8	1.386	0	
bond	00000001_2	C8 C7	Not unusual (enough hits	20000	1.417	1.383	0.019	1.808	0.034	0.882	1.685	1.383	0	
bond	00000001_2	O1 N1	Unusual (enough hits)	476	1.295	1.241	0.019	2.851	0.055	1.169	1.356	1.241	0.001	
bond	00000001_2	O2 N1	Unusual (enough hits)	476	1.295	1.241	0.019	2.819	0.054	1.169	1.356	1.241	0	
bond	00000001_2	C1 N2	Unusual (enough hits)	38	1.28	1.345	0.012	5.564	0.065	1.322	1.369	1.343	0.042	
bond	00000001_2	C1 N3	Unusual (enough hits)	23	1.404	1.351	0.021	2.523	0.054	1.327	1.394	1.344	0.011	
bond	00000001_2	C1 N4	Unusual (enough hits)	56	1.405	1.335	0.02	3.452	0.07	1.304	1.41	1.331	0.005	
bond	00000001_2	C8 C4	Unusual (enough hits)	479	1.417	1.373	0.022	2.039	0.045	1.267	1.455	1.373	0.002	
bond	00000001_2	C5 C6	Unusual (enough hits)	560	1.432	1.381	0.017	3.011	0.051	1.279	1.497	1.382	0.003	
bond	00000001_2	C9 C6	Unusual (enough hits)	10549	1.549	1.51	0.019	2.108	0.039	1.278	1.842	1.51	0	
bond	00000001_3	N2 N1	Not unusual (enough hits	218	1.364	1.342	0.035	0.638	0.022	1.286	1.462	1.336	0.001	
bond	00000001_3	C3 N3	Not unusual (enough hits	1978	1.461	1.468	0.023	0.298	0.007	1.336	1.699	1.468	0	
bond	00000001_3	C9 N3	Not unusual (enough hits	931	1.476	1.465	0.015	0.725	0.011	1.386	1.561	1.465	0	
bond	00000001_3	C2 N4	Not unusual (enough hits	1745	1.447	1.457	0.022	0.471	0.01	1.204	1.687	1.458	0	
bond	00000001_3	C3 C2	Not unusual (enough hits	252	1.538	1.521	0.02	0.886	0.017	1.452	1.629	1.52	0	
bond	00000001_3	C4 CL1	Not unusual (enough hits	743	1.705	1.738	0.019	1.761	0.033	1.561	1.806	1.74	0.001	
bond	00000001_3	C4 N6	Not unusual (enough hits	245	1.337	1.321	0.025	0.61	0.015	1.254	1.422	1.317	0	

bond	00000001_3	C5 N6	Not unusual (enough hits	2818	1.339	1.34	0.022	0.072	0.002	1.05	1.584	1.337	0	
bond	00000001_3	C7 C6	Not unusual (enough hits	14050	1.415	1.384	0.022	1.4	0.031	0.618	1.8	1.386	0	
bond	00000001_3	C9 C6	Not unusual (enough hits	10549	1.533	1.51	0.019	1.219	0.023	1.278	1.842	1.51	0	
bond	00000001_3	C8 C7	Not unusual (enough hits	20000	1.416	1.383	0.019	1.763	0.033	0.882	1.685	1.383	0	
bond	00000001_3	O1 N1	Unusual (enough hits)	476	1.286	1.241	0.019	2.359	0.045	1.169	1.356	1.241	0.001	
bond	00000001_3	O2 N1	Unusual (enough hits)	476	1.309	1.241	0.019	3.57	0.068	1.169	1.356	1.241	0.012	
bond	00000001_3	C1 N2	Unusual (enough hits)	38	1.276	1.345	0.012	5.949	0.07	1.322	1.369	1.343	0.046	
bond	00000001_3	C1 N3	Unusual (enough hits)	23	1.416	1.351	0.021	3.059	0.065	1.327	1.394	1.344	0.022	
bond	00000001_3	C1 N4	Unusual (enough hits)	56	1.406	1.335	0.02	3.523	0.071	1.304	1.41	1.331	0.004	
bond	00000001_3	C8 C4	Unusual (enough hits)	479	1.42	1.373	0.022	2.186	0.048	1.267	1.455	1.373	0.001	
bond	00000001_3	C5 C6	Unusual (enough hits)	560	1.429	1.381	0.017	2.824	0.048	1.279	1.497	1.382	0.006	
bond	00000001_4	N2 N1	Not unusual (enough hits	218	1.368	1.342	0.035	0.742	0.026	1.286	1.462	1.336	0	
bond	00000001_4	C3 N3	Not unusual (enough hits	1978	1.464	1.468	0.023	0.196	0.004	1.336	1.699	1.468	0	
bond	00000001_4	C9 N3	Not unusual (enough hits	931	1.469	1.465	0.015	0.287	0.004	1.386	1.561	1.465	0	
bond	00000001_4	C2 N4	Not unusual (enough hits	1745	1.463	1.457	0.022	0.256	0.006	1.204	1.687	1.458	0	
bond	00000001_4	C3 C2	Not unusual (enough hits	252	1.542	1.521	0.02	1.071	0.021	1.452	1.629	1.52	0	
bond	00000001_4	C4 CL1	Not unusual (enough hits	743	1.735	1.738	0.019	0.186	0.003	1.561	1.806	1.74	0	
bond	00000001_4	C4 N6	Not unusual (enough hits	245	1.338	1.321	0.025	0.652	0.016	1.254	1.422	1.317	0	
bond	00000001_4	C8 C4	Not unusual (enough hits	479	1.413	1.373	0.022	1.84	0.04	1.267	1.455	1.373	0	
bond	00000001_4	C5 N6	Not unusual (enough hits	2818	1.35	1.34	0.022	0.427	0.01	1.05	1.584	1.337	0	
bond	00000001_4	C7 C6	Not unusual (enough hits	14050	1.416	1.384	0.022	1.438	0.032	0.618	1.8	1.386	0	
bond	00000001_4	C9 C6	Not unusual (enough hits	10549	1.538	1.51	0.019	1.489	0.028	1.278	1.842	1.51	0	
bond	00000001_4	C8 C7	Not unusual (enough hits	20000	1.415	1.383	0.019	1.718	0.032	0.882	1.685	1.383	0	
bond	00000001_4	O1 N1	Unusual (enough hits)	476	1.287	1.241	0.019	2.429	0.046	1.169	1.356	1.241	0	
bond	00000001_4	O2 N1	Unusual (enough hits)	476	1.295	1.241	0.019	2.849	0.055	1.169	1.356	1.241	0.001	
bond	00000001_4	C1 N2	Unusual (enough hits)	38	1.286	1.345	0.012	5.096	0.06	1.322	1.369	1.343	0.037	
bond	00000001_4	C1 N3	Unusual (enough hits)	23	1.416	1.351	0.021	3.088	0.066	1.327	1.394	1.344	0.023	
bond	00000001_4	C1 N4	Unusual (enough hits)	56	1.412	1.335	0.02	3.84	0.078	1.304	1.41	1.331	0.003	
bond	00000001_4	C5 C6	Unusual (enough hits)	560	1.43	1.381	0.017	2.912	0.049	1.279	1.497	1.382	0.004	
bond	00000001_5	N2 N1	Not unusual (enough hits	218	1.354	1.342	0.035	0.341	0.012	1.286	1.462	1.336	0	
bond	00000001_5	C3 N3	Not unusual (enough hits	1978	1.466	1.468	0.023	0.084	0.002	1.336	1.699	1.468	0	
bond	00000001_5	C9 N3	Not unusual (enough hits	931	1.463	1.465	0.015	0.131	0.002	1.386	1.561	1.465	0	
bond	00000001_5	C2 N4	Not unusual (enough hits	1745	1.462	1.457	0.022	0.193	0.004	1.204	1.687	1.458	0	
bond	00000001_5	C3 C2	Not unusual (enough hits	252	1.539	1.521	0.02	0.929	0.018	1.452	1.629	1.52	0	
bond	00000001_5	C4 CL1	Not unusual (enough hits	743	1.726	1.738	0.019	0.664	0.012	1.561	1.806	1.74	0	
bond	00000001_5	C4 N6	Not unusual (enough hits	245	1.338	1.321	0.025	0.655	0.016	1.254	1.422	1.317	0	
bond	00000001_5	C5 N6	Not unusual (enough hits	2818	1.336	1.34	0.022	0.204	0.005	1.05	1.584	1.337	0	
bond	00000001_5	C7 C6	Not unusual (enough hits	14050	1.421	1.384	0.022	1.708	0.037	0.618	1.8	1.386	0	
bond	00000001_5	C9 C6	Not unusual (enough hits	10549	1.527	1.51	0.019	0.895	0.017	1.278	1.842	1.51	0	
bond	00000001_5	C8 C7	Not unusual (enough hits	20000	1.409	1.383	0.019	1.364	0.025	0.882	1.685	1.383	0	
bond	00000001_5	O1 N1	Unusual (enough hits)	476	1.283	1.241	0.019	2.204	0.042	1.169	1.356	1.241	0.002	
bond	00000001_5	O2 N1	Unusual (enough hits)	476	1.299	1.241	0.019	3.058	0.059	1.169	1.356	1.241	0.002	
bond	00000001_5	C1 N2	Unusual (enough hits)	38	1.274	1.345	0.012	6.086	0.071	1.322	1.369	1.343	0.048	
bond	00000001_5	C1 N3	Unusual (enough hits)	23	1.409	1.351	0.021	2.728	0.058	1.327	1.394	1.344	0.015	
bond	00000001_5	C1 N4	Unusual (enough hits)	56	1.411	1.335	0.02	3.751	0.076	1.304	1.41	1.331	0.001	

bond	00000001_5	C8 C4	Unusual (enough hits)	479	1.421	1.373	0.022	2.217	0.049	1.267	1.455	1.373	0.002	
bond	00000001_5	C5 C6	Unusual (enough hits)	560	1.428	1.381	0.017	2.819	0.048	1.279	1.497	1.382	0.006	
angle	00000001_1	O2 N1 O1	Not unusual (enough hits	234	118.184	121.526	2.164	1.544	3.342	116.275	131.091	121.113	0.039	
angle	00000001_1	O1 N1 N2	Not unusual (enough hits	430	118.366	119.288	4.121	0.224	0.922	112.759	126.082	117.049	0.114	
angle	00000001_1	O2 N1 N2	Not unusual (enough hits	430	123.441	119.288	4.121	1.008	4.153	112.759	126.082	117.049	0.007	
angle	00000001_1	C3 N3 C1	Not unusual (enough hits	23	108.21	109.675	2.799	0.524	1.466	104.343	112.076	111.094	0.866	
angle	00000001_1	C9 N3 C3	Not unusual (enough hits	109	123.095	120.505	2.722	0.952	2.59	110.736	125.952	121.036	0.007	
angle	00000001_1	N3 C1 N2	Not unusual (enough hits	16	124.006	118.565	3.722	1.462	5.44	116.421	131.83	117.249	4.135	
angle	00000001_1	N4 C1 N3	Not unusual (enough hits	19	110.62	109.894	0.771	0.941	0.726	107.953	111.238	110.048	0.056	
angle	00000001_1	C2 N4 C1	Not unusual (enough hits	53	109.692	110.972	2.593	0.494	1.28	105.927	114.592	111.774	0.08	
angle	00000001_1	C2 C3 N3	Not unusual (enough hits	85	106.129	102.951	1.651	1.925	3.178	99.561	108.169	102.882	0.31	
angle	00000001_1	CL1 C4 N6	Not unusual (enough hits	239	119.193	116.229	2.378	1.247	2.964	106.087	140.591	115.898	0.317	
angle	00000001_1	C8 C4 CL1	Not unusual (enough hits	437	119.527	119.088	2.36	0.186	0.439	96.671	128.568	119.178	0.01	
angle	00000001_1	C6 C5 N6	Not unusual (enough hits	225	121.242	123.744	1.746	1.433	2.502	117.703	127.597	124.357	0.093	
angle	00000001_1	C7 C6 C5	Not unusual (enough hits	495	117.275	117.075	1.499	0.134	0.201	105.829	123.29	116.994	0.003	
angle	00000001_1	C9 C6 C5	Not unusual (enough hits	155	121.994	121.018	1.641	0.594	0.975	113.768	126.783	120.987	0.006	
angle	00000001_1	C9 C6 C7	Not unusual (enough hits	10997	120.731	120.774	1.905	0.023	0.043	90.622	143.824	120.777	0	
angle	00000001_1	C8 C7 C6	Not unusual (enough hits	11395	120.045	121.039	1.437	0.692	0.994	93.35	147.791	121.028	0	
angle	00000001_1	C7 C8 C4	Not unusual (enough hits	289	118.172	117.43	0.964	0.769	0.741	114.685	123.178	117.353	0.003	
angle	00000001_1	C1 N2 N1	Unusual (enough hits)	38	134.617	116.494	1.659	10.927	18.123	113.273	119.271	116.712	15.346	
angle	00000001_1	C9 N3 C1	Unusual (enough hits)	15	128.692	124.917	0.706	5.347	3.774	123.364	126.201	124.859	2.49	
angle	00000001_1	N4 C1 N2	Unusual (enough hits)	15	125.326	132.6	1.547	4.701	7.274	128.968	134.4	133.08	3.642	
angle	00000001_1	C3 C2 N4	Unusual (enough hits)	191	105.34	102.619	1.341	2.029	2.72	94.971	107.419	102.75	0.03	
angle	00000001_1	C8 C4 N6	Unusual (enough hits)	167	121.279	124.711	1.675	2.048	3.432	117.068	127.876	125.155	0.029	
angle	00000001_1	C5 N6 C4	Unusual (enough hits)	179	121.986	116.435	1.303	4.261	5.551	112.785	121.37	116.186	0.616	
angle	00000001_1	C6 C9 N3	Unusual (enough hits)	764	117.698	113.088	1.717	2.685	4.611	104.07	122.755	113.045	0.246	
angle	00000001_2	O2 N1 O1	Not unusual (enough hits	234	118.571	121.526	2.164	1.366	2.956	116.275	131.091	121.113	0.018	
angle	00000001_2	O1 N1 N2	Not unusual (enough hits	430	118.32	119.288	4.121	0.235	0.968	112.759	126.082	117.049	0.068	
angle	00000001_2	O2 N1 N2	Not unusual (enough hits	430	123.077	119.288	4.121	0.92	3.79	112.759	126.082	117.049	0.01	
angle	00000001_2	C3 N3 C1	Not unusual (enough hits	23	108.597	109.675	2.799	0.385	1.079	104.343	112.076	111.094	1.253	
angle	00000001_2	C9 N3 C3	Not unusual (enough hits	109	123.07	120.505	2.722	0.942	2.565	110.736	125.952	121.036	0.019	
angle	00000001_2	N3 C1 N2	Not unusual (enough hits	16	122.976	118.565	3.722	1.185	4.411	116.421	131.83	117.249	3.106	
angle	00000001_2	N4 C1 N3	Not unusual (enough hits	19	110.863	109.894	0.771	1.257	0.969	107.953	111.238	110.048	0.014	
angle	00000001_2	C2 N4 C1	Not unusual (enough hits	53	109.615	110.972	2.593	0.523	1.357	105.927	114.592	111.774	0.012	
angle	00000001_2	C3 C2 N4	Not unusual (enough hits	191	104.978	102.619	1.341	1.759	2.359	94.971	107.419	102.75	0.087	
angle	00000001_2	C2 C3 N3	Not unusual (enough hits	85	105.896	102.951	1.651	1.784	2.944	99.561	108.169	102.882	0.077	
angle	00000001_2	CL1 C4 N6	Not unusual (enough hits	239	119.629	116.229	2.378	1.43	3.4	106.087	140.591	115.898	0.057	
angle	00000001_2	C8 C4 CL1	Not unusual (enough hits	437	119.461	119.088	2.36	0.158	0.373	96.671	128.568	119.178	0.003	
angle	00000001_2	C6 C5 N6	Not unusual (enough hits	225	120.977	123.744	1.746	1.585	2.767	117.703	127.597	124.357	0.034	
angle	00000001_2	C7 C6 C5	Not unusual (enough hits	495	117.499	117.075	1.499	0.283	0.424	105.829	123.29	116.994	0	
angle	00000001_2	C9 C6 C5	Not unusual (enough hits	155	122.095	121.018	1.641	0.656	1.077	113.768	126.783	120.987	0.009	
angle	00000001_2	C9 C6 C7	Not unusual (enough hits	10997	120.403	120.774	1.905	0.195	0.371	90.622	143.824	120.777	0	
angle	00000001_2	C8 C7 C6	Not unusual (enough hits	11395	119.993	121.039	1.437	0.728	1.046	93.35	147.791	121.028	0	
angle	00000001_2	C7 C8 C4	Not unusual (enough hits	289	118.491	117.43	0.964	1.101	1.061	114.685	123.178	117.353	0.014	
angle	00000001_2	C1 N2 N1	Unusual (enough hits)	38	134.495	116.494	1.659	10.853	18	113.273	119.271	116.712	15.223	

angle	00000001_2	C9 N3 C1	Unusual (enough hits)	15	128.297	124.917	0.706	4.787	3.379	123.364	126.201	124.859	2.095	
angle	00000001_2	N4 C1 N2	Unusual (enough hits)	15	125.992	132.6	1.547	4.271	6.608	128.968	134.4	133.08	2.976	
angle	00000001_2	C8 C4 N6	Unusual (enough hits)	167	120.91	124.711	1.675	2.269	3.801	117.068	127.876	125.155	0.087	
angle	00000001_2	C5 N6 C4	Unusual (enough hits)	179	122.13	116.435	1.303	4.372	5.695	112.785	121.37	116.186	0.76	
angle	00000001_2	C6 C9 N3	Unusual (enough hits)	764	116.999	113.088	1.717	2.279	3.912	104.07	122.755	113.045	0.042	
angle	00000001_3	O2 N1 O1	Not unusual (enough hits	234	118.525	121.526	2.164	1.387	3.001	116.275	131.091	121.113	0.028	
angle	00000001_3	O1 N1 N2	Not unusual (enough hits	430	118.142	119.288	4.121	0.278	1.146	112.759	126.082	117.049	0.11	
angle	00000001_3	O2 N1 N2	Not unusual (enough hits	430	123.329	119.288	4.121	0.981	4.041	112.759	126.082	117.049	0.003	
angle	00000001_3	C3 N3 C1	Not unusual (enough hits	23	108.078	109.675	2.799	0.571	1.597	104.343	112.076	111.094	0.734	
angle	00000001_3	C9 N3 C3	Not unusual (enough hits	109	123.303	120.505	2.722	1.028	2.798	110.736	125.952	121.036	0.015	
angle	00000001_3	N3 C1 N2	Not unusual (enough hits	16	123.962	118.565	3.722	1.45	5.396	116.421	131.83	117.249	4.091	
angle	00000001_3	N4 C1 N3	Not unusual (enough hits	19	111.05	109.894	0.771	1.499	1.156	107.953	111.238	110.048	0.187	
angle	00000001_3	C2 N4 C1	Not unusual (enough hits	53	109.423	110.972	2.593	0.597	1.549	105.927	114.592	111.774	0.039	
angle	00000001_3	C2 C3 N3	Not unusual (enough hits	85	106.02	102.951	1.651	1.859	3.069	99.561	108.169	102.882	0.201	
angle	00000001_3	CL1 C4 N6	Not unusual (enough hits	239	119.57	116.229	2.378	1.405	3.341	106.087	140.591	115.898	0.003	
angle	00000001_3	C8 C4 CL1	Not unusual (enough hits	437	119.737	119.088	2.36	0.275	0.649	96.671	128.568	119.178	0.001	
angle	00000001_3	C6 C5 N6	Not unusual (enough hits	225	120.578	123.744	1.746	1.814	3.166	117.703	127.597	124.357	0	
angle	00000001_3	C7 C6 C5	Not unusual (enough hits	495	118.332	117.075	1.499	0.839	1.258	105.829	123.29	116.994	0.016	
angle	00000001_3	C9 C6 C5	Not unusual (enough hits	155	120.953	121.018	1.641	0.04	0.066	113.768	126.783	120.987	0.004	
angle	00000001_3	C9 C6 C7	Not unusual (enough hits	10997	120.712	120.774	1.905	0.033	0.062	90.622	143.824	120.777	0	
angle	00000001_3	C8 C7 C6	Not unusual (enough hits	11395	119.216	121.039	1.437	1.269	1.823	93.35	147.791	121.028	0	
angle	00000001_3	C7 C8 C4	Not unusual (enough hits	289	118.614	117.43	0.964	1.228	1.184	114.685	123.178	117.353	0.017	
angle	00000001_3	C6 C9 N3	Not unusual (enough hits	764	113.559	113.088	1.717	0.275	0.471	104.07	122.755	113.045	0.003	
angle	00000001_3	C1 N2 N1	Unusual (enough hits)	38	132.081	116.494	1.659	9.398	15.587	113.273	119.271	116.712	12.81	
angle	00000001_3	C9 N3 C1	Unusual (enough hits)	15	128.619	124.917	0.706	5.244	3.702	123.364	126.201	124.859	2.418	
angle	00000001_3	N4 C1 N2	Unusual (enough hits)	15	124.988	132.6	1.547	4.92	7.612	128.968	134.4	133.08	3.98	
angle	00000001_3	C3 C2 N4	Unusual (enough hits)	191	105.429	102.619	1.341	2.095	2.809	94.971	107.419	102.75	0.016	
angle	00000001_3	C8 C4 N6	Unusual (enough hits)	167	120.693	124.711	1.675	2.398	4.018	117.068	127.876	125.155	0.063	
angle	00000001_3	C5 N6 C4	Unusual (enough hits)	179	122.565	116.435	1.303	4.706	6.13	112.785	121.37	116.186	1.195	
angle	00000001_4	O2 N1 O1	Not unusual (enough hits	234	118.304	121.526	2.164	1.489	3.222	116.275	131.091	121.113	0.082	
angle	00000001_4	O1 N1 N2	Not unusual (enough hits	430	118.131	119.288	4.121	0.281	1.157	112.759	126.082	117.049	0.121	
angle	00000001_4	O2 N1 N2	Not unusual (enough hits	430	123.563	119.288	4.121	1.037	4.276	112.759	126.082	117.049	0.01	
angle	00000001_4	C3 N3 C1	Not unusual (enough hits	23	108.88	109.675	2.799	0.284	0.796	104.343	112.076	111.094	1.378	
angle	00000001_4	C9 N3 C3	Not unusual (enough hits	109	123.388	120.505	2.722	1.059	2.883	110.736	125.952	121.036	0.069	
angle	00000001_4	N3 C1 N2	Not unusual (enough hits	16	123.136	118.565	3.722	1.228	4.57	116.421	131.83	117.249	3.265	
angle	00000001_4	N4 C1 N3	Not unusual (enough hits	19	110.582	109.894	0.771	0.892	0.688	107.953	111.238	110.048	0.018	
angle	00000001_4	C2 N4 C1	Not unusual (enough hits	53	109.465	110.972	2.593	0.581	1.506	105.927	114.592	111.774	0.004	
angle	00000001_4	C3 C2 N4	Not unusual (enough hits	191	105.201	102.619	1.341	1.925	2.582	94.971	107.419	102.75	0.016	
angle	00000001_4	C2 C3 N3	Not unusual (enough hits	85	105.871	102.951	1.651	1.768	2.919	99.561	108.169	102.882	0.051	
angle	00000001_4	CL1 C4 N6	Not unusual (enough hits	239	119.392	116.229	2.378	1.33	3.163	106.087	140.591	115.898	0.181	
angle	00000001_4	C8 C4 CL1	Not unusual (enough hits	437	119.327	119.088	2.36	0.101	0.239	96.671	128.568	119.178	0.002	
angle	00000001_4	C6 C5 N6	Not unusual (enough hits	225	121.057	123.744	1.746	1.539	2.687	117.703	127.597	124.357	0.025	
angle	00000001_4	C7 C6 C5	Not unusual (enough hits	495	117.344	117.075	1.499	0.18	0.27	105.829	123.29	116.994	0	
angle	00000001_4	C9 C6 C5	Not unusual (enough hits	155	121.823	121.018	1.641	0.49	0.804	113.768	126.783	120.987	0.026	
angle	00000001_4	C9 C6 C7	Not unusual (enough hits	10997	120.832	120.774	1.905	0.03	0.058	90.622	143.824	120.777	0	

angle	00000001_4	C8 C7 C6	Not unusual (enough hits	11395	120.215	121.039	1.437	0.573	0.824	93.35	147.791	121.028	0	
angle	00000001_4	C7 C8 C4	Not unusual (enough hits	289	118.216	117.43	0.964	0.815	0.786	114.685	123.178	117.353	0.018	
angle	00000001_4	C1 N2 N1	Unusual (enough hits)	38	135.035	116.494	1.659	11.179	18.541	113.273	119.271	116.712	15.764	
angle	00000001_4	C9 N3 C1	Unusual (enough hits)	15	127.733	124.917	0.706	3.988	2.815	123.364	126.201	124.859	1.531	
angle	00000001_4	N4 C1 N2	Unusual (enough hits)	15	126.276	132.6	1.547	4.087	6.324	128.968	134.4	133.08	2.692	
angle	00000001_4	C8 C4 N6	Unusual (enough hits)	167	121.279	124.711	1.675	2.049	3.432	117.068	127.876	125.155	0.029	
angle	00000001_4	C5 N6 C4	Unusual (enough hits)	179	121.883	116.435	1.303	4.182	5.448	112.785	121.37	116.186	0.513	
angle	00000001_4	C6 C9 N3	Unusual (enough hits)	764	116.679	113.088	1.717	2.092	3.592	104.07	122.755	113.045	0.234	
angle	00000001_5	O2 N1 O1	Not unusual (enough hits	234	118.888	121.526	2.164	1.219	2.639	116.275	131.091	121.113	0.162	
angle	00000001_5	O1 N1 N2	Not unusual (enough hits	430	117.614	119.288	4.121	0.406	1.674	112.759	126.082	117.049	0.039	
angle	00000001_5	O2 N1 N2	Not unusual (enough hits	430	123.498	119.288	4.121	1.022	4.21	112.759	126.082	117.049	0.006	
angle	00000001_5	C3 N3 C1	Not unusual (enough hits	23	108.599	109.675	2.799	0.385	1.076	104.343	112.076	111.094	1.255	
angle	00000001_5	C9 N3 C3	Not unusual (enough hits	109	123.513	120.505	2.722	1.105	3.008	110.736	125.952	121.036	0.177	
angle	00000001_5	N3 C1 N2	Not unusual (enough hits	16	122.463	118.565	3.722	1.047	3.898	116.421	131.83	117.249	2.593	
angle	00000001_5	N4 C1 N3	Not unusual (enough hits	19	110.96	109.894	0.771	1.383	1.066	107.953	111.238	110.048	0.111	
angle	00000001_5	C2 N4 C1	Not unusual (enough hits	53	109.369	110.972	2.593	0.618	1.603	105.927	114.592	111.774	0.076	
angle	00000001_5	C3 C2 N4	Not unusual (enough hits	191	105.079	102.619	1.341	1.834	2.459	94.971	107.419	102.75	0.013	
angle	00000001_5	C2 C3 N3	Not unusual (enough hits	85	105.991	102.951	1.651	1.841	3.039	99.561	108.169	102.882	0.172	
angle	00000001_5	CL1 C4 N6	Not unusual (enough hits	239	118.911	116.229	2.378	1.128	2.682	106.087	140.591	115.898	0.035	
angle	00000001_5	C8 C4 CL1	Not unusual (enough hits	437	119.839	119.088	2.36	0.318	0.751	96.671	128.568	119.178	0.001	
angle	00000001_5	C6 C5 N6	Not unusual (enough hits	225	120.969	123.744	1.746	1.59	2.775	117.703	127.597	124.357	0.042	
angle	00000001_5	C7 C6 C5	Not unusual (enough hits	495	117.899	117.075	1.499	0.55	0.825	105.829	123.29	116.994	0	
angle	00000001_5	C9 C6 C5	Not unusual (enough hits	155	121.058	121.018	1.641	0.024	0.04	113.768	126.783	120.987	0.003	
angle	00000001_5	C9 C6 C7	Not unusual (enough hits	10997	121.042	120.774	1.905	0.141	0.268	90.622	143.824	120.777	0	
angle	00000001_5	C8 C7 C6	Not unusual (enough hits	11395	119.584	121.039	1.437	1.013	1.455	93.35	147.791	121.028	0	
angle	00000001_5	C7 C8 C4	Not unusual (enough hits	289	118.228	117.43	0.964	0.827	0.797	114.685	123.178	117.353	0.007	
angle	00000001_5	C6 C9 N3	Not unusual (enough hits	764	115.386	113.088	1.717	1.339	2.299	104.07	122.755	113.045	0	
angle	00000001_5	C1 N2 N1	Unusual (enough hits)	38	135.763	116.494	1.659	11.618	19.269	113.273	119.271	116.712	16.492	
angle	00000001_5	C9 N3 C1	Unusual (enough hits)	15	127.886	124.917	0.706	4.205	2.969	123.364	126.201	124.859	1.685	
angle	00000001_5	N4 C1 N2	Unusual (enough hits)	15	126.57	132.6	1.547	3.897	6.03	128.968	134.4	133.08	2.397	
angle	00000001_5	C8 C4 N6	Unusual (enough hits)	167	121.25	124.711	1.675	2.066	3.461	117.068	127.876	125.155	0.058	
angle	00000001_5	C5 N6 C4	Unusual (enough hits)	179	122.07	116.435	1.303	4.326	5.635	112.785	121.37	116.186	0.7	
torsion	00000001_1	O1 N1 N2 C1	Not unusual (enough hits	382	178.73								0.027	0.487
torsion	00000001_1	O2 N1 N2 C1	Not unusual (enough hits	382	−2.387								0.009	0.479
torsion	00000001_1	N3 C1 N2 N1	Not unusual (enough hits	66	−179.808								0.074	0.833
torsion	00000001_1	N4 C1 N2 N1	Not unusual (enough hits	40	2.967								0.061	0.7
torsion	00000001_1	C6 C9 N3 C1	Not unusual (enough hits	48	88.961								0.066	0.208
torsion	00000001_1	C6 C9 N3 C3	Not unusual (enough hits	182	−90.294								0.395	0.143
torsion	00000001_1	C5 C6 C9 N3	Not unusual (enough hits	349	39.165								0.307	0.072
torsion	00000001_1	C7 C6 C9 N3	Not unusual (enough hits	10853	−140.937								0.008	0.119
torsion	00000001_2	O1 N1 N2 C1	Not unusual (enough hits	382	−177.216								0.008	0.492
torsion	00000001_2	O2 N1 N2 C1	Not unusual (enough hits	382	4.881								0.006	0.487
torsion	00000001_2	N3 C1 N2 N1	Not unusual (enough hits	66	179.219								0.041	0.833
torsion	00000001_2	N4 C1 N2 N1	Not unusual (enough hits	40	−5.938								0.157	0.7
torsion	00000001_2	C5 C6 C9 N3	Not unusual (enough hits	349	45.508								0.362	0.106

torsion	00000001_2	C7 C6 C9 N3	Not unusual (enough hits	10853	-135.118								0.012	0.126
torsion	00000001_2	C6 C9 N3 C1	Unusual (enough hits)	48	77.543								2.471	0.042
torsion	00000001_2	C6 C9 N3 C3	Unusual (enough hits)	182	-104.924								0.86	0.038
torsion	00000001_3	O1 N1 N2 C1	Not unusual (enough hits	382	-179.918								0.032	0.476
torsion	00000001_3	O2 N1 N2 C1	Not unusual (enough hits	382	-0.612								0.007	0.466
torsion	00000001_3	N3 C1 N2 N1	Not unusual (enough hits	66	178.974								0.016	0.833
torsion	00000001_3	N4 C1 N2 N1	Not unusual (enough hits	40	-1.161								0.022	0.7
torsion	00000001_3	C6 C9 N3 C1	Not unusual (enough hits	48	86.968								0.389	0.188
torsion	00000001_3	C6 C9 N3 C3	Not unusual (enough hits	182	-93.146								0.919	0.088
torsion	00000001_3	C5 C6 C9 N3	Not unusual (enough hits	349	68.134								0.11	0.138
torsion	00000001_3	C7 C6 C9 N3	Not unusual (enough hits	10853	-111.205								0.007	0.128
torsion	00000001_4	O1 N1 N2 C1	Not unusual (enough hits	382	179.609								0.027	0.482
torsion	00000001_4	O2 N1 N2 C1	Not unusual (enough hits	382	-0.839								0.019	0.466
torsion	00000001_4	N3 C1 N2 N1	Not unusual (enough hits	66	179.945								0.037	0.818
torsion	00000001_4	N4 C1 N2 N1	Not unusual (enough hits	40	0.969								0.027	0.7
torsion	00000001_4	C6 C9 N3 C1	Not unusual (enough hits	48	85.478								1.879	0.188
torsion	00000001_4	C6 C9 N3 C3	Not unusual (enough hits	182	-94.307								0.205	0.093
torsion	00000001_4	C5 C6 C9 N3	Not unusual (enough hits	349	37.819								1.039	0.08
torsion	00000001_4	C7 C6 C9 N3	Not unusual (enough hits	10853	-141.895								0.01	0.118
torsion	00000001_5	O1 N1 N2 C1	Not unusual (enough hits	382	-179.17								0.032	0.482
torsion	00000001_5	O2 N1 N2 C1	Not unusual (enough hits	382	1.039								0.04	0.466
torsion	00000001_5	N3 C1 N2 N1	Not unusual (enough hits	66	179.489								0.045	0.833
torsion	00000001_5	N4 C1 N2 N1	Not unusual (enough hits	40	-1.463								0.029	0.7
torsion	00000001_5	C6 C9 N3 C1	Not unusual (enough hits	48	86.62								0.737	0.188
torsion	00000001_5	C6 C9 N3 C3	Not unusual (enough hits	182	-93.992								0.074	0.088
torsion	00000001_5	C5 C6 C9 N3	Not unusual (enough hits	349	68.286								0.043	0.135
torsion	00000001_5	C7 C6 C9 N3	Not unusual (enough hits	10853	-111.874								0.005	0.128
ring	00000001_1	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.412	16.221			0.771
ring	00000001_1	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.078	8.296			1
ring	00000001_2	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.425	15.971			0.8
ring	00000001_2	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.07	8.301			1
ring	00000001_3	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.735	16.357			0.771
ring	00000001_3	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.071	8.273			1
ring	00000001_4	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.58	16.339			0.771
ring	00000001_4	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.149	8.144			1
ring	00000001_5	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.462	16.262			0.771
ring	00000001_5	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.087	8.294			1

Table 2. Geometry Analysis by Mogul of Imidacloprid in Complex with Gln55Arg Mutant of Ls-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	｜z-score｜	｜x - mean｜	Minimum	Maximum	Median	｜d(min)｜	Local density
bond	00000001_1	N2 N1	Not unusual (enough hits	218	1.361	1.342	0.035	0.553	0.019	1.286	1.462	1.336	0	
bond	00000001_1	C3 N3	Not unusual (enough hits	1978	1.469	1.468	0.023	0.011	0	1.336	1.699	1.468	0	
bond	00000001_1	C9 N3	Not unusual (enough hits	931	1.473	1.465	0.015	0.543	0.008	1.386	1.561	1.465	0	
bond	00000001_1	C2 N4	Not unusual (enough hits	1745	1.468	1.457	0.022	0.469	0.01	1.204	1.687	1.458	0	
bond	00000001_1	C3 C2	Not unusual (enough hits	252	1.545	1.521	0.02	1.244	0.024	1.452	1.629	1.52	0	
bond	00000001_1	C4 CL1	Not unusual (enough hits	743	1.739	1.738	0.019	0.066	0.001	1.561	1.806	1.74	0	
bond	00000001_1	C4 N6	Not unusual (enough hits	245	1.35	1.321	0.025	1.121	0.028	1.254	1.422	1.317	0.002	
bond	00000001_1	C5 N6	Not unusual (enough hits	2818	1.343	1.34	0.022	0.14	0.003	1.05	1.584	1.337	0	
bond	00000001_1	C7 C6	Not unusual (enough hits	14050	1.426	1.384	0.022	1.892	0.042	0.618	1.8	1.386	0	
bond	00000001_1	C9 C6	Not unusual (enough hits	10549	1.537	1.51	0.019	1.46	0.027	1.278	1.842	1.51	0	
bond	00000001_1	C8 C7	Not unusual (enough hits	20000	1.417	1.383	0.019	1.806	0.033	0.882	1.685	1.383	0	
bond	00000001_1	O1 N1	Unusual (enough hits)	476	1.282	1.241	0.019	2.154	0.041	1.169	1.356	1.241	0.002	
bond	00000001_1	O2 N1	Unusual (enough hits)	476	1.295	1.241	0.019	2.83	0.054	1.169	1.356	1.241	0	
bond	00000001_1	C1 N2	Unusual (enough hits)	38	1.278	1.345	0.012	5.716	0.067	1.322	1.369	1.343	0.044	
bond	00000001_1	C1 N3	Unusual (enough hits)	23	1.419	1.351	0.021	3.22	0.069	1.327	1.394	1.344	0.025	
bond	00000001_1	C1 N4	Unusual (enough hits)	56	1.413	1.335	0.02	3.846	0.078	1.304	1.41	1.331	0.003	
bond	00000001_1	C8 C4	Unusual (enough hits)	479	1.421	1.373	0.022	2.189	0.048	1.267	1.455	1.373	0.002	
bond	00000001_1	C5 C6	Unusual (enough hits)	560	1.429	1.381	0.017	2.877	0.048	1.279	1.497	1.382	0.005	
bond	00000001_2	N2 N1	Not unusual (enough hits	218	1.376	1.342	0.035	0.988	0.034	1.286	1.462	1.336	0.004	
bond	00000001_2	C3 N3	Not unusual (enough hits	1978	1.474	1.468	0.023	0.26	0.006	1.336	1.699	1.468	0	
bond	00000001_2	C9 N3	Not unusual (enough hits	931	1.476	1.465	0.015	0.677	0.01	1.386	1.561	1.465	0	
bond	00000001_2	C2 N4	Not unusual (enough hits	1745	1.464	1.457	0.022	0.313	0.007	1.204	1.687	1.458	0	
bond	00000001_2	C3 C2	Not unusual (enough hits	252	1.539	1.521	0.02	0.913	0.018	1.452	1.629	1.52	0	
bond	00000001_2	C4 CL1	Not unusual (enough hits	743	1.749	1.738	0.019	0.582	0.011	1.561	1.806	1.74	0	
bond	00000001_2	C4 N6	Not unusual (enough hits	245	1.355	1.321	0.025	1.321	0.033	1.254	1.422	1.317	0.002	
bond	00000001_2	C8 C4	Not unusual (enough hits	479	1.414	1.373	0.022	1.869	0.041	1.267	1.455	1.373	0	
bond	00000001_2	C5 N6	Not unusual (enough hits	2818	1.355	1.34	0.022	0.673	0.015	1.05	1.584	1.337	0	
bond	00000001_2	C7 C6	Not unusual (enough hits	14050	1.423	1.384	0.022	1.76	0.039	0.618	1.8	1.386	0	
bond	00000001_2	C8 C7	Not unusual (enough hits	20000	1.417	1.383	0.019	1.832	0.034	0.882	1.685	1.383	0	
bond	00000001_2	O1 N1	Unusual (enough hits)	476	1.294	1.241	0.019	2.77	0.053	1.169	1.356	1.241	0.001	
bond	00000001_2	O2 N1	Unusual (enough hits)	476	1.297	1.241	0.019	2.931	0.056	1.169	1.356	1.241	0	
bond	00000001_2	C1 N2	Unusual (enough hits)	38	1.29	1.345	0.012	4.691	0.055	1.322	1.369	1.343	0.032	
bond	00000001_2	C1 N3	Unusual (enough hits)	23	1.42	1.351	0.021	3.252	0.069	1.327	1.394	1.344	0.026	
bond	00000001_2	C1 N4	Unusual (enough hits)	56	1.411	1.335	0.02	3.756	0.076	1.304	1.41	1.331	0.001	
bond	00000001_2	C5 C6	Unusual (enough hits)	560	1.436	1.381	0.017	3.245	0.055	1.279	1.497	1.382	0.001	
bond	00000001_2	C9 C6	Unusual (enough hits)	10549	1.553	1.51	0.019	2.311	0.043	1.278	1.842	1.51	0	
bond	00000001_3	N2 N1	Not unusual (enough hits	218	1.358	1.342	0.035	0.475	0.016	1.286	1.462	1.336	0	

bond	00000001_3	C3 N3	Not unusual (enough hits	1978	1.464	1.468	0.023	0.17	0.004	1.336	1.699	1.468	0	
bond	00000001_3	C9 N3	Not unusual (enough hits	931	1.472	1.465	0.015	0.466	0.007	1.386	1.561	1.465	0	
bond	00000001_3	C2 N4	Not unusual (enough hits	1745	1.457	1.457	0.022	0.009	0	1.204	1.687	1.458	0	
bond	00000001_3	C3 C2	Not unusual (enough hits	252	1.538	1.521	0.02	0.877	0.017	1.452	1.629	1.52	0	
bond	00000001_3	C4 CL1	Not unusual (enough hits	743	1.721	1.738	0.019	0.917	0.017	1.561	1.806	1.74	0	
bond	00000001_3	C4 N6	Not unusual (enough hits	245	1.348	1.321	0.025	1.057	0.027	1.254	1.422	1.317	0.004	
bond	00000001_3	C5 N6	Not unusual (enough hits	2818	1.345	1.34	0.022	0.232	0.005	1.05	1.584	1.337	0	
bond	00000001_3	C7 C6	Not unusual (enough hits	14050	1.425	1.384	0.022	1.849	0.041	0.618	1.8	1.386	0	
bond	00000001_3	C9 C6	Not unusual (enough hits	10549	1.525	1.51	0.019	0.802	0.015	1.278	1.842	1.51	0	
bond	00000001_3	O1 N1	Unusual (enough hits)	476	1.284	1.241	0.019	2.241	0.043	1.169	1.356	1.241	0.002	
bond	00000001_3	O2 N1	Unusual (enough hits)	476	1.298	1.241	0.019	3.011	0.058	1.169	1.356	1.241	0.001	
bond	00000001_3	C1 N2	Unusual (enough hits)	38	1.275	1.345	0.012	6.002	0.07	1.322	1.369	1.343	0.047	
bond	00000001_3	C1 N3	Unusual (enough hits)	23	1.401	1.351	0.021	2.382	0.051	1.327	1.394	1.344	0.008	
bond	00000001_3	C1 N4	Unusual (enough hits)	56	1.407	1.335	0.02	3.591	0.073	1.304	1.41	1.331	0.002	
bond	00000001_3	C8 C4	Unusual (enough hits)	479	1.418	1.373	0.022	2.082	0.046	1.267	1.455	1.373	0.001	
bond	00000001_3	C5 C6	Unusual (enough hits)	560	1.423	1.381	0.017	2.524	0.043	1.279	1.497	1.382	0.006	
bond	00000001_3	C8 C7	Unusual (enough hits)	20000	1.421	1.383	0.019	2.026	0.038	0.882	1.685	1.383	0	
bond	00000001_4	N2 N1	Not unusual (enough hits	218	1.359	1.342	0.035	0.491	0.017	1.286	1.462	1.336	0	
bond	00000001_4	C3 N3	Not unusual (enough hits	1978	1.46	1.468	0.023	0.358	0.008	1.336	1.699	1.468	0	
bond	00000001_4	C9 N3	Not unusual (enough hits	931	1.458	1.465	0.015	0.438	0.007	1.386	1.561	1.465	0	
bond	00000001_4	C2 N4	Not unusual (enough hits	1745	1.467	1.457	0.022	0.445	0.01	1.204	1.687	1.458	0	
bond	00000001_4	C3 C2	Not unusual (enough hits	252	1.541	1.521	0.02	1.02	0.02	1.452	1.629	1.52	0	
bond	00000001_4	C4 CL1	Not unusual (enough hits	743	1.741	1.738	0.019	0.15	0.003	1.561	1.806	1.74	0	
bond	00000001_4	C4 N6	Not unusual (enough hits	245	1.351	1.321	0.025	1.181	0.03	1.254	1.422	1.317	0.001	
bond	00000001_4	C8 C4	Not unusual (enough hits	479	1.414	1.373	0.022	1.896	0.042	1.267	1.455	1.373	0	
bond	00000001_4	C5 N6	Not unusual (enough hits	2818	1.353	1.34	0.022	0.566	0.013	1.05	1.584	1.337	0	
bond	00000001_4	C7 C6	Not unusual (enough hits	14050	1.411	1.384	0.022	1.228	0.027	0.618	1.8	1.386	0	
bond	00000001_4	C9 C6	Not unusual (enough hits	10549	1.527	1.51	0.019	0.917	0.017	1.278	1.842	1.51	0	
bond	00000001_4	C8 C7	Not unusual (enough hits	20000	1.412	1.383	0.019	1.553	0.029	0.882	1.685	1.383	0	
bond	00000001_4	O1 N1	Unusual (enough hits)	476	1.292	1.241	0.019	2.647	0.051	1.169	1.356	1.241	0.001	
bond	00000001_4	O2 N1	Unusual (enough hits)	476	1.296	1.241	0.019	2.901	0.056	1.169	1.356	1.241	0.001	
bond	00000001_4	C1 N2	Unusual (enough hits)	38	1.286	1.345	0.012	5.08	0.059	1.322	1.369	1.343	0.036	
bond	00000001_4	C1 N3	Unusual (enough hits)	23	1.419	1.351	0.021	3.22	0.069	1.327	1.394	1.344	0.025	
bond	00000001_4	C1 N4	Unusual (enough hits)	56	1.412	1.335	0.02	3.822	0.077	1.304	1.41	1.331	0.002	
bond	00000001_4	C5 C6	Unusual (enough hits)	560	1.433	1.381	0.017	3.118	0.053	1.279	1.497	1.382	0.001	
bond	00000001_5	N2 N1	Not unusual (enough hits	218	1.358	1.342	0.035	0.454	0.016	1.286	1.462	1.336	0.001	
bond	00000001_5	C3 N3	Not unusual (enough hits	1978	1.463	1.468	0.023	0.239	0.005	1.336	1.699	1.468	0	
bond	00000001_5	C9 N3	Not unusual (enough hits	931	1.474	1.465	0.015	0.591	0.009	1.386	1.561	1.465	0	
bond	00000001_5	C2 N4	Not unusual (enough hits	1745	1.46	1.457	0.022	0.094	0.002	1.204	1.687	1.458	0	

bond	00000001_5	C3 C2	Not unusual (enough hits	252	1.546	1.521	0.02	1.269	0.025	1.452	1.629	1.52	0	
bond	00000001_5	C4 CL1	Not unusual (enough hits	743	1.737	1.738	0.019	0.058	0.001	1.561	1.806	1.74	0	
bond	00000001_5	C4 N6	Not unusual (enough hits	245	1.353	1.321	0.025	1.261	0.032	1.254	1.422	1.317	0	
bond	00000001_5	C5 N6	Not unusual (enough hits	2818	1.35	1.34	0.022	0.446	0.01	1.05	1.584	1.337	0	
bond	00000001_5	C7 C6	Not unusual (enough hits	14050	1.423	1.384	0.022	1.758	0.039	0.618	1.8	1.386	0	
bond	00000001_5	C9 C6	Not unusual (enough hits	10549	1.537	1.51	0.019	1.464	0.027	1.278	1.842	1.51	0	
bond	00000001_5	C8 C7	Not unusual (enough hits	20000	1.412	1.383	0.019	1.532	0.028	0.882	1.685	1.383	0	
bond	00000001_5	O1 N1	Unusual (enough hits)	476	1.289	1.241	0.019	2.508	0.048	1.169	1.356	1.241	0.001	
bond	00000001_5	O2 N1	Unusual (enough hits)	476	1.291	1.241	0.019	2.644	0.051	1.169	1.356	1.241	0.002	
bond	00000001_5	C1 N2	Unusual (enough hits)	38	1.281	1.345	0.012	5.475	0.064	1.322	1.369	1.343	0.041	
bond	00000001_5	C1 N3	Unusual (enough hits)	23	1.415	1.351	0.021	3.031	0.065	1.327	1.394	1.344	0.021	
bond	00000001_5	C1 N4	Unusual (enough hits)	56	1.409	1.335	0.02	3.69	0.075	1.304	1.41	1.331	0	
bond	00000001_5	C8 C4	Unusual (enough hits)	479	1.421	1.373	0.022	2.22	0.049	1.267	1.455	1.373	0.002	
bond	00000001_5	C5 C6	Unusual (enough hits)	560	1.439	1.381	0.017	3.439	0.058	1.279	1.497	1.382	0.005	
angle	00000001_1	O2 N1 O1	Not unusual (enough hits	234	118.588	121.526	2.164	1.358	2.938	116.275	131.091	121.113	0.035	
angle	00000001_1	O1 N1 N2	Not unusual (enough hits	430	118.15	119.288	4.121	0.276	1.137	112.759	126.082	117.049	0.102	
angle	00000001_1	O2 N1 N2	Not unusual (enough hits	430	123.261	119.288	4.121	0.964	3.973	112.759	126.082	117.049	0.01	
angle	00000001_1	C3 N3 C1	Not unusual (enough hits	23	108.556	109.675	2.799	0.4	1.119	104.343	112.076	111.094	1.212	
angle	00000001_1	C9 N3 C3	Not unusual (enough hits	109	123.567	120.505	2.722	1.125	3.062	110.736	125.952	121.036	0.123	
angle	00000001_1	N3 C1 N2	Not unusual (enough hits	16	123.188	118.565	3.722	1.242	4.623	116.421	131.83	117.249	3.318	
angle	00000001_1	N4 C1 N3	Not unusual (enough hits	19	111.084	109.894	0.771	1.543	1.19	107.953	111.238	110.048	0.153	
angle	00000001_1	C2 N4 C1	Not unusual (enough hits	53	109.145	110.972	2.593	0.705	1.827	105.927	114.592	111.774	0.034	
angle	00000001_1	C2 C3 N3	Not unusual (enough hits	85	105.888	102.951	1.651	1.779	2.936	99.561	108.169	102.882	0.069	
angle	00000001_1	CL1 C4 N6	Not unusual (enough hits	239	119.604	116.229	2.378	1.419	3.375	106.087	140.591	115.898	0.032	
angle	00000001_1	C8 C4 CL1	Not unusual (enough hits	437	119.71	119.088	2.36	0.263	0.622	96.671	128.568	119.178	0.009	
angle	00000001_1	C6 C5 N6	Not unusual (enough hits	225	121.106	123.744	1.746	1.511	2.638	117.703	127.597	124.357	0.043	
angle	00000001_1	C7 C6 C5	Not unusual (enough hits	495	117.626	117.075	1.499	0.368	0.551	105.829	123.29	116.994	0	
angle	00000001_1	C9 C6 C5	Not unusual (enough hits	155	121.358	121.018	1.641	0.207	0.339	113.768	126.783	120.987	0.01	
angle	00000001_1	C9 C6 C7	Not unusual (enough hits	10997	121.016	120.774	1.905	0.127	0.242	90.622	143.824	120.777	0	
angle	00000001_1	C8 C7 C6	Not unusual (enough hits	11395	119.809	121.039	1.437	0.856	1.23	93.35	147.791	121.028	0	
angle	00000001_1	C7 C8 C4	Not unusual (enough hits	289	118.511	117.43	0.964	1.121	1.081	114.685	123.178	117.353	0.034	
angle	00000001_1	C6 C9 N3	Not unusual (enough hits	764	115.639	113.088	1.717	1.486	2.551	104.07	122.755	113.045	0.004	
angle	00000001_1	C1 N2 N1	Unusual (enough hits)	38	134.518	116.494	1.659	10.867	18.024	113.273	119.271	116.712	15.247	
angle	00000001_1	C9 N3 C1	Unusual (enough hits)	15	127.877	124.917	0.706	4.193	2.96	123.364	126.201	124.859	1.676	
angle	00000001_1	N4 C1 N2	Unusual (enough hits)	15	125.726	132.6	1.547	4.443	6.874	128.968	134.4	133.08	3.242	
angle	00000001_1	C3 C2 N4	Unusual (enough hits)	191	105.327	102.619	1.341	2.019	2.708	94.971	107.419	102.75	0.042	
angle	00000001_1	C8 C4 N6	Unusual (enough hits)	167	120.685	124.711	1.675	2.403	4.026	117.068	127.876	125.155	0.055	
angle	00000001_1	C5 N6 C4	Unusual (enough hits)	179	122.263	116.435	1.303	4.473	5.828	112.785	121.37	116.186	0.893	
angle	00000001_2	O2 N1 O1	Not unusual (enough hits	234	118.16	121.526	2.164	1.555	3.366	116.275	131.091	121.113	0.062	

angle	00000001_2	O1 N1 N2	Not unusual (enough hits	430	118.615	119.288	4.121	0.163	0.673	112.759	126.082	117.049	0.289	
angle	00000001_2	O2 N1 N2	Not unusual (enough hits	430	123.224	119.288	4.121	0.955	3.937	112.759	126.082	117.049	0.001	
angle	00000001_2	C3 N3 C1	Not unusual (enough hits	23	108.662	109.675	2.799	0.362	1.013	104.343	112.076	111.094	1.318	
angle	00000001_2	C9 N3 C3	Not unusual (enough hits	109	122.959	120.505	2.722	0.902	2.455	110.736	125.952	121.036	0.008	
angle	00000001_2	N3 C1 N2	Not unusual (enough hits	16	123.922	118.565	3.722	1.439	5.357	116.421	131.83	117.249	4.052	
angle	00000001_2	N4 C1 N3	Not unusual (enough hits	19	110.407	109.894	0.771	0.665	0.513	107.953	111.238	110.048	0.08	
angle	00000001_2	C2 N4 C1	Not unusual (enough hits	53	109.901	110.972	2.593	0.413	1.07	105.927	114.592	111.774	0.113	
angle	00000001_2	C3 C2 N4	Not unusual (enough hits	191	105.126	102.619	1.341	1.869	2.507	94.971	107.419	102.75	0.06	
angle	00000001_2	C2 C3 N3	Not unusual (enough hits	85	105.903	102.951	1.651	1.788	2.951	99.561	108.169	102.882	0.084	
angle	00000001_2	CL1 C4 N6	Not unusual (enough hits	239	119.914	116.229	2.378	1.55	3.685	106.087	140.591	115.898	0.06	
angle	00000001_2	C8 C4 CL1	Not unusual (enough hits	437	119.252	119.088	2.36	0.069	0.164	96.671	128.568	119.178	0	
angle	00000001_2	C6 C5 N6	Not unusual (enough hits	225	121.036	123.744	1.746	1.552	2.709	117.703	127.597	124.357	0.004	
angle	00000001_2	C7 C6 C5	Not unusual (enough hits	495	117.218	117.075	1.499	0.096	0.143	105.829	123.29	116.994	0.004	
angle	00000001_2	C9 C6 C5	Not unusual (enough hits	155	122.677	121.018	1.641	1.011	1.658	113.768	126.783	120.987	0.053	
angle	00000001_2	C9 C6 C7	Not unusual (enough hits	10997	120.105	120.774	1.905	0.351	0.669	90.622	143.824	120.777	0	
angle	00000001_2	C8 C7 C6	Not unusual (enough hits	11395	120.393	121.039	1.437	0.45	0.646	93.35	147.791	121.028	0	
angle	00000001_2	C7 C8 C4	Not unusual (enough hits	289	118.581	117.43	0.964	1.194	1.151	114.685	123.178	117.353	0.05	
angle	00000001_2	C1 N2 N1	Unusual (enough hits)	38	134.339	116.494	1.659	10.759	17.845	113.273	119.271	116.712	15.068	
angle	00000001_2	C9 N3 C1	Unusual (enough hits)	15	128.376	124.917	0.706	4.899	3.459	123.364	126.201	124.859	2.175	
angle	00000001_2	N4 C1 N2	Unusual (enough hits)	15	125.668	132.6	1.547	4.48	6.932	128.968	134.4	133.08	3.3	
angle	00000001_2	C8 C4 N6	Unusual (enough hits)	167	120.834	124.711	1.675	2.314	3.877	117.068	127.876	125.155	0.011	
angle	00000001_2	C5 N6 C4	Unusual (enough hits)	179	121.938	116.435	1.303	4.224	5.503	112.785	121.37	116.186	0.568	
angle	00000001_2	C6 C9 N3	Unusual (enough hits)	764	117.21	113.088	1.717	2.401	4.122	104.07	122.755	113.045	0.008	
angle	00000001_3	O2 N1 O1	Not unusual (enough hits	234	118.816	121.526	2.164	1.252	2.71	116.275	131.091	121.113	0.194	
angle	00000001_3	O1 N1 N2	Not unusual (enough hits	430	117.949	119.288	4.121	0.325	1.339	112.759	126.082	117.049	0.036	
angle	00000001_3	O2 N1 N2	Not unusual (enough hits	430	123.234	119.288	4.121	0.958	3.946	112.759	126.082	117.049	0.006	
angle	00000001_3	C3 N3 C1	Not unusual (enough hits	23	108.675	109.675	2.799	0.357	1	104.343	112.076	111.094	1.331	
angle	00000001_3	C9 N3 C3	Not unusual (enough hits	109	123.637	120.505	2.722	1.151	3.132	110.736	125.952	121.036	0.053	
angle	00000001_3	N3 C1 N2	Not unusual (enough hits	16	123.099	118.565	3.722	1.218	4.533	116.421	131.83	117.249	3.229	
angle	00000001_3	N4 C1 N3	Not unusual (enough hits	19	111.078	109.894	0.771	1.535	1.184	107.953	111.238	110.048	0.159	
angle	00000001_3	C2 N4 C1	Not unusual (enough hits	53	109.354	110.972	2.593	0.624	1.617	105.927	114.592	111.774	0.062	
angle	00000001_3	C3 C2 N4	Not unusual (enough hits	191	105.062	102.619	1.341	1.822	2.443	94.971	107.419	102.75	0.003	
angle	00000001_3	C2 C3 N3	Not unusual (enough hits	85	105.829	102.951	1.651	1.743	2.878	99.561	108.169	102.882	0.01	
angle	00000001_3	CL1 C4 N6	Not unusual (enough hits	239	120.009	116.229	2.378	1.59	3.78	106.087	140.591	115.898	0.035	
angle	00000001_3	C8 C4 CL1	Not unusual (enough hits	437	119.224	119.088	2.36	0.058	0.136	96.671	128.568	119.178	0.002	
angle	00000001_3	C6 C5 N6	Not unusual (enough hits	225	120.767	123.744	1.746	1.705	2.977	117.703	127.597	124.357	0.042	
angle	00000001_3	C7 C6 C5	Not unusual (enough hits	495	118.169	117.075	1.499	0.73	1.095	105.829	123.29	116.994	0.017	
angle	00000001_3	C9 C6 C5	Not unusual (enough hits	155	120.381	121.018	1.641	0.389	0.638	113.768	126.783	120.987	0.015	
angle	00000001_3	C9 C6 C7	Not unusual (enough hits	10997	121.448	120.774	1.905	0.354	0.674	90.622	143.824	120.777	0	

angle	00000001_3	C8 C7 C6	Not unusual (enough hits	11395	119.459	121.039	1.437	1.1	1.581	93.35	147.791	121.028	0.001	
angle	00000001_3	C7 C8 C4	Not unusual (enough hits	289	118.448	117.43	0.964	1.056	1.018	114.685	123.178	117.353	0.029	
angle	00000001_3	C6 C9 N3	Not unusual (enough hits	764	112.552	113.088	1.717	0.312	0.536	104.07	122.755	113.045	0.003	
angle	00000001_3	C1 N2 N1	Unusual (enough hits)	38	134.112	116.494	1.659	10.622	17.617	113.273	119.271	116.712	14.84	
angle	00000001_3	C9 N3 C1	Unusual (enough hits)	15	127.687	124.917	0.706	3.923	2.77	123.364	126.201	124.859	1.486	
angle	00000001_3	N4 C1 N2	Unusual (enough hits)	15	125.821	132.6	1.547	4.381	6.779	128.968	134.4	133.08	3.147	
angle	00000001_3	C8 C4 N6	Unusual (enough hits)	167	120.767	124.711	1.675	2.354	3.944	117.068	127.876	125.155	0.056	
angle	00000001_3	C5 N6 C4	Unusual (enough hits)	179	122.39	116.435	1.303	4.571	5.955	112.785	121.37	116.186	1.02	
angle	00000001_4	O2 N1 O1	Not unusual (enough hits	234	118.616	121.526	2.164	1.345	2.91	116.275	131.091	121.113	0.007	
angle	00000001_4	O1 N1 N2	Not unusual (enough hits	430	118.008	119.288	4.121	0.311	1.28	112.759	126.082	117.049	0.095	
angle	00000001_4	O2 N1 N2	Not unusual (enough hits	430	123.37	119.288	4.121	0.991	4.083	112.759	126.082	117.049	0.005	
angle	00000001_4	C3 N3 C1	Not unusual (enough hits	23	109.053	109.675	2.799	0.222	0.622	104.343	112.076	111.094	1.204	
angle	00000001_4	C9 N3 C3	Not unusual (enough hits	109	122.94	120.505	2.722	0.895	2.436	110.736	125.952	121.036	0.002	
angle	00000001_4	N3 C1 N2	Not unusual (enough hits	16	122.918	118.565	3.722	1.17	4.353	116.421	131.83	117.249	3.048	
angle	00000001_4	N4 C1 N3	Not unusual (enough hits	19	110.569	109.894	0.771	0.876	0.675	107.953	111.238	110.048	0.006	
angle	00000001_4	C2 N4 C1	Not unusual (enough hits	53	109.19	110.972	2.593	0.687	1.782	105.927	114.592	111.774	0.079	
angle	00000001_4	C2 C3 N3	Not unusual (enough hits	85	105.801	102.951	1.651	1.726	2.849	99.561	108.169	102.882	0.019	
angle	00000001_4	CL1 C4 N6	Not unusual (enough hits	239	120.074	116.229	2.378	1.617	3.845	106.087	140.591	115.898	0.1	
angle	00000001_4	C8 C4 CL1	Not unusual (enough hits	437	119.111	119.088	2.36	0.01	0.022	96.671	128.568	119.178	0.005	
angle	00000001_4	C6 C5 N6	Not unusual (enough hits	225	120.52	123.744	1.746	1.847	3.224	117.703	127.597	124.357	0.027	
angle	00000001_4	C7 C6 C5	Not unusual (enough hits	495	117.922	117.075	1.499	0.565	0.847	105.829	123.29	116.994	0.009	
angle	00000001_4	C9 C6 C5	Not unusual (enough hits	155	122.599	121.018	1.641	0.963	1.58	113.768	126.783	120.987	0.019	
angle	00000001_4	C9 C6 C7	Not unusual (enough hits	10997	119.478	120.774	1.905	0.681	1.296	90.622	143.824	120.777	0	
angle	00000001_4	C8 C7 C6	Not unusual (enough hits	11395	120.199	121.039	1.437	0.585	0.841	93.35	147.791	121.028	0	
angle	00000001_4	C7 C8 C4	Not unusual (enough hits	289	118.563	117.43	0.964	1.175	1.132	114.685	123.178	117.353	0.068	
angle	00000001_4	C1 N2 N1	Unusual (enough hits)	38	134.722	116.494	1.659	10.99	18.228	113.273	119.271	116.712	15.451	
angle	00000001_4	C9 N3 C1	Unusual (enough hits)	15	128.001	124.917	0.706	4.369	3.084	123.364	126.201	124.859	1.8	
angle	00000001_4	N4 C1 N2	Unusual (enough hits)	15	126.495	132.6	1.547	3.946	6.105	128.968	134.4	133.08	2.473	
angle	00000001_4	C3 C2 N4	Unusual (enough hits)	191	105.381	102.619	1.341	2.059	2.761	94.971	107.419	102.75	0.011	
angle	00000001_4	C8 C4 N6	Unusual (enough hits)	167	120.813	124.711	1.675	2.327	3.898	117.068	127.876	125.155	0.01	
angle	00000001_4	C5 N6 C4	Unusual (enough hits)	179	121.983	116.435	1.303	4.259	5.548	112.785	121.37	116.186	0.613	
angle	00000001_4	C6 C9 N3	Unusual (enough hits)	764	116.842	113.088	1.717	2.187	3.755	104.07	122.755	113.045	0.071	
angle	00000001_5	O2 N1 O1	Not unusual (enough hits	234	119.036	121.526	2.164	1.151	2.49	116.275	131.091	121.113	0.013	
angle	00000001_5	O1 N1 N2	Not unusual (enough hits	430	118.15	119.288	4.121	0.276	1.137	112.759	126.082	117.049	0.102	
angle	00000001_5	O2 N1 N2	Not unusual (enough hits	430	122.812	119.288	4.121	0.855	3.525	112.759	126.082	117.049	0.001	
angle	00000001_5	C3 N3 C1	Not unusual (enough hits	23	108.424	109.675	2.799	0.447	1.251	104.343	112.076	111.094	1.08	
angle	00000001_5	C9 N3 C3	Not unusual (enough hits	109	122.971	120.505	2.722	0.906	2.467	110.736	125.952	121.036	0.02	
angle	00000001_5	N3 C1 N2	Not unusual (enough hits	16	123.371	118.565	3.722	1.291	4.806	116.421	131.83	117.249	3.501	
angle	00000001_5	N4 C1 N3	Not unusual (enough hits	19	111.167	109.894	0.771	1.65	1.273	107.953	111.238	110.048	0.071	

angle	00000001_5	C2 N4 C1	Not unusual (enough hits	53	109.254	110.972	2.593	0.663	1.718	105.927	114.592	111.774	0.039	
angle	00000001_5	C3 C2 N4	Not unusual (enough hits	191	105.188	102.619	1.341	1.916	2.569	94.971	107.419	102.75	0.029	
angle	00000001_5	C2 C3 N3	Not unusual (enough hits	85	105.965	102.951	1.651	1.826	3.014	99.561	108.169	102.882	0.146	
angle	00000001_5	CL1 C4 N6	Not unusual (enough hits	239	119.256	116.229	2.378	1.273	3.027	106.087	140.591	115.898	0.317	
angle	00000001_5	C8 C4 CL1	Not unusual (enough hits	437	119.791	119.088	2.36	0.298	0.703	96.671	128.568	119.178	0	
angle	00000001_5	C6 C5 N6	Not unusual (enough hits	225	120.651	123.744	1.746	1.772	3.093	117.703	127.597	124.357	0.03	
angle	00000001_5	C7 C6 C5	Not unusual (enough hits	495	117.629	117.075	1.499	0.37	0.555	105.829	123.29	116.994	0.004	
angle	00000001_5	C9 C6 C5	Not unusual (enough hits	155	122.575	121.018	1.641	0.948	1.556	113.768	126.783	120.987	0.005	
angle	00000001_5	C9 C6 C7	Not unusual (enough hits	10997	119.793	120.774	1.905	0.515	0.981	90.622	143.824	120.777	0	
angle	00000001_5	C8 C7 C6	Not unusual (enough hits	11395	120.305	121.039	1.437	0.511	0.735	93.35	147.791	121.028	0	
angle	00000001_5	C7 C8 C4	Not unusual (enough hits	289	118.353	117.43	0.964	0.957	0.922	114.685	123.178	117.353	0.034	
angle	00000001_5	C1 N2 N1	Unusual (enough hits)	38	133.765	116.494	1.659	10.413	17.271	113.273	119.271	116.712	14.494	
angle	00000001_5	C9 N3 C1	Unusual (enough hits)	15	128.603	124.917	0.706	5.22	3.685	123.364	126.201	124.859	2.401	
angle	00000001_5	N4 C1 N2	Unusual (enough hits)	15	125.459	132.6	1.547	4.615	7.141	128.968	134.4	133.08	3.509	
angle	00000001_5	C8 C4 N6	Unusual (enough hits)	167	120.953	124.711	1.675	2.243	3.758	117.068	127.876	125.155	0.13	
angle	00000001_5	C5 N6 C4	Unusual (enough hits)	179	122.108	116.435	1.303	4.355	5.673	112.785	121.37	116.186	0.738	
angle	00000001_5	C6 C9 N3	Unusual (enough hits)	764	117.637	113.088	1.717	2.65	4.55	104.07	122.755	113.045	0.305	
torsion	00000001_1	O1 N1 N2 C1	Not unusual (enough hits	382	−179.81								0.005	0.479
torsion	00000001_1	O2 N1 N2 C1	Not unusual (enough hits	382	0.08								0.03	0.463
torsion	00000001_1	N3 C1 N2 N1	Not unusual (enough hits	66	−179.814								0.068	0.833
torsion	00000001_1	N4 C1 N2 N1	Not unusual (enough hits	40	0.723								0.004	0.7
torsion	00000001_1	C6 C9 N3 C1	Not unusual (enough hits	48	87.381								0.025	0.188
torsion	00000001_1	C6 C9 N3 C3	Not unusual (enough hits	182	−92.374								1.023	0.11
torsion	00000001_1	C5 C6 C9 N3	Not unusual (enough hits	349	60.183								0.093	0.163
torsion	00000001_1	C7 C6 C9 N3	Not unusual (enough hits	10853	−119.769								0.002	0.135
torsion	00000001_2	O1 N1 N2 C1	Not unusual (enough hits	382	179.978								0.017	0.476
torsion	00000001_2	O2 N1 N2 C1	Not unusual (enough hits	382	0.037								0.002	0.461
torsion	00000001_2	N3 C1 N2 N1	Not unusual (enough hits	66	−179.12								0.017	0.833
torsion	00000001_2	N4 C1 N2 N1	Not unusual (enough hits	40	1.576								0.084	0.7
torsion	00000001_2	C6 C9 N3 C1	Not unusual (enough hits	48	82.332								2.318	0.125
torsion	00000001_2	C6 C9 N3 C3	Not unusual (enough hits	182	−97.056								0.844	0.082
torsion	00000001_2	C5 C6 C9 N3	Not unusual (enough hits	349	26.521								0.066	0.1
torsion	00000001_2	C7 C6 C9 N3	Not unusual (enough hits	10853	−153.609								0.009	0.103
torsion	00000001_3	O1 N1 N2 C1	Not unusual (enough hits	382	179.816								0.001	0.479
torsion	00000001_3	O2 N1 N2 C1	Not unusual (enough hits	382	−0.463								0.011	0.466
torsion	00000001_3	N3 C1 N2 N1	Not unusual (enough hits	66	−179.906								0.002	0.833
torsion	00000001_3	N4 C1 N2 N1	Not unusual (enough hits	40	0.608								0.119	0.7
torsion	00000001_3	C6 C9 N3 C1	Not unusual (enough hits	48	83.938								3.419	0.146
torsion	00000001_3	C6 C9 N3 C3	Not unusual (enough hits	182	−95.599								0.26	0.082

torsion	00000001_3	C5 C6 C9 N3	Not unusual (enough hits	349	66.584								0.108	0.14
torsion	00000001_3	C7 C6 C9 N3	Not unusual (enough hits	10853	−112.877								0.002	0.129
torsion	00000001_4	O1 N1 N2 C1	Not unusual (enough hits	382	−179.204								0.062	0.482
torsion	00000001_4	O2 N1 N2 C1	Not unusual (enough hits	382	1.64								0.005	0.474
torsion	00000001_4	N3 C1 N2 N1	Not unusual (enough hits	66	179.783								0.099	0.833
torsion	00000001_4	N4 C1 N2 N1	Not unusual (enough hits	40	−1.887								0.006	0.7
torsion	00000001_4	C6 C9 N3 C1	Not unusual (enough hits	48	82.986								2.972	0.146
torsion	00000001_4	C6 C9 N3 C3	Not unusual (enough hits	182	−97.926								1.714	0.082
torsion	00000001_4	C5 C6 C9 N3	Not unusual (enough hits	349	62.598								0.332	0.152
torsion	00000001_4	C7 C6 C9 N3	Not unusual (enough hits	10853	−117.828								0.003	0.135
torsion	00000001_5	O1 N1 N2 C1	Not unusual (enough hits	382	−179.301								0.022	0.482
torsion	00000001_5	O2 N1 N2 C1	Not unusual (enough hits	382	1.035								0.044	0.466
torsion	00000001_5	N3 C1 N2 N1	Not unusual (enough hits	66	−179.999								0.091	0.818
torsion	00000001_5	N4 C1 N2 N1	Not unusual (enough hits	40	−0.668								0.059	0.7
torsion	00000001_5	C6 C9 N3 C1	Not unusual (enough hits	48	80.268								0.254	0.104
torsion	00000001_5	C6 C9 N3 C3	Not unusual (enough hits	182	−100.313								0.851	0.066
torsion	00000001_5	C5 C6 C9 N3	Not unusual (enough hits	349	61.752								0.032	0.158
torsion	00000001_5	C7 C6 C9 N3	Not unusual (enough hits	10853	−118.906								0.003	0.135
ring	00000001_1	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.687	16.38			0.771
ring	00000001_1	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.059	8.312			1
ring	00000001_2	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.656	16.354			0.771
ring	00000001_2	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.027	8.369			1
ring	00000001_3	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.591	16.32			0.771
ring	00000001_3	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.06	8.321			1
ring	00000001_4	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.374	16.214			0.771
ring	00000001_4	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.08	8.291			1
ring	00000001_5	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.553	16.336			0.771
ring	00000001_5	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.073	8.245			1

Table 3. Geometry Analysis by Mogul of Clothianidin in Complex with Wild-Type *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	|z-score|	|x - mean|	Minimum	Maximum	Median	|d(min)|	Local density
bond	00000001_1	C1 N	Not unusual (enough hits	1811	1.457	1.448	0.028	0.342	0.01	1.141	1.787	1.446	0	
bond	00000001_1	C N2	Not unusual (enough hits	24	1.327	1.351	0.014	1.766	0.024	1.314	1.377	1.353	0.01	
bond	00000001_1	C3 N1	Not unusual (enough hits	2631	1.454	1.452	0.017	0.122	0.002	1.243	1.584	1.452	0	
bond	00000001_1	N2 N5	Not unusual (enough hits	218	1.356	1.342	0.035	0.402	0.014	1.286	1.462	1.336	0	
bond	00000001_1	C1 C2	Not unusual (enough hits	15	1.501	1.499	0.011	0.198	0.002	1.483	1.52	1.5	0.001	
bond	00000001_1	C2 S	Not unusual (enough hits	496	1.722	1.727	0.034	0.157	0.005	1.424	1.854	1.727	0	
bond	00000001_1	C4 S	Not unusual (enough hits	28	1.703	1.717	0.008	1.84	0.014	1.7	1.733	1.716	0.003	
bond	00000001_1	C4 CL	Not unusual (enough hits	34	1.711	1.713	0.005	0.441	0.002	1.703	1.721	1.715	0	
bond	00000001_1	C5 N4	Not unusual (enough hits	384	1.38	1.369	0.018	0.615	0.011	1.304	1.426	1.371	0	
bond	00000001_1	O1 N5	Not unusual (enough hits	476	1.25	1.241	0.019	0.469	0.009	1.169	1.356	1.241	0	
bond	00000001_1	O2 N5	Not unusual (enough hits	476	1.257	1.241	0.019	0.848	0.016	1.169	1.356	1.241	0	
bond	00000001_1	C N	Unusual (enough hits)	57	1.387	1.334	0.026	2.012	0.052	1.174	1.371	1.335	0.016	
bond	00000001_1	C N1	Unusual (enough hits)	32	1.389	1.327	0.025	2.514	0.063	1.22	1.379	1.329	0.01	
bond	00000001_1	C5 C2	Unusual (enough hits)	32	1.388	1.348	0.01	4.122	0.04	1.318	1.366	1.349	0.022	
bond	00000001_1	C4 N4	Unusual (enough hits)	25	1.313	1.282	0.007	4.368	0.031	1.267	1.297	1.281	0.016	
bond	00000001_2	C1 N	Not unusual (enough hits	1811	1.446	1.448	0.028	0.059	0.002	1.141	1.787	1.446	0	
bond	00000001_2	C N2	Not unusual (enough hits	24	1.332	1.351	0.014	1.402	0.019	1.314	1.377	1.353	0.005	
bond	00000001_2	C3 N1	Not unusual (enough hits	2631	1.452	1.452	0.017	0.024	0	1.243	1.584	1.452	0	
bond	00000001_2	N2 N5	Not unusual (enough hits	218	1.37	1.342	0.035	0.815	0.028	1.286	1.462	1.336	0	
bond	00000001_2	C1 C2	Not unusual (enough hits	15	1.497	1.499	0.011	0.199	0.002	1.483	1.52	1.5	0	
bond	00000001_2	C2 S	Not unusual (enough hits	496	1.709	1.727	0.034	0.539	0.018	1.424	1.854	1.727	0	
bond	00000001_2	C4 CL	Not unusual (enough hits	34	1.707	1.713	0.005	1.395	0.007	1.703	1.721	1.715	0	
bond	00000001_2	C5 N4	Not unusual (enough hits	384	1.385	1.369	0.018	0.877	0.016	1.304	1.426	1.371	0	
bond	00000001_2	O1 N5	Not unusual (enough hits	476	1.252	1.241	0.019	0.586	0.011	1.169	1.356	1.241	0	
bond	00000001_2	O2 N5	Not unusual (enough hits	476	1.256	1.241	0.019	0.797	0.015	1.169	1.356	1.241	0	
bond	00000001_2	C N	Unusual (enough hits)	57	1.388	1.334	0.026	2.04	0.053	1.174	1.371	1.335	0.017	
bond	00000001_2	C N1	Unusual (enough hits)	32	1.387	1.327	0.025	2.413	0.06	1.22	1.379	1.329	0.008	
bond	00000001_2	C5 C2	Unusual (enough hits)	32	1.391	1.348	0.01	4.468	0.043	1.318	1.366	1.349	0.025	
bond	00000001_2	C4 S	Unusual (enough hits)	28	1.699	1.717	0.008	2.355	0.018	1.7	1.733	1.716	0.001	
bond	00000001_2	C4 N4	Unusual (enough hits)	25	1.317	1.282	0.007	4.965	0.035	1.267	1.297	1.281	0.02	
bond	00000001_3	C N	Not unusual (enough hits	57	1.364	1.334	0.026	1.136	0.03	1.174	1.371	1.335	0.001	
bond	00000001_3	C1 N	Not unusual (enough hits	1811	1.441	1.448	0.028	0.221	0.006	1.141	1.787	1.446	0	
bond	00000001_3	C3 N1	Not unusual (enough hits	2631	1.453	1.452	0.017	0.077	0.001	1.243	1.584	1.452	0	
bond	00000001_3	N2 N5	Not unusual (enough hits	218	1.344	1.342	0.035	0.066	0.002	1.286	1.462	1.336	0	
bond	00000001_3	C1 C2	Not unusual (enough hits	15	1.485	1.499	0.011	1.394	0.015	1.483	1.52	1.5	0	
bond	00000001_3	C2 S	Not unusual (enough hits	496	1.707	1.727	0.034	0.601	0.02	1.424	1.854	1.727	0	
bond	00000001_3	C5 N4	Not unusual (enough hits	384	1.373	1.369	0.018	0.204	0.004	1.304	1.426	1.371	0	
bond	00000001_3	O1 N5	Not unusual (enough hits	476	1.253	1.241	0.019	0.62	0.012	1.169	1.356	1.241	0	
bond	00000001_3	O2 N5	Not unusual (enough hits	476	1.25	1.241	0.019	0.497	0.01	1.169	1.356	1.241	0	
bond	00000001_3	C N1	Unusual (enough hits)	32	1.39	1.327	0.025	2.563	0.064	1.22	1.379	1.329	0.012	
bond	00000001_3	C N2	Unusual (enough hits)	24	1.317	1.351	0.014	2.514	0.034	1.314	1.377	1.353	0.003	
bond	00000001_3	C5 C2	Unusual (enough hits)	32	1.385	1.348	0.01	3.832	0.037	1.318	1.366	1.349	0.019	
bond	00000001_3	C4 S	Unusual (enough hits)	28	1.683	1.717	0.008	4.518	0.034	1.7	1.733	1.716	0.017	

bond	00000001_3	C4 N4	Unusual (enough hits)	25	1.312	1.282	0.007	4.237	0.03	1.267	1.297	1.281	0.015	
bond	00000001_3	C4 CL	Unusual (enough hits)	34	1.697	1.713	0.005	3.294	0.016	1.703	1.721	1.715	0.005	
bond	00000001_4	C1 N	Not unusual (enough hits	1811	1.455	1.448	0.028	0.248	0.007	1.141	1.787	1.446	0	
bond	00000001_4	C N2	Not unusual (enough hits	24	1.329	1.351	0.014	1.614	0.022	1.314	1.377	1.353	0.008	
bond	00000001_4	C3 N1	Not unusual (enough hits	2631	1.45	1.452	0.017	0.14	0.002	1.243	1.584	1.452	0	
bond	00000001_4	N2 N5	Not unusual (enough hits	218	1.354	1.342	0.035	0.34	0.012	1.286	1.462	1.336	0	
bond	00000001_4	C1 C2	Not unusual (enough hits	15	1.486	1.499	0.011	1.289	0.014	1.483	1.52	1.5	0	
bond	00000001_4	C2 S	Not unusual (enough hits	496	1.71	1.727	0.034	0.504	0.017	1.424	1.854	1.727	0	
bond	00000001_4	C5 N4	Not unusual (enough hits	384	1.375	1.369	0.018	0.313	0.006	1.304	1.426	1.371	0	
bond	00000001_4	O1 N5	Not unusual (enough hits	476	1.25	1.241	0.019	0.455	0.009	1.169	1.356	1.241	0	
bond	00000001_4	O2 N5	Not unusual (enough hits	476	1.25	1.241	0.019	0.487	0.009	1.169	1.356	1.241	0	
bond	00000001_4	C N	Unusual (enough hits)	57	1.393	1.334	0.026	2.255	0.059	1.174	1.371	1.335	0.022	
bond	00000001_4	C N1	Unusual (enough hits)	32	1.389	1.327	0.025	2.485	0.062	1.22	1.379	1.329	0.01	
bond	00000001_4	C5 C2	Unusual (enough hits)	32	1.382	1.348	0.01	3.453	0.033	1.318	1.366	1.349	0.015	
bond	00000001_4	C4 S	Unusual (enough hits)	28	1.694	1.717	0.008	3.068	0.023	1.7	1.733	1.716	0.006	
bond	00000001_4	C4 N4	Unusual (enough hits)	25	1.313	1.282	0.007	4.38	0.031	1.267	1.297	1.281	0.016	
bond	00000001_4	C4 CL	Unusual (enough hits)	34	1.699	1.713	0.005	3.001	0.014	1.703	1.721	1.715	0.004	
bond	00000001_5	C N	Not unusual (enough hits	57	1.372	1.334	0.026	1.447	0.038	1.174	1.371	1.335	0.001	
bond	00000001_5	C1 N	Not unusual (enough hits	1811	1.455	1.448	0.028	0.247	0.007	1.141	1.787	1.446	0	
bond	00000001_5	C3 N1	Not unusual (enough hits	2631	1.449	1.452	0.017	0.204	0.004	1.243	1.584	1.452	0	
bond	00000001_5	N2 N5	Not unusual (enough hits	218	1.346	1.342	0.035	0.116	0.004	1.286	1.462	1.336	0	
bond	00000001_5	C1 C2	Not unusual (enough hits	15	1.497	1.499	0.011	0.264	0.003	1.483	1.52	1.5	0.001	
bond	00000001_5	C2 S	Not unusual (enough hits	496	1.709	1.727	0.034	0.536	0.018	1.424	1.854	1.727	0	
bond	00000001_5	C5 N4	Not unusual (enough hits	384	1.376	1.369	0.018	0.366	0.007	1.304	1.426	1.371	0	
bond	00000001_5	O1 N5	Not unusual (enough hits	476	1.262	1.241	0.019	1.079	0.021	1.169	1.356	1.241	0	
bond	00000001_5	O2 N5	Not unusual (enough hits	476	1.258	1.241	0.019	0.872	0.017	1.169	1.356	1.241	0	
bond	00000001_5	C N1	Unusual (enough hits)	32	1.394	1.327	0.025	2.723	0.068	1.22	1.379	1.329	0.016	
bond	00000001_5	C N2	Unusual (enough hits)	24	1.313	1.351	0.014	2.841	0.039	1.314	1.377	1.353	0.001	
bond	00000001_5	C5 C2	Unusual (enough hits)	32	1.392	1.348	0.01	4.502	0.043	1.318	1.366	1.349	0.025	
bond	00000001_5	C4 S	Unusual (enough hits)	28	1.686	1.717	0.008	4.053	0.031	1.7	1.733	1.716	0.014	
bond	00000001_5	C4 N4	Unusual (enough hits)	25	1.309	1.282	0.007	3.848	0.027	1.267	1.297	1.281	0.012	
bond	00000001_5	C4 CL	Unusual (enough hits)	34	1.693	1.713	0.005	4.28	0.02	1.703	1.721	1.715	0.01	
angle	00000001_1	C1 N C	Not unusual (enough hits	23	124.476	122.525	0.976	1.999	1.951	119.921	124.647	122.528	0.17	
angle	00000001_1	N C N2	Not unusual (enough hits	17	118.165	116.791	5.244	0.262	1.374	111.877	127.156	113.426	0.276	
angle	00000001_1	C2 C1 N	Not unusual (enough hits	54	114.595	112.659	2.516	0.769	1.935	105.384	119.945	112.805	0.246	
angle	00000001_1	C1 C2 S	Not unusual (enough hits	65	120.765	121.721	1.903	0.502	0.956	116.682	126.834	121.976	0.01	
angle	00000001_1	C5 C2 S	Not unusual (enough hits	28	109.215	108.891	0.338	0.957	0.324	108.29	109.609	108.895	0.054	
angle	00000001_1	C2 S C4	Not unusual (enough hits	25	88.896	88.532	0.254	1.432	0.364	88.113	89.118	88.507	0.051	
angle	00000001_1	CL C4 S	Not unusual (enough hits	28	119.886	120.016	0.787	0.165	0.13	117.738	121.007	120.051	0.024	
angle	00000001_1	CL C4 N4	Not unusual (enough hits	25	122.411	122.906	0.345	1.437	0.496	122.36	123.648	122.862	0.019	
angle	00000001_1	C5 N4 C4	Not unusual (enough hits	25	108.159	108.622	0.389	1.19	0.463	107.984	109.398	108.602	0.003	
angle	00000001_1	O1 N5 N2	Not unusual (enough hits	430	117.241	119.288	4.121	0.497	2.047	112.759	126.082	117.049	0.025	
angle	00000001_1	O2 N5 N2	Not unusual (enough hits	430	120.729	119.288	4.121	0.35	1.442	112.759	126.082	117.049	0.347	
angle	00000001_1	O2 N5 O1	Not unusual (enough hits	234	122.028	121.526	2.164	0.232	0.502	116.275	131.091	121.113	0.001	
angle	00000001_1	N C N1	Unusual (enough hits)	24	108.309	119.399	1.03	10.767	11.09	118.274	123.867	119.262	9.965	

angle	00000001_1	N1 C N2	Unusual (enough hits)	20	133.519	117.685	6.06	2.613	15.834	111.877	128.566	115.23	4.953	
angle	00000001_1	C3 N1 C	Unusual (enough hits)	31	130.355	123.883	2.525	2.563	6.472	120.489	135.488	123.773	4.398	
angle	00000001_1	C N2 N5	Unusual (enough hits)	24	122.409	117.666	2.009	2.361	4.743	115.027	121.105	117.558	1.305	
angle	00000001_1	C1 C2 C5	Unusual (enough hits)	20	130.02	127.821	0.602	3.656	2.199	126.411	128.891	127.785	1.13	
angle	00000001_1	S C4 N4	Unusual (enough hits)	25	117.703	116.884	0.405	2.023	0.819	116.195	117.616	116.931	0.088	
angle	00000001_1	C2 C5 N4	Unusual (enough hits)	28	116.026	117.048	0.444	2.3	1.022	116.164	117.79	117.046	0.138	
angle	00000001_2	N C N2	Not unusual (enough hits	17	119.673	116.791	5.244	0.55	2.882	111.877	127.156	113.426	0.38	
angle	00000001_2	C N2 N5	Not unusual (enough hits	24	121.419	117.666	2.009	1.868	3.753	115.027	121.105	117.558	0.314	
angle	00000001_2	C2 C1 N	Not unusual (enough hits	54	113.641	112.659	2.516	0.39	0.982	105.384	119.945	112.805	0.047	
angle	00000001_2	C1 C2 S	Not unusual (enough hits	65	119.91	121.721	1.903	0.951	1.81	116.682	126.834	121.976	0.012	
angle	00000001_2	C5 C2 S	Not unusual (enough hits	28	109.3	108.891	0.338	1.207	0.408	108.29	109.609	108.895	0.032	
angle	00000001_2	S C4 N4	Not unusual (enough hits	25	117.347	116.884	0.405	1.143	0.463	116.195	117.616	116.931	0.013	
angle	00000001_2	CL C4 S	Not unusual (enough hits	28	119.65	120.016	0.787	0.465	0.366	117.738	121.007	120.051	0.082	
angle	00000001_2	CL C4 N4	Not unusual (enough hits	25	123.003	122.906	0.345	0.279	0.096	122.36	123.648	122.862	0.011	
angle	00000001_2	C5 N4 C4	Not unusual (enough hits	25	108.098	108.622	0.389	1.346	0.524	107.984	109.398	108.602	0.01	
angle	00000001_2	O1 N5 N2	Not unusual (enough hits	430	118.056	119.288	4.121	0.299	1.231	112.759	126.082	117.049	0.144	
angle	00000001_2	O2 N5 N2	Not unusual (enough hits	430	120.344	119.288	4.121	0.256	1.056	112.759	126.082	117.049	0.039	
angle	00000001_2	O2 N5 O1	Not unusual (enough hits	234	121.6	121.526	2.164	0.034	0.073	116.275	131.091	121.113	0.002	
angle	00000001_2	C1 N C	Unusual (enough hits)	23	125.729	122.525	0.976	3.282	3.203	119.921	124.647	122.528	1.082	
angle	00000001_2	N C N1	Unusual (enough hits)	24	107.312	119.399	1.03	11.735	12.087	118.274	123.867	119.262	10.962	
angle	00000001_2	N1 C N2	Unusual (enough hits)	20	133.011	117.685	6.06	2.529	15.326	111.877	128.566	115.23	4.445	
angle	00000001_2	C3 N1 C	Unusual (enough hits)	31	129.789	123.883	2.525	2.339	5.906	120.489	135.488	123.773	3.832	
angle	00000001_2	C1 C2 C5	Unusual (enough hits)	20	130.79	127.821	0.602	4.935	2.969	126.411	128.891	127.785	1.899	
angle	00000001_2	C2 S C4	Unusual (enough hits)	25	89.481	88.532	0.254	3.732	0.949	88.113	89.118	88.507	0.363	
angle	00000001_2	C2 C5 N4	Unusual (enough hits)	28	115.774	117.048	0.444	2.868	1.275	116.164	117.79	117.046	0.39	
angle	00000001_3	C1 N C	Not unusual (enough hits	23	123.161	122.525	0.976	0.651	0.636	119.921	124.647	122.528	0.044	
angle	00000001_3	N C N2	Not unusual (enough hits	17	117.462	116.791	5.244	0.128	0.671	111.877	127.156	113.426	0.428	
angle	00000001_3	C2 C1 N	Not unusual (enough hits	54	112.727	112.659	2.516	0.027	0.067	105.384	119.945	112.805	0.046	
angle	00000001_3	C1 C2 S	Not unusual (enough hits	65	120.322	121.721	1.903	0.735	1.398	116.682	126.834	121.976	0.106	
angle	00000001_3	C2 S C4	Not unusual (enough hits	25	88.861	88.532	0.254	1.292	0.329	88.113	89.118	88.507	0.044	
angle	00000001_3	CL C4 S	Not unusual (enough hits	28	119.269	120.016	0.787	0.949	0.747	117.738	121.007	120.051	0.01	
angle	00000001_3	CL C4 N4	Not unusual (enough hits	25	122.636	122.906	0.345	0.785	0.271	122.36	123.648	122.862	0.047	
angle	00000001_3	C5 N4 C4	Not unusual (enough hits	25	107.946	108.622	0.389	1.738	0.677	107.984	109.398	108.602	0.038	
angle	00000001_3	O1 N5 N2	Not unusual (enough hits	430	117.25	119.288	4.121	0.495	2.038	112.759	126.082	117.049	0.035	
angle	00000001_3	O2 N5 N2	Not unusual (enough hits	430	120.221	119.288	4.121	0.226	0.933	112.759	126.082	117.049	0.039	
angle	00000001_3	O2 N5 O1	Not unusual (enough hits	234	122.529	121.526	2.164	0.464	1.003	116.275	131.091	121.113	0.005	
angle	00000001_3	N C N1	Unusual (enough hits)	24	108.573	119.399	1.03	10.51	10.826	118.274	123.867	119.262	9.701	
angle	00000001_3	N1 C N2	Unusual (enough hits)	20	133.963	117.685	6.06	2.686	16.278	111.877	128.566	115.23	5.397	
angle	00000001_3	C3 N1 C	Unusual (enough hits)	31	130.652	123.883	2.525	2.681	6.769	120.489	135.488	123.773	4.695	
angle	00000001_3	C N2 N5	Unusual (enough hits)	24	122.034	117.666	2.009	2.174	4.368	115.027	121.105	117.558	0.93	
angle	00000001_3	C1 C2 C5	Unusual (enough hits)	20	130.057	127.821	0.602	3.717	2.236	126.411	128.891	127.785	1.166	
angle	00000001_3	C5 C2 S	Unusual (enough hits)	28	109.62	108.891	0.338	2.156	0.729	108.29	109.609	108.895	0.011	
angle	00000001_3	S C4 N4	Unusual (enough hits)	25	118.095	116.884	0.405	2.991	1.211	116.195	117.616	116.931	0.479	
angle	00000001_3	C2 C5 N4	Unusual (enough hits)	28	115.478	117.048	0.444	3.535	1.571	116.164	117.79	117.046	0.687	
angle	00000001_4	N C N2	Not unusual (enough hits	17	118.32	116.791	5.244	0.291	1.529	111.877	127.156	113.426	0.121	

angle	00000001_4	C2 C1 N	Not unusual (enough hits	54	114.16	112.659	2.516	0.596	1.5	105.384	119.945	112.805	0.037	
angle	00000001_4	C1 C2 S	Not unusual (enough hits	65	120.507	121.721	1.903	0.638	1.214	116.682	126.834	121.976	0.069	
angle	00000001_4	C5 C2 S	Not unusual (enough hits	28	109.504	108.891	0.338	1.812	0.613	108.29	109.609	108.895	0.105	
angle	00000001_4	C2 S C4	Not unusual (enough hits	25	88.876	88.532	0.254	1.354	0.344	88.113	89.118	88.507	0.06	
angle	00000001_4	CL C4 S	Not unusual (enough hits	28	119.737	120.016	0.787	0.355	0.279	117.738	121.007	120.051	0.001	
angle	00000001_4	CL C4 N4	Not unusual (enough hits	25	122.509	122.906	0.345	1.153	0.398	122.36	123.648	122.862	0.011	
angle	00000001_4	C5 N4 C4	Not unusual (enough hits	25	107.917	108.622	0.389	1.811	0.705	107.984	109.398	108.602	0.066	
angle	00000001_4	O1 N5 N2	Not unusual (enough hits	430	117.561	119.288	4.121	0.419	1.727	112.759	126.082	117.049	0.014	
angle	00000001_4	O2 N5 N2	Not unusual (enough hits	430	120.404	119.288	4.121	0.271	1.116	112.759	126.082	117.049	0.021	
angle	00000001_4	O2 N5 O1	Not unusual (enough hits	234	122.032	121.526	2.164	0.234	0.506	116.275	131.091	121.113	0.003	
angle	00000001_4	C1 N C	Unusual (enough hits)	23	124.487	122.525	0.976	2.009	1.962	119.921	124.647	122.528	0.16	
angle	00000001_4	N C N1	Unusual (enough hits)	24	108.199	119.399	1.03	10.874	11.2	118.274	123.867	119.262	10.075	
angle	00000001_4	N1 C N2	Unusual (enough hits)	20	133.48	117.685	6.06	2.606	15.795	111.877	128.566	115.23	4.914	
angle	00000001_4	C3 N1 C	Unusual (enough hits)	31	130.175	123.883	2.525	2.492	6.292	120.489	135.488	123.773	4.218	
angle	00000001_4	C N2 N5	Unusual (enough hits)	24	122.621	117.666	2.009	2.466	4.955	115.027	121.105	117.558	1.516	
angle	00000001_4	C1 C2 C5	Unusual (enough hits)	20	129.989	127.821	0.602	3.604	2.168	126.411	128.891	127.785	1.098	
angle	00000001_4	S C4 N4	Unusual (enough hits)	25	117.754	116.884	0.405	2.149	0.87	116.195	117.616	116.931	0.139	
angle	00000001_4	C2 C5 N4	Unusual (enough hits)	28	115.948	117.048	0.444	2.477	1.101	116.164	117.79	117.046	0.217	
angle	00000001_5	C1 N C	Not unusual (enough hits	23	122.96	122.525	0.976	0.445	0.434	119.921	124.647	122.528	0.078	
angle	00000001_5	N C N2	Not unusual (enough hits	17	117.109	116.791	5.244	0.061	0.318	111.877	127.156	113.426	0.075	
angle	00000001_5	C2 C1 N	Not unusual (enough hits	54	113.392	112.659	2.516	0.291	0.732	105.384	119.945	112.805	0.032	
angle	00000001_5	C1 C2 S	Not unusual (enough hits	65	120.507	121.721	1.903	0.638	1.214	116.682	126.834	121.976	0.069	
angle	00000001_5	C5 C2 S	Not unusual (enough hits	28	109.011	108.891	0.338	0.353	0.119	108.29	109.609	108.895	0.012	
angle	00000001_5	CL C4 S	Not unusual (enough hits	28	119.467	120.016	0.787	0.698	0.549	117.738	121.007	120.051	0.029	
angle	00000001_5	CL C4 N4	Not unusual (enough hits	25	122.735	122.906	0.345	0.497	0.171	122.36	123.648	122.862	0.001	
angle	00000001_5	C5 N4 C4	Not unusual (enough hits	25	108.161	108.622	0.389	1.184	0.461	107.984	109.398	108.602	0.005	
angle	00000001_5	O1 N5 N2	Not unusual (enough hits	430	117.04	119.288	4.121	0.545	2.248	112.759	126.082	117.049	0.009	
angle	00000001_5	O2 N5 N2	Not unusual (enough hits	430	120.174	119.288	4.121	0.215	0.886	112.759	126.082	117.049	0.087	
angle	00000001_5	O2 N5 O1	Not unusual (enough hits	234	122.786	121.526	2.164	0.582	1.26	116.275	131.091	121.113	0.038	
angle	00000001_5	N C N1	Unusual (enough hits)	24	109.588	119.399	1.03	9.526	9.811	118.274	123.867	119.262	8.686	
angle	00000001_5	N1 C N2	Unusual (enough hits)	20	133.303	117.685	6.06	2.577	15.619	111.877	128.566	115.23	4.737	
angle	00000001_5	C3 N1 C	Unusual (enough hits)	31	131.44	123.883	2.525	2.993	7.557	120.489	135.488	123.773	4.048	
angle	00000001_5	C N2 N5	Unusual (enough hits)	24	122.121	117.666	2.009	2.217	4.454	115.027	121.105	117.558	1.016	
angle	00000001_5	C1 C2 C5	Unusual (enough hits)	20	130.482	127.821	0.602	4.423	2.661	126.411	128.891	127.785	1.591	
angle	00000001_5	C2 S C4	Unusual (enough hits)	25	89.342	88.532	0.254	3.185	0.81	88.113	89.118	88.507	0.224	
angle	00000001_5	S C4 N4	Unusual (enough hits)	25	117.798	116.884	0.405	2.257	0.914	116.195	117.616	116.931	0.182	
angle	00000001_5	C2 C5 N4	Unusual (enough hits)	28	115.688	117.048	0.444	3.061	1.361	116.164	117.79	117.046	0.476	
torsion	00000001_1	N1 C N C1	Not unusual (enough hits	46	−179.866								0.004	0.565
torsion	00000001_1	N2 C N C1	Not unusual (enough hits	49	−0.719								0.045	0.531
torsion	00000001_1	C2 C1 N C	Not unusual (enough hits	53	106.173								4.229	0.113
torsion	00000001_1	N C N1 C3	Not unusual (enough hits	132	−0.709								0.027	0.379
torsion	00000001_1	N2 C N1 C3	Not unusual (enough hits	31	−179.671								0.008	0.613
torsion	00000001_1	N C N2 N5	Not unusual (enough hits	38	−179.884								0.011	0.789
torsion	00000001_1	N1 C N2 N5	Not unusual (enough hits	38	−1.001								0.144	0.211
torsion	00000001_1	O1 N5 N2 C	Not unusual (enough hits	382	−179.56								0.01	0.482

torsion	00000001_1	O2 N5 N2 C	Not unusual (enough hits	382	0.935								0.005	0.466
torsion	00000001_1	S C2 C1 N	Unusual (enough hits)	59	−178.381								46.258	0
torsion	00000001_1	C5 C2 C1 N	Unusual (enough hits)	133	1.761								0.912	0.03
torsion	00000001_2	N1 C N C1	Not unusual (enough hits	46	179.777								0	0.565
torsion	00000001_2	N2 C N C1	Not unusual (enough hits	49	0.378								0.059	0.531
torsion	00000001_2	C2 C1 N C	Not unusual (enough hits	53	105.549								3.605	0.113
torsion	00000001_2	N C N1 C3	Not unusual (enough hits	132	0.042								0.017	0.379
torsion	00000001_2	N2 C N1 C3	Not unusual (enough hits	31	179.327								0.017	0.613
torsion	00000001_2	N C N2 N5	Not unusual (enough hits	38	179.666								0.179	0.789
torsion	00000001_2	N1 C N2 N5	Not unusual (enough hits	38	0.452								0.314	0.211
torsion	00000001_2	O1 N5 N2 C	Not unusual (enough hits	382	−179.756								0.029	0.479
torsion	00000001_2	O2 N5 N2 C	Not unusual (enough hits	382	−0.033								0.001	0.461
torsion	00000001_2	S C2 C1 N	Unusual (enough hits)	59	−174.714								42.591	0
torsion	00000001_2	C5 C2 C1 N	Unusual (enough hits)	133	5.134								1.548	0.03
torsion	00000001_3	N1 C N C1	Not unusual (enough hits	46	−179.643								0.006	0.565
torsion	00000001_3	N2 C N C1	Not unusual (enough hits	49	−0.081								0.067	0.531
torsion	00000001_3	C2 C1 N C	Not unusual (enough hits	53	106.902								4.164	0.113
torsion	00000001_3	N C N1 C3	Not unusual (enough hits	132	−0.198								0.172	0.379
torsion	00000001_3	N2 C N1 C3	Not unusual (enough hits	31	−179.658								0.005	0.613
torsion	00000001_3	N C N2 N5	Not unusual (enough hits	38	−179.858								0.015	0.789
torsion	00000001_3	N1 C N2 N5	Not unusual (enough hits	38	−0.435								0.298	0.211
torsion	00000001_3	O1 N5 N2 C	Not unusual (enough hits	382	−179.42								0.009	0.482
torsion	00000001_3	O2 N5 N2 C	Not unusual (enough hits	382	0.566								0.002	0.466
torsion	00000001_3	S C2 C1 N	Unusual (enough hits)	59	176.384								44.262	0
torsion	00000001_3	C5 C2 C1 N	Unusual (enough hits)	133	−3.31								0.03	0.03
torsion	00000001_4	N1 C N C1	Not unusual (enough hits	46	179.514								0.036	0.587
torsion	00000001_4	N2 C N C1	Not unusual (enough hits	49	−0.116								0.033	0.531
torsion	00000001_4	C2 C1 N C	Not unusual (enough hits	53	106.645								4.421	0.113
torsion	00000001_4	N C N1 C3	Not unusual (enough hits	132	−0.014								0.011	0.379
torsion	00000001_4	N2 C N1 C3	Not unusual (enough hits	31	179.537								0.126	0.613
torsion	00000001_4	N C N2 N5	Not unusual (enough hits	38	179.212								0.181	0.789
torsion	00000001_4	N1 C N2 N5	Not unusual (enough hits	38	−0.305								0.167	0.211
torsion	00000001_4	O1 N5 N2 C	Not unusual (enough hits	382	−179.827								0	0.479
torsion	00000001_4	O2 N5 N2 C	Not unusual (enough hits	382	−0.428								0.002	0.466
torsion	00000001_4	S C2 C1 N	Unusual (enough hits)	59	−166.831								34.708	0
torsion	00000001_4	C5 C2 C1 N	Unusual (enough hits)	133	13.31								5.496	0.015
torsion	00000001_5	N1 C N C1	Not unusual (enough hits	46	−179.669								0.005	0.565
torsion	00000001_5	N2 C N C1	Not unusual (enough hits	49	0.237								0.03	0.531
torsion	00000001_5	C2 C1 N C	Not unusual (enough hits	53	104.795								2.851	0.113
torsion	00000001_5	N C N1 C3	Not unusual (enough hits	132	0.048								0.022	0.379
torsion	00000001_5	N2 C N1 C3	Not unusual (enough hits	31	−179.837								0.019	0.613
torsion	00000001_5	N C N2 N5	Not unusual (enough hits	38	−179.692								0.181	0.789
torsion	00000001_5	N1 C N2 N5	Not unusual (enough hits	38	0.186								0.049	0.211
torsion	00000001_5	O1 N5 N2 C	Not unusual (enough hits	382	−179.693								0.032	0.482
torsion	00000001_5	O2 N5 N2 C	Not unusual (enough hits	382	0.358								0.007	0.466

torsion	00000001_5	S C2 C1 N	Unusual (enough hits)	59	150.222								18.099	0
torsion	00000001_5	C5 C2 C1 N	Unusual (enough hits)	133	−29.591								3.017	0.03
ring	00000001_1	C2 S C4 N4 C5	Not unusual (enough hits	56						0.034	1.479			1
ring	00000001_2	C2 S C4 N4 C5	Not unusual (enough hits	56						0.057	1.358			1
ring	00000001_3	C2 S C4 N4 C5	Not unusual (enough hits	56						0.009	1.309			1
ring	00000001_4	C2 S C4 N4 C5	Not unusual (enough hits	56						0.043	1.453			1
ring	00000001_5	C2 S C4 N4 C5	Not unusual (enough hits	56						0.067	1.416			1

Table 4. Geometry Analysis by Mogul of Clothianidin in Complex with Gln55Arg Mutant of *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	| z-score |	| x - mean |	Minimum	Maximum	Median	| d(min) |	Local density
bond	00000001_1	C N	Not unusual (enough hits	57	1.334	1.334	0.026	0.033	0.001	1.174	1.371	1.335	0	
bond	00000001_1	C1 N	Not unusual (enough hits	1811	1.448	1.448	0.028	0.001	0	1.141	1.787	1.446	0	
bond	00000001_1	C N1	Not unusual (enough hits	32	1.326	1.327	0.025	0.026	0.001	1.22	1.379	1.329	0.001	
bond	00000001_1	C N2	Not unusual (enough hits	24	1.349	1.351	0.014	0.169	0.002	1.314	1.377	1.353	0.001	
bond	00000001_1	C3 N1	Not unusual (enough hits	2631	1.447	1.452	0.017	0.314	0.005	1.243	1.584	1.452	0	
bond	00000001_1	N2 N5	Not unusual (enough hits	218	1.283	1.342	0.035	1.703	0.059	1.286	1.462	1.336	0.004	
bond	00000001_1	C2 S	Not unusual (enough hits	496	1.714	1.727	0.034	0.409	0.014	1.424	1.854	1.727	0	
bond	00000001_1	C5 C2	Not unusual (enough hits	32	1.345	1.348	0.01	0.38	0.004	1.318	1.366	1.349	0	
bond	00000001_1	C4 S	Not unusual (enough hits	28	1.711	1.717	0.008	0.795	0.006	1.7	1.733	1.716	0	
bond	00000001_1	C4 N4	Not unusual (enough hits	25	1.278	1.282	0.007	0.533	0.004	1.267	1.297	1.281	0	
bond	00000001_1	C4 CL	Not unusual (enough hits	34	1.712	1.713	0.005	0.27	0.001	1.703	1.721	1.715	0.001	
bond	00000001_1	C5 N4	Not unusual (enough hits	384	1.365	1.369	0.018	0.216	0.004	1.304	1.426	1.371	0	
bond	00000001_1	O1 N5	Not unusual (enough hits	476	1.238	1.241	0.019	0.17	0.003	1.169	1.356	1.241	0	
bond	00000001_1	O2 N5	Not unusual (enough hits	476	1.234	1.241	0.019	0.366	0.007	1.169	1.356	1.241	0	
bond	00000001_1	C1 C2	Unusual (enough hits)	15	1.417	1.499	0.011	7.828	0.083	1.483	1.52	1.5	0.067	
bond	00000001_2	C N	Not unusual (enough hits	57	1.331	1.334	0.026	0.118	0.003	1.174	1.371	1.335	0	
bond	00000001_2	C1 N	Not unusual (enough hits	1811	1.444	1.448	0.028	0.142	0.004	1.141	1.787	1.446	0	
bond	00000001_2	C N1	Not unusual (enough hits	32	1.329	1.327	0.025	0.11	0.003	1.22	1.379	1.329	0	
bond	00000001_2	C N2	Not unusual (enough hits	24	1.354	1.351	0.014	0.213	0.003	1.314	1.377	1.353	0.001	
bond	00000001_2	C3 N1	Not unusual (enough hits	2631	1.45	1.452	0.017	0.098	0.002	1.243	1.584	1.452	0	
bond	00000001_2	N2 N5	Not unusual (enough hits	218	1.292	1.342	0.035	1.441	0.05	1.286	1.462	1.336	0.002	
bond	00000001_2	C2 S	Not unusual (enough hits	496	1.705	1.727	0.034	0.673	0.023	1.424	1.854	1.727	0.001	
bond	00000001_2	C5 C2	Not unusual (enough hits	32	1.348	1.348	0.01	0.039	0	1.318	1.366	1.349	0	
bond	00000001_2	C4 S	Not unusual (enough hits	28	1.708	1.717	0.008	1.259	0.01	1.7	1.733	1.716	0	
bond	00000001_2	C4 N4	Not unusual (enough hits	25	1.278	1.282	0.007	0.615	0.004	1.267	1.297	1.281	0	
bond	00000001_2	C4 CL	Not unusual (enough hits	34	1.711	1.713	0.005	0.486	0.002	1.703	1.721	1.715	0	
bond	00000001_2	C5 N4	Not unusual (enough hits	384	1.363	1.369	0.018	0.346	0.006	1.304	1.426	1.371	0	
bond	00000001_2	O1 N5	Not unusual (enough hits	476	1.235	1.241	0.019	0.305	0.006	1.169	1.356	1.241	0	
bond	00000001_2	O2 N5	Not unusual (enough hits	476	1.236	1.241	0.019	0.257	0.005	1.169	1.356	1.241	0	
bond	00000001_2	C1 C2	Unusual (enough hits)	15	1.429	1.499	0.011	6.615	0.07	1.483	1.52	1.5	0.054	
bond	00000001_3	C N	Not unusual (enough hits	57	1.338	1.334	0.026	0.14	0.004	1.174	1.371	1.335	0.001	
bond	00000001_3	C1 N	Not unusual (enough hits	1811	1.445	1.448	0.028	0.092	0.003	1.141	1.787	1.446	0	
bond	00000001_3	C N1	Not unusual (enough hits	32	1.33	1.327	0.025	0.152	0.004	1.22	1.379	1.329	0	
bond	00000001_3	C N2	Not unusual (enough hits	24	1.357	1.351	0.014	0.43	0.006	1.314	1.377	1.353	0	
bond	00000001_3	C3 N1	Not unusual (enough hits	2631	1.453	1.452	0.017	0.025	0	1.243	1.584	1.452	0	
bond	00000001_3	N2 N5	Not unusual (enough hits	218	1.354	1.342	0.035	0.344	0.012	1.286	1.462	1.336	0	
bond	00000001_3	C2 S	Not unusual (enough hits	496	1.723	1.727	0.034	0.141	0.005	1.424	1.854	1.727	0	

bond	00000001_3	C5 C2	Not unusual (enough hits	32	1.349	1.348	0.01	0.114	0.001	1.318	1.366	1.349	0	
bond	00000001_3	C4 S	Not unusual (enough hits	28	1.716	1.717	0.008	0.148	0.001	1.7	1.733	1.716	0	
bond	00000001_3	C4 N4	Not unusual (enough hits	25	1.282	1.282	0.007	0.061	0	1.267	1.297	1.281	0	
bond	00000001_3	C4 CL	Not unusual (enough hits	34	1.714	1.713	0.005	0.123	0.001	1.703	1.721	1.715	0.001	
bond	00000001_3	C5 N4	Not unusual (enough hits	384	1.374	1.369	0.018	0.27	0.005	1.304	1.426	1.371	0	
bond	00000001_3	O1 N5	Not unusual (enough hits	476	1.245	1.241	0.019	0.193	0.004	1.169	1.356	1.241	0	
bond	00000001_3	O2 N5	Not unusual (enough hits	476	1.246	1.241	0.019	0.282	0.005	1.169	1.356	1.241	0	
bond	00000001_3	C1 C2	Unusual (enough hits)	15	1.476	1.499	0.011	2.173	0.023	1.483	1.52	1.5	0.007	
bond	00000001_4	C N	Not unusual (enough hits	57	1.333	1.334	0.026	0.073	0.002	1.174	1.371	1.335	0	
bond	00000001_4	C1 N	Not unusual (enough hits	1811	1.443	1.448	0.028	0.164	0.005	1.141	1.787	1.446	0	
bond	00000001_4	C N1	Not unusual (enough hits	32	1.326	1.327	0.025	0.022	0.001	1.22	1.379	1.329	0.001	
bond	00000001_4	C N2	Not unusual (enough hits	24	1.346	1.351	0.014	0.386	0.005	1.314	1.377	1.353	0	
bond	00000001_4	C3 N1	Not unusual (enough hits	2631	1.447	1.452	0.017	0.277	0.005	1.243	1.584	1.452	0	
bond	00000001_4	N2 N5	Not unusual (enough hits	218	1.31	1.342	0.035	0.936	0.032	1.286	1.462	1.336	0	
bond	00000001_4	C2 S	Not unusual (enough hits	496	1.711	1.727	0.034	0.469	0.016	1.424	1.854	1.727	0	
bond	00000001_4	C5 C2	Not unusual (enough hits	32	1.346	1.348	0.01	0.234	0.002	1.318	1.366	1.349	0	
bond	00000001_4	C4 S	Not unusual (enough hits	28	1.708	1.717	0.008	1.221	0.009	1.7	1.733	1.716	0	
bond	00000001_4	C4 N4	Not unusual (enough hits	25	1.277	1.282	0.007	0.649	0.005	1.267	1.297	1.281	0.001	
bond	00000001_4	C4 CL	Not unusual (enough hits	34	1.712	1.713	0.005	0.266	0.001	1.703	1.721	1.715	0.001	
bond	00000001_4	C5 N4	Not unusual (enough hits	384	1.366	1.369	0.018	0.208	0.004	1.304	1.426	1.371	0	
bond	00000001_4	O1 N5	Not unusual (enough hits	476	1.237	1.241	0.019	0.212	0.004	1.169	1.356	1.241	0	
bond	00000001_4	O2 N5	Not unusual (enough hits	476	1.23	1.241	0.019	0.543	0.01	1.169	1.356	1.241	0	
bond	00000001_4	C1 C2	Unusual (enough hits)	15	1.466	1.499	0.011	3.183	0.034	1.483	1.52	1.5	0.018	
bond	00000001_5	C N	Not unusual (enough hits	57	1.338	1.334	0.026	0.131	0.003	1.174	1.371	1.335	0.001	
bond	00000001_5	C1 N	Not unusual (enough hits	1811	1.444	1.448	0.028	0.115	0.003	1.141	1.787	1.446	0	
bond	00000001_5	C N1	Not unusual (enough hits	32	1.331	1.327	0.025	0.178	0.004	1.22	1.379	1.329	0	
bond	00000001_5	C N2	Not unusual (enough hits	24	1.355	1.351	0.014	0.26	0.004	1.314	1.377	1.353	0	
bond	00000001_5	C3 N1	Not unusual (enough hits	2631	1.452	1.452	0.017	0.007	0	1.243	1.584	1.452	0	
bond	00000001_5	N2 N5	Not unusual (enough hits	218	1.343	1.342	0.035	0.036	0.001	1.286	1.462	1.336	0	
bond	00000001_5	C1 C2	Not unusual (enough hits	15	1.482	1.499	0.011	1.601	0.017	1.483	1.52	1.5	0.001	
bond	00000001_5	C2 S	Not unusual (enough hits	496	1.724	1.727	0.034	0.085	0.003	1.424	1.854	1.727	0	
bond	00000001_5	C5 C2	Not unusual (enough hits	32	1.349	1.348	0.01	0.093	0.001	1.318	1.366	1.349	0	
bond	00000001_5	C4 S	Not unusual (enough hits	28	1.717	1.717	0.008	0.009	0	1.7	1.733	1.716	0	
bond	00000001_5	C4 N4	Not unusual (enough hits	25	1.283	1.282	0.007	0.106	0.001	1.267	1.297	1.281	0.001	
bond	00000001_5	C4 CL	Not unusual (enough hits	34	1.714	1.713	0.005	0.072	0	1.703	1.721	1.715	0.001	
bond	00000001_5	C5 N4	Not unusual (enough hits	384	1.377	1.369	0.018	0.404	0.007	1.304	1.426	1.371	0	
bond	00000001_5	O1 N5	Not unusual (enough hits	476	1.245	1.241	0.019	0.226	0.004	1.169	1.356	1.241	0	
bond	00000001_5	O2 N5	Not unusual (enough hits	476	1.246	1.241	0.019	0.284	0.005	1.169	1.356	1.241	0	
angle	00000001_1	C1 N C	Not unusual (enough hits	23	123.651	122.525	0.976	1.153	1.126	119.921	124.647	122.528	0.077	

angle	00000001_1	N C N1	Not unusual (enough hits	24	119.059	119.399	1.03	0.33	0.34	118.274	123.867	119.262	0.006	
angle	00000001_1	N C N2	Not unusual (enough hits	17	115.208	116.791	5.244	0.302	1.583	111.877	127.156	113.426	1.782	
angle	00000001_1	N1 C N2	Not unusual (enough hits	20	125.699	117.685	6.06	1.322	8.014	111.877	128.566	115.23	0.585	
angle	00000001_1	C3 N1 C	Not unusual (enough hits	31	122.442	123.883	2.525	0.571	1.441	120.489	135.488	123.773	0.1	
angle	00000001_1	C2 C1 N	Not unusual (enough hits	54	110.289	112.659	2.516	0.942	2.371	105.384	119.945	112.805	0.123	
angle	00000001_1	C1 C2 S	Not unusual (enough hits	65	123.168	121.721	1.903	0.76	1.447	116.682	126.834	121.976	0.032	
angle	00000001_1	C1 C2 C5	Not unusual (enough hits	20	127.9	127.821	0.602	0.132	0.079	126.411	128.891	127.785	0.032	
angle	00000001_1	C5 C2 S	Not unusual (enough hits	28	108.88	108.891	0.338	0.033	0.011	108.29	109.609	108.895	0.021	
angle	00000001_1	C2 S C4	Not unusual (enough hits	25	88.474	88.532	0.254	0.23	0.058	88.113	89.118	88.507	0.024	
angle	00000001_1	S C4 N4	Not unusual (enough hits	25	116.781	116.884	0.405	0.253	0.102	116.195	117.616	116.931	0.009	
angle	00000001_1	CL C4 S	Not unusual (enough hits	28	120.171	120.016	0.787	0.197	0.155	117.738	121.007	120.051	0.068	
angle	00000001_1	CL C4 N4	Not unusual (enough hits	25	123.047	122.906	0.345	0.406	0.14	122.36	123.648	122.862	0.033	
angle	00000001_1	C5 N4 C4	Not unusual (enough hits	25	108.657	108.622	0.389	0.09	0.035	107.984	109.398	108.602	0.005	
angle	00000001_1	C2 C5 N4	Not unusual (enough hits	28	117.204	117.048	0.444	0.35	0.156	116.164	117.79	117.046	0.029	
angle	00000001_1	O1 N5 N2	Not unusual (enough hits	430	113.363	119.288	4.121	1.438	5.925	112.759	126.082	117.049	0.048	
angle	00000001_1	O2 N5 N2	Not unusual (enough hits	430	124.679	119.288	4.121	1.308	5.391	112.759	126.082	117.049	0.001	
angle	00000001_1	O2 N5 O1	Not unusual (enough hits	234	121.958	121.526	2.164	0.2	0.432	116.275	131.091	121.113	0.042	
angle	00000001_1	C N2 N5	Unusual (enough hits)	24	122.041	117.666	2.009	2.178	4.375	115.027	121.105	117.558	0.937	
angle	00000001_2	C1 N C	Not unusual (enough hits	23	123.73	122.525	0.976	1.234	1.204	119.921	124.647	122.528	0.156	
angle	00000001_2	N C N1	Not unusual (enough hits	24	118.978	119.399	1.03	0.409	0.421	118.274	123.867	119.262	0.018	
angle	00000001_2	N C N2	Not unusual (enough hits	17	115.009	116.791	5.244	0.34	1.782	111.877	127.156	113.426	1.583	
angle	00000001_2	N1 C N2	Not unusual (enough hits	20	126.002	117.685	6.06	1.372	8.317	111.877	128.566	115.23	0.282	
angle	00000001_2	C3 N1 C	Not unusual (enough hits	31	122.875	123.883	2.525	0.399	1.008	120.489	135.488	123.773	0.053	
angle	00000001_2	C N2 N5	Not unusual (enough hits	24	121.626	117.666	2.009	1.971	3.959	115.027	121.105	117.558	0.521	
angle	00000001_2	C2 C1 N	Not unusual (enough hits	54	107.732	112.659	2.516	1.958	4.927	105.384	119.945	112.805	0.801	
angle	00000001_2	C1 C2 S	Not unusual (enough hits	65	122.629	121.721	1.903	0.477	0.908	116.682	126.834	121.976	0.049	
angle	00000001_2	C1 C2 C5	Not unusual (enough hits	20	128.355	127.821	0.602	0.887	0.534	126.411	128.891	127.785	0.05	
angle	00000001_2	C5 C2 S	Not unusual (enough hits	28	108.94	108.891	0.338	0.142	0.048	108.29	109.609	108.895	0.003	
angle	00000001_2	C2 S C4	Not unusual (enough hits	25	88.581	88.532	0.254	0.193	0.049	88.113	89.118	88.507	0.029	
angle	00000001_2	S C4 N4	Not unusual (enough hits	25	116.868	116.884	0.405	0.039	0.016	116.195	117.616	116.931	0.037	
angle	00000001_2	CL C4 S	Not unusual (enough hits	28	120.066	120.016	0.787	0.063	0.05	117.738	121.007	120.051	0.037	
angle	00000001_2	CL C4 N4	Not unusual (enough hits	25	123.034	122.906	0.345	0.371	0.128	122.36	123.648	122.862	0.021	
angle	00000001_2	C5 N4 C4	Not unusual (enough hits	25	108.508	108.622	0.389	0.294	0.115	107.984	109.398	108.602	0.019	
angle	00000001_2	C2 C5 N4	Not unusual (enough hits	28	117.1	117.048	0.444	0.116	0.052	116.164	117.79	117.046	0.005	
angle	00000001_2	O1 N5 N2	Not unusual (enough hits	430	115.494	119.288	4.121	0.921	3.794	112.759	126.082	117.049	0	
angle	00000001_2	O2 N5 N2	Not unusual (enough hits	430	123.834	119.288	4.121	1.103	4.547	112.759	126.082	117.049	0.003	
angle	00000001_2	O2 N5 O1	Not unusual (enough hits	234	120.665	121.526	2.164	0.398	0.861	116.275	131.091	121.113	0.002	
angle	00000001_3	C1 N C	Not unusual (enough hits	23	123.454	122.525	0.976	0.951	0.929	119.921	124.647	122.528	0.022	
angle	00000001_3	N C N1	Not unusual (enough hits	24	119.099	119.399	1.03	0.291	0.3	118.274	123.867	119.262	0.001	

angle	00000001_3	N C N2	Not unusual (enough hits	17	116.458	116.791	5.244	0.063	0.333	111.877	127.156	113.426	0.576	
angle	00000001_3	N1 C N2	Not unusual (enough hits	20	124.435	117.685	6.06	1.114	6.75	111.877	128.566	115.23	0.551	
angle	00000001_3	C3 N1 C	Not unusual (enough hits	31	123.498	123.883	2.525	0.152	0.385	120.489	135.488	123.773	0.009	
angle	00000001_3	C N2 N5	Not unusual (enough hits	24	119.767	117.666	2.009	1.046	2.101	115.027	121.105	117.558	0.048	
angle	00000001_3	C1 C2 S	Not unusual (enough hits	65	123.294	121.721	1.903	0.827	1.574	116.682	126.834	121.976	0.01	
angle	00000001_3	C1 C2 C5	Not unusual (enough hits	20	127.876	127.821	0.602	0.092	0.056	126.411	128.891	127.785	0.008	
angle	00000001_3	C5 C2 S	Not unusual (enough hits	28	108.816	108.891	0.338	0.223	0.075	108.29	109.609	108.895	0.001	
angle	00000001_3	C2 S C4	Not unusual (enough hits	25	88.497	88.532	0.254	0.139	0.035	88.113	89.118	88.507	0.01	
angle	00000001_3	S C4 N4	Not unusual (enough hits	25	116.902	116.884	0.405	0.046	0.019	116.195	117.616	116.931	0.029	
angle	00000001_3	CL C4 S	Not unusual (enough hits	28	120.048	120.016	0.787	0.041	0.032	117.738	121.007	120.051	0.049	
angle	00000001_3	CL C4 N4	Not unusual (enough hits	25	123.027	122.906	0.345	0.35	0.121	122.36	123.648	122.862	0.013	
angle	00000001_3	C5 N4 C4	Not unusual (enough hits	25	108.63	108.622	0.389	0.019	0.007	107.984	109.398	108.602	0.027	
angle	00000001_3	C2 C5 N4	Not unusual (enough hits	28	117.152	117.048	0.444	0.234	0.104	116.164	117.79	117.046	0.021	
angle	00000001_3	O1 N5 N2	Not unusual (enough hits	430	117.374	119.288	4.121	0.464	1.914	112.759	126.082	117.049	0.024	
angle	00000001_3	O2 N5 N2	Not unusual (enough hits	430	122.199	119.288	4.121	0.706	2.911	112.759	126.082	117.049	0.04	
angle	00000001_3	O2 N5 O1	Not unusual (enough hits	234	120.419	121.526	2.164	0.511	1.107	116.275	131.091	121.113	0.002	
angle	00000001_3	C2 C1 N	Unusual (enough hits)	54	105.755	112.659	2.516	2.744	6.905	105.384	119.945	112.805	0.371	
angle	00000001_4	C1 N C	Not unusual (enough hits	23	122.958	122.525	0.976	0.444	0.433	119.921	124.647	122.528	0.077	
angle	00000001_4	N C N1	Not unusual (enough hits	24	119.003	119.399	1.03	0.384	0.396	118.274	123.867	119.262	0.043	
angle	00000001_4	N C N2	Not unusual (enough hits	17	116.544	116.791	5.244	0.047	0.247	111.877	127.156	113.426	0.491	
angle	00000001_4	N1 C N2	Not unusual (enough hits	20	124.395	117.685	6.06	1.107	6.71	111.877	128.566	115.23	0.511	
angle	00000001_4	C3 N1 C	Not unusual (enough hits	31	122.598	123.883	2.525	0.509	1.285	120.489	135.488	123.773	0.162	
angle	00000001_4	C2 C1 N	Not unusual (enough hits	54	111.398	112.659	2.516	0.501	1.261	105.384	119.945	112.805	0.004	
angle	00000001_4	C1 C2 S	Not unusual (enough hits	65	123.144	121.721	1.903	0.748	1.423	116.682	126.834	121.976	0.008	
angle	00000001_4	C1 C2 C5	Not unusual (enough hits	20	127.952	127.821	0.602	0.218	0.131	126.411	128.891	127.785	0.069	
angle	00000001_4	C5 C2 S	Not unusual (enough hits	28	108.826	108.891	0.338	0.192	0.065	108.29	109.609	108.895	0.005	
angle	00000001_4	C2 S C4	Not unusual (enough hits	25	88.543	88.532	0.254	0.043	0.011	88.113	89.118	88.507	0.036	
angle	00000001_4	S C4 N4	Not unusual (enough hits	25	116.895	116.884	0.405	0.026	0.011	116.195	117.616	116.931	0.036	
angle	00000001_4	CL C4 S	Not unusual (enough hits	28	120.106	120.016	0.787	0.115	0.09	117.738	121.007	120.051	0.003	
angle	00000001_4	CL C4 N4	Not unusual (enough hits	25	122.997	122.906	0.345	0.263	0.091	122.36	123.648	122.862	0.014	
angle	00000001_4	C5 N4 C4	Not unusual (enough hits	25	108.577	108.622	0.389	0.115	0.045	107.984	109.398	108.602	0.023	
angle	00000001_4	C2 C5 N4	Not unusual (enough hits	28	117.156	117.048	0.444	0.242	0.107	116.164	117.79	117.046	0.018	
angle	00000001_4	O1 N5 N2	Not unusual (enough hits	430	115.981	119.288	4.121	0.803	3.307	112.759	126.082	117.049	0.01	
angle	00000001_4	O2 N5 N2	Not unusual (enough hits	430	123.112	119.288	4.121	0.928	3.824	112.759	126.082	117.049	0.002	
angle	00000001_4	O2 N5 O1	Not unusual (enough hits	234	120.652	121.526	2.164	0.404	0.874	116.275	131.091	121.113	0.01	
angle	00000001_4	C N2 N5	Unusual (enough hits)	24	121.917	117.666	2.009	2.116	4.25	115.027	121.105	117.558	0.812	
angle	00000001_5	C1 N C	Not unusual (enough hits	23	122.485	122.525	0.976	0.041	0.04	119.921	124.647	122.528	0.01	
angle	00000001_5	N C N1	Not unusual (enough hits	24	119.158	119.399	1.03	0.234	0.241	118.274	123.867	119.262	0.025	
angle	00000001_5	N C N2	Not unusual (enough hits	17	112.705	116.791	5.244	0.779	4.086	111.877	127.156	113.426	0.115	

angle	00000001_5	N1 C N2	Not unusual (enough hits	20	128.137	117.685	6.06	1.725	10.452	111.877	128.566	115.23	0.429	
angle	00000001_5	C3 N1 C	Not unusual (enough hits	31	123.772	123.883	2.525	0.044	0.111	120.489	135.488	123.773	0.001	
angle	00000001_5	C N2 N5	Not unusual (enough hits	24	120.344	117.666	2.009	1.333	2.678	115.027	121.105	117.558	0.268	
angle	00000001_5	C2 C1 N	Not unusual (enough hits	54	109.661	112.659	2.516	1.192	2.998	105.384	119.945	112.805	0.219	
angle	00000001_5	C1 C2 S	Not unusual (enough hits	65	123.066	121.721	1.903	0.707	1.346	116.682	126.834	121.976	0.033	
angle	00000001_5	C1 C2 C5	Not unusual (enough hits	20	127.946	127.821	0.602	0.208	0.125	126.411	128.891	127.785	0.075	
angle	00000001_5	C5 C2 S	Not unusual (enough hits	28	108.877	108.891	0.338	0.044	0.015	108.29	109.609	108.895	0.017	
angle	00000001_5	C2 S C4	Not unusual (enough hits	25	88.486	88.532	0.254	0.181	0.046	88.113	89.118	88.507	0.021	
angle	00000001_5	S C4 N4	Not unusual (enough hits	25	116.878	116.884	0.405	0.016	0.006	116.195	117.616	116.931	0.047	
angle	00000001_5	CL C4 S	Not unusual (enough hits	28	120.036	120.016	0.787	0.025	0.02	117.738	121.007	120.051	0.037	
angle	00000001_5	CL C4 N4	Not unusual (enough hits	25	123.04	122.906	0.345	0.388	0.134	122.36	123.648	122.862	0.026	
angle	00000001_5	C5 N4 C4	Not unusual (enough hits	25	108.656	108.622	0.389	0.086	0.033	107.984	109.398	108.602	0.007	
angle	00000001_5	C2 C5 N4	Not unusual (enough hits	28	117.088	117.048	0.444	0.09	0.04	116.164	117.79	117.046	0	
angle	00000001_5	O1 N5 N2	Not unusual (enough hits	430	116.425	119.288	4.121	0.695	2.863	112.759	126.082	117.049	0.001	
angle	00000001_5	O2 N5 N2	Not unusual (enough hits	430	122.773	119.288	4.121	0.846	3.485	112.759	126.082	117.049	0.008	
angle	00000001_5	O2 N5 O1	Not unusual (enough hits	234	120.792	121.526	2.164	0.339	0.734	116.275	131.091	121.113	0.003	
torsion	00000001_1	N1 C N C1	Not unusual (enough hits	46	177.781								0.387	0.587
torsion	00000001_1	N2 C N C1	Not unusual (enough hits	49	−4.241								0.052	0.592
torsion	00000001_1	C2 C1 N C	Not unusual (enough hits	53	97.316								1.164	0.226
torsion	00000001_1	N C N1 C3	Not unusual (enough hits	132	−4.261								0.006	0.379
torsion	00000001_1	N2 C N1 C3	Not unusual (enough hits	31	177.992								0.088	0.613
torsion	00000001_1	N C N2 N5	Not unusual (enough hits	38	179.829								0.044	0.789
torsion	00000001_1	N1 C N2 N5	Not unusual (enough hits	38	−2.347								0.266	0.211
torsion	00000001_1	O1 N5 N2 C	Not unusual (enough hits	382	179.064								0.017	0.487
torsion	00000001_1	O2 N5 N2 C	Not unusual (enough hits	382	−0.821								0	0.466
torsion	00000001_1	S C2 C1 N	Unusual (enough hits)	59	−146.703								14.58	0
torsion	00000001_1	C5 C2 C1 N	Unusual (enough hits)	133	36.206								1.12	0.023
torsion	00000001_2	N1 C N C1	Not unusual (enough hits	46	−178.803								0.297	0.587
torsion	00000001_2	N2 C N C1	Not unusual (enough hits	49	2.333								0.112	0.551
torsion	00000001_2	C2 C1 N C	Not unusual (enough hits	53	108.743								2.323	0.113
torsion	00000001_2	N C N1 C3	Not unusual (enough hits	132	0.372								0.346	0.379
torsion	00000001_2	N2 C N1 C3	Not unusual (enough hits	31	179.099								0.091	0.613
torsion	00000001_2	N C N2 N5	Not unusual (enough hits	38	−178.969								0.061	0.789
torsion	00000001_2	N1 C N2 N5	Not unusual (enough hits	38	2.259								0.178	0.211
torsion	00000001_2	O1 N5 N2 C	Not unusual (enough hits	382	179.842								0.003	0.479
torsion	00000001_2	O2 N5 N2 C	Not unusual (enough hits	382	0.767								0.007	0.466
torsion	00000001_2	S C2 C1 N	Unusual (enough hits)	59	169.944								37.821	0
torsion	00000001_2	C5 C2 C1 N	Unusual (enough hits)	133	−6.5								1.314	0.03
torsion	00000001_3	N1 C N C1	Not unusual (enough hits	46	−178.189								0.021	0.587

torsion	00000001_3	N2 C N C1	Not unusual (enough hits	49	2.793								0.206	0.551
torsion	00000001_3	C2 C1 N C	Not unusual (enough hits	53	103.326								1.382	0.132
torsion	00000001_3	N C N1 C3	Not unusual (enough hits	132	−0.193								0.167	0.379
torsion	00000001_3	N2 C N1 C3	Not unusual (enough hits	31	178.741								0.158	0.613
torsion	00000001_3	N C N2 N5	Not unusual (enough hits	38	179.147								0.117	0.789
torsion	00000001_3	N1 C N2 N5	Not unusual (enough hits	38	0.188								0.051	0.211
torsion	00000001_3	O1 N5 N2 C	Not unusual (enough hits	382	179.764								0.021	0.479
torsion	00000001_3	O2 N5 N2 C	Not unusual (enough hits	382	−1.243								0.008	0.466
torsion	00000001_3	S C2 C1 N	Unusual (enough hits)	59	−143.967								11.844	0
torsion	00000001_3	C5 C2 C1 N	Unusual (enough hits)	133	34.566								1.958	0.03
torsion	00000001_4	N1 C N C1	Not unusual (enough hits	46	−179.399								0.079	0.587
torsion	00000001_4	N2 C N C1	Not unusual (enough hits	49	3.255								0.231	0.571
torsion	00000001_4	C2 C1 N C	Not unusual (enough hits	53	100.99								0.669	0.132
torsion	00000001_4	N C N1 C3	Not unusual (enough hits	132	2.468								0.041	0.379
torsion	00000001_4	N2 C N1 C3	Not unusual (enough hits	31	179.59								0.073	0.613
torsion	00000001_4	N C N2 N5	Not unusual (enough hits	38	−178.563								0.005	0.789
torsion	00000001_4	N1 C N2 N5	Not unusual (enough hits	38	4.251								0.394	0.211
torsion	00000001_4	O1 N5 N2 C	Not unusual (enough hits	382	−177.165								0.021	0.495
torsion	00000001_4	O2 N5 N2 C	Not unusual (enough hits	382	8.611								0.115	0.495
torsion	00000001_4	S C2 C1 N	Unusual (enough hits)	59	−149.349								17.226	0
torsion	00000001_4	C5 C2 C1 N	Unusual (enough hits)	133	34.212								1.604	0.03
torsion	00000001_5	N1 C N C1	Not unusual (enough hits	46	−179.957								0.087	0.565
torsion	00000001_5	N2 C N C1	Not unusual (enough hits	49	0.269								0.002	0.531
torsion	00000001_5	C2 C1 N C	Not unusual (enough hits	53	79.322								0.002	0.434
torsion	00000001_5	N C N1 C3	Not unusual (enough hits	132	−1.264								0.128	0.379
torsion	00000001_5	N2 C N1 C3	Not unusual (enough hits	31	178.471								0.053	0.613
torsion	00000001_5	N C N2 N5	Not unusual (enough hits	38	179.208								0.178	0.789
torsion	00000001_5	N1 C N2 N5	Not unusual (enough hits	38	−0.541								0.316	0.211
torsion	00000001_5	O1 N5 N2 C	Not unusual (enough hits	382	179.805								0.001	0.479
torsion	00000001_5	O2 N5 N2 C	Not unusual (enough hits	382	−1.336								0.043	0.466
torsion	00000001_5	S C2 C1 N	Unusual (enough hits)	59	−137.798								5.675	0.017
torsion	00000001_5	C5 C2 C1 N	Unusual (enough hits)	133	46.474								0.714	0.023
ring	00000001_1	C2 S C4 N4 C5	Not unusual (enough hits	56						0.138	1.214			1
ring	00000001_2	C2 S C4 N4 C5	Not unusual (enough hits	56						0.042	1.12			1
ring	00000001_3	C2 S C4 N4 C5	Not unusual (enough hits	56						0.064	1.143			1
ring	00000001_4	C2 S C4 N4 C5	Not unusual (enough hits	56						0.04	1.185			1
ring	00000001_5	C2 S C4 N4 C5	Not unusual (enough hits	56						0.138	1.235			1

Table 5. Geometry Analysis by Mogul of Thiacloprid in Complex with Wild-Type *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	| z-score |	| x - mean |	Minimum	Maximum	Median	| d(min) |	Local density
bond	00000001_1	C11 N4	Not unusual (enough hits	270	1.16	1.154	0.026	0.262	0.007	1.037	1.411	1.153	0	
bond	00000001_1	C8 N21	Not unusual (enough hits	20	1.291	1.31	0.012	1.56	0.019	1.294	1.336	1.309	0.003	
bond	00000001_1	C8 N3	Not unusual (enough hits	18	1.339	1.353	0.03	0.451	0.013	1.321	1.39	1.333	0.006	
bond	00000001_1	C9 N3	Not unusual (enough hits	1978	1.47	1.468	0.023	0.096	0.002	1.336	1.699	1.468	0	
bond	00000001_1	C7 S1	Not unusual (enough hits	1363	1.753	1.803	0.034	1.476	0.05	1.305	1.92	1.808	0.001	
bond	00000001_1	C7 C9	Not unusual (enough hits	329	1.533	1.505	0.028	0.996	0.028	1.349	1.653	1.509	0	
bond	00000001_1	C10 N3	Not unusual (enough hits	931	1.46	1.465	0.015	0.303	0.005	1.386	1.561	1.465	0	
bond	00000001_1	C10 C4	Not unusual (enough hits	10549	1.519	1.51	0.019	0.468	0.009	1.278	1.842	1.51	0	
bond	00000001_1	C3 C4	Not unusual (enough hits	560	1.414	1.381	0.017	1.961	0.033	1.279	1.497	1.382	0	
bond	00000001_1	C3 N2	Not unusual (enough hits	2818	1.364	1.34	0.022	1.046	0.023	1.05	1.584	1.337	0	
bond	00000001_1	C5 C4	Not unusual (enough hits	14050	1.428	1.384	0.022	1.997	0.044	0.618	1.8	1.386	0	
bond	00000001_1	C11 N21	Unusual (enough hits)	236	1.228	1.324	0.018	5.455	0.096	1.266	1.419	1.324	0.039	
bond	00000001_1	C8 S1	Unusual (enough hits)	176	1.668	1.752	0.019	4.419	0.085	1.681	1.81	1.75	0.014	
bond	00000001_1	C6 C5	Unusual (enough hits)	20000	1.422	1.383	0.019	2.112	0.039	0.882	1.685	1.383	0	
bond	00000001_1	C1 N2	Unusual (enough hits)	245	1.384	1.321	0.025	2.478	0.062	1.254	1.422	1.317	0	
bond	00000001_1	C6 C1	Unusual (enough hits)	479	1.42	1.373	0.022	2.169	0.047	1.267	1.455	1.373	0.001	
bond	00000001_1	C1 CL11	Unusual (enough hits)	743	1.79	1.738	0.019	2.799	0.052	1.561	1.806	1.74	0.004	
bond	00000001_2	C11 N4	Not unusual (enough hits	270	1.162	1.154	0.026	0.327	0.008	1.037	1.411	1.153	0	
bond	00000001_2	C8 N21	Not unusual (enough hits	20	1.291	1.31	0.012	1.55	0.019	1.294	1.336	1.309	0.003	
bond	00000001_2	C8 N3	Not unusual (enough hits	18	1.341	1.353	0.03	0.387	0.011	1.321	1.39	1.333	0.008	
bond	00000001_2	C9 N3	Not unusual (enough hits	1978	1.473	1.468	0.023	0.224	0.005	1.336	1.699	1.468	0	
bond	00000001_2	C7 S1	Not unusual (enough hits	1363	1.754	1.803	0.034	1.432	0.048	1.305	1.92	1.808	0	
bond	00000001_2	C7 C9	Not unusual (enough hits	329	1.533	1.505	0.028	0.974	0.028	1.349	1.653	1.509	0	
bond	00000001_2	C10 N3	Not unusual (enough hits	931	1.476	1.465	0.015	0.689	0.011	1.386	1.561	1.465	0	
bond	00000001_2	C10 C4	Not unusual (enough hits	10549	1.525	1.51	0.019	0.796	0.015	1.278	1.842	1.51	0	
bond	00000001_2	C3 C4	Not unusual (enough hits	560	1.413	1.381	0.017	1.932	0.033	1.279	1.497	1.382	0	
bond	00000001_2	C3 N2	Not unusual (enough hits	2818	1.366	1.34	0.022	1.138	0.026	1.05	1.584	1.337	0	
bond	00000001_2	C5 C4	Not unusual (enough hits	14050	1.424	1.384	0.022	1.831	0.04	0.618	1.8	1.386	0	
bond	00000001_2	C11 N21	Unusual (enough hits)	236	1.227	1.324	0.018	5.512	0.097	1.266	1.419	1.324	0.04	
bond	00000001_2	C8 S1	Unusual (enough hits)	176	1.67	1.752	0.019	4.265	0.082	1.681	1.81	1.75	0.011	
bond	00000001_2	C6 C5	Unusual (enough hits)	20000	1.425	1.383	0.019	2.263	0.042	0.882	1.685	1.383	0	
bond	00000001_2	C1 N2	Unusual (enough hits)	245	1.379	1.321	0.025	2.274	0.057	1.254	1.422	1.317	0.001	
bond	00000001_2	C6 C1	Unusual (enough hits)	479	1.42	1.373	0.022	2.175	0.048	1.267	1.455	1.373	0.001	
bond	00000001_2	C1 CL11	Unusual (enough hits)	743	1.797	1.738	0.019	3.187	0.059	1.561	1.806	1.74	0.003	
bond	00000001_3	C11 N4	Not unusual (enough hits	270	1.159	1.154	0.026	0.215	0.006	1.037	1.411	1.153	0	
bond	00000001_3	C8 N21	Not unusual (enough hits	20	1.293	1.31	0.012	1.402	0.017	1.294	1.336	1.309	0.001	
bond	00000001_3	C8 N3	Not unusual (enough hits	18	1.343	1.353	0.03	0.329	0.01	1.321	1.39	1.333	0.009	

bond	00000001_3	C9 N3	Not unusual (enough hits	1978	1.482	1.468	0.023	0.61	0.014	1.336	1.699	1.468	0	
bond	00000001_3	C7 S1	Not unusual (enough hits	1363	1.761	1.803	0.034	1.25	0.042	1.305	1.92	1.808	0	
bond	00000001_3	C7 C9	Not unusual (enough hits	329	1.538	1.505	0.028	1.167	0.033	1.349	1.653	1.509	0.001	
bond	00000001_3	C10 N3	Not unusual (enough hits	931	1.465	1.465	0.015	0.013	0	1.386	1.561	1.465	0	
bond	00000001_3	C10 C4	Not unusual (enough hits	10549	1.522	1.51	0.019	0.647	0.012	1.278	1.842	1.51	0	
bond	00000001_3	C3 C4	Not unusual (enough hits	560	1.407	1.381	0.017	1.565	0.026	1.279	1.497	1.382	0	
bond	00000001_3	C3 N2	Not unusual (enough hits	2818	1.361	1.34	0.022	0.915	0.021	1.05	1.584	1.337	0	
bond	00000001_3	C5 C4	Not unusual (enough hits	14050	1.416	1.384	0.022	1.476	0.032	0.618	1.8	1.386	0	
bond	00000001_3	C1 N2	Not unusual (enough hits	245	1.367	1.321	0.025	1.805	0.045	1.254	1.422	1.317	0	
bond	00000001_3	C6 C1	Not unusual (enough hits	479	1.416	1.373	0.022	1.994	0.044	1.267	1.455	1.373	0.002	
bond	00000001_3	C11 N21	Unusual (enough hits)	236	1.225	1.324	0.018	5.637	0.099	1.266	1.419	1.324	0.042	
bond	00000001_3	C8 S1	Unusual (enough hits)	176	1.673	1.752	0.019	4.153	0.08	1.681	1.81	1.75	0.009	
bond	00000001_3	C6 C5	Unusual (enough hits)	20000	1.428	1.383	0.019	2.419	0.045	0.882	1.685	1.383	0	
bond	00000001_3	C1 CL11	Unusual (enough hits)	743	1.786	1.738	0.019	2.565	0.048	1.561	1.806	1.74	0.001	
bond	00000001_4	C11 N4	Not unusual (enough hits	270	1.155	1.154	0.026	0.055	0.001	1.037	1.411	1.153	0	
bond	00000001_4	C8 N21	Not unusual (enough hits	20	1.294	1.31	0.012	1.25	0.015	1.294	1.336	1.309	0	
bond	00000001_4	C8 N3	Not unusual (enough hits	18	1.342	1.353	0.03	0.375	0.011	1.321	1.39	1.333	0.008	
bond	00000001_4	C9 N3	Not unusual (enough hits	1978	1.471	1.468	0.023	0.102	0.002	1.336	1.699	1.468	0	
bond	00000001_4	C7 S1	Not unusual (enough hits	1363	1.755	1.803	0.034	1.423	0.048	1.305	1.92	1.808	0	
bond	00000001_4	C7 C9	Not unusual (enough hits	329	1.533	1.505	0.028	1.001	0.028	1.349	1.653	1.509	0	
bond	00000001_4	C10 N3	Not unusual (enough hits	931	1.464	1.465	0.015	0.06	0.001	1.386	1.561	1.465	0	
bond	00000001_4	C10 C4	Not unusual (enough hits	10549	1.521	1.51	0.019	0.585	0.011	1.278	1.842	1.51	0	
bond	00000001_4	C3 C4	Not unusual (enough hits	560	1.413	1.381	0.017	1.873	0.032	1.279	1.497	1.382	0.001	
bond	00000001_4	C3 N2	Not unusual (enough hits	2818	1.36	1.34	0.022	0.886	0.02	1.05	1.584	1.337	0	
bond	00000001_4	C5 C4	Not unusual (enough hits	14050	1.427	1.384	0.022	1.956	0.043	0.618	1.8	1.386	0	
bond	00000001_4	C11 N21	Unusual (enough hits)	236	1.222	1.324	0.018	5.798	0.102	1.266	1.419	1.324	0.045	
bond	00000001_4	C8 S1	Unusual (enough hits)	176	1.672	1.752	0.019	4.192	0.081	1.681	1.81	1.75	0.009	
bond	00000001_4	C6 C5	Unusual (enough hits)	20000	1.421	1.383	0.019	2.055	0.038	0.882	1.685	1.383	0	
bond	00000001_4	C1 N2	Unusual (enough hits)	245	1.378	1.321	0.025	2.235	0.056	1.254	1.422	1.317	0.002	
bond	00000001_4	C6 C1	Unusual (enough hits)	479	1.421	1.373	0.022	2.222	0.049	1.267	1.455	1.373	0.002	
bond	00000001_4	C1 CL11	Unusual (enough hits)	743	1.783	1.738	0.019	2.41	0.045	1.561	1.806	1.74	0.002	
bond	00000001_5	C11 N4	Not unusual (enough hits	270	1.164	1.154	0.026	0.407	0.01	1.037	1.411	1.153	0	
bond	00000001_5	C8 N3	Not unusual (enough hits	18	1.336	1.353	0.03	0.581	0.017	1.321	1.39	1.333	0.002	
bond	00000001_5	C9 N3	Not unusual (enough hits	1978	1.474	1.468	0.023	0.263	0.006	1.336	1.699	1.468	0	
bond	00000001_5	C7 S1	Not unusual (enough hits	1363	1.754	1.803	0.034	1.451	0.049	1.305	1.92	1.808	0	
bond	00000001_5	C7 C9	Not unusual (enough hits	329	1.532	1.505	0.028	0.954	0.027	1.349	1.653	1.509	0.001	
bond	00000001_5	C10 N3	Not unusual (enough hits	931	1.461	1.465	0.015	0.246	0.004	1.386	1.561	1.465	0	
bond	00000001_5	C10 C4	Not unusual (enough hits	10549	1.52	1.51	0.019	0.549	0.01	1.278	1.842	1.51	0	
bond	00000001_5	C3 C4	Not unusual (enough hits	560	1.41	1.381	0.017	1.747	0.029	1.279	1.497	1.382	0	

bond	00000001_5	C3 N2	Not unusual (enough hits	2818	1.363	1.34	0.022	1	0.022	1.05	1.584	1.337	0	
bond	00000001_5	C5 C4	Not unusual (enough hits	14050	1.422	1.384	0.022	1.714	0.038	0.618	1.8	1.386	0	
bond	00000001_5	C6 C1	Not unusual (enough hits	479	1.416	1.373	0.022	1.98	0.043	1.267	1.455	1.373	0.001	
bond	00000001_5	C11 N21	Unusual (enough hits)	236	1.227	1.324	0.018	5.478	0.097	1.266	1.419	1.324	0.039	
bond	00000001_5	C8 N21	Unusual (enough hits)	20	1.283	1.31	0.012	2.177	0.026	1.294	1.336	1.309	0.011	
bond	00000001_5	C8 S1	Unusual (enough hits)	176	1.664	1.752	0.019	4.579	0.088	1.681	1.81	1.75	0.017	
bond	00000001_5	C6 C5	Unusual (enough hits)	20000	1.423	1.383	0.019	2.154	0.04	0.882	1.685	1.383	0	
bond	00000001_5	C1 N2	Unusual (enough hits)	245	1.374	1.321	0.025	2.11	0.053	1.254	1.422	1.317	0	
bond	00000001_5	C1 CL11	Unusual (enough hits)	743	1.785	1.738	0.019	2.543	0.047	1.561	1.806	1.74	0.001	
angle	00000001_1	N21 C11 N4	Not unusual (enough hits	229	179.059	172.864	3.874	1.599	6.195	129.202	177.69	173.256	1.369	
angle	00000001_1	S1 C8 N21	Not unusual (enough hits	15	125.25	125.758	0.568	0.892	0.507	124.171	126.665	125.769	0.131	
angle	00000001_1	N3 C8 N21	Not unusual (enough hits	15	123.939	122.137	1.552	1.161	1.802	119.21	125.039	122.189	0.208	
angle	00000001_1	S1 C8 N3	Not unusual (enough hits	17	110.81	112.335	0.891	1.71	1.525	111.047	114.313	112.241	0.237	
angle	00000001_1	C9 N3 C8	Not unusual (enough hits	17	118	114.613	1.854	1.827	3.387	111.633	116.76	115.197	1.241	
angle	00000001_1	C10 N3 C8	Not unusual (enough hits	17	124.122	123.878	2.748	0.089	0.245	120.755	131.475	123.652	0.134	
angle	00000001_1	C10 N3 C9	Not unusual (enough hits	109	117.876	120.505	2.722	0.966	2.629	110.736	125.952	121.036	0.001	
angle	00000001_1	C7 C9 N3	Not unusual (enough hits	37	107.32	106.737	2.199	0.265	0.583	101.643	111.558	106.948	0.161	
angle	00000001_1	C9 C7 S1	Not unusual (enough hits	245	106.425	106.659	2.153	0.109	0.234	100.728	118.537	106.294	0.013	
angle	00000001_1	C10 C4 C3	Not unusual (enough hits	155	119.483	121.018	1.641	0.936	1.536	113.768	126.783	120.987	0.038	
angle	00000001_1	C10 C4 C5	Not unusual (enough hits	10997	121.324	120.774	1.905	0.289	0.55	90.622	143.824	120.777	0	
angle	00000001_1	C5 C4 C3	Not unusual (enough hits	495	119.185	117.075	1.499	1.407	2.11	105.829	123.29	116.994	0.004	
angle	00000001_1	C6 C5 C4	Not unusual (enough hits	11395	119.588	121.039	1.437	1.01	1.451	93.35	147.791	121.028	0	
angle	00000001_1	C5 C6 C1	Not unusual (enough hits	289	118.871	117.43	0.964	1.494	1.44	114.685	123.178	117.353	0.021	
angle	00000001_1	CL11 C1 N2	Not unusual (enough hits	239	119.448	116.229	2.378	1.354	3.219	106.087	140.591	115.898	0.124	
angle	00000001_1	C6 C1 CL11	Not unusual (enough hits	437	120.611	119.088	2.36	0.645	1.523	96.671	128.568	119.178	0.002	
angle	00000001_1	C11 N21 C8	Unusual (enough hits)	19	123.643	118.367	1.142	4.619	5.276	116.537	121.811	118.22	1.832	
angle	00000001_1	C7 S1 C8	Unusual (enough hits)	103	97.444	91.388	1.578	3.838	6.056	86.226	98.264	91.466	0.82	
angle	00000001_1	C4 C10 N3	Unusual (enough hits)	764	116.894	113.088	1.717	2.217	3.806	104.07	122.755	113.045	0.02	
angle	00000001_1	C4 C3 N2	Unusual (enough hits)	225	120.236	123.744	1.746	2.01	3.509	117.703	127.597	124.357	0.072	
angle	00000001_1	C3 N2 C1	Unusual (enough hits)	179	122.179	116.435	1.303	4.409	5.744	112.785	121.37	116.186	0.809	
angle	00000001_1	C6 C1 N2	Unusual (enough hits)	167	119.938	124.711	1.675	2.849	4.773	117.068	127.876	125.155	0.036	
angle	00000001_2	N21 C11 N4	Not unusual (enough hits	229	178.995	172.864	3.874	1.582	6.131	129.202	177.69	173.256	1.304	
angle	00000001_2	S1 C8 N21	Not unusual (enough hits	15	125.41	125.758	0.568	0.612	0.348	124.171	126.665	125.769	0.029	
angle	00000001_2	N3 C8 N21	Not unusual (enough hits	15	123.591	122.137	1.552	0.937	1.454	119.21	125.039	122.189	0.085	
angle	00000001_2	S1 C8 N3	Not unusual (enough hits	17	110.999	112.335	0.891	1.499	1.336	111.047	114.313	112.241	0.048	
angle	00000001_2	C9 N3 C8	Not unusual (enough hits	17	117.753	114.613	1.854	1.693	3.139	111.633	116.76	115.197	0.993	
angle	00000001_2	C10 N3 C8	Not unusual (enough hits	17	123.912	123.878	2.748	0.013	0.035	120.755	131.475	123.652	0.011	
angle	00000001_2	C10 N3 C9	Not unusual (enough hits	109	118.334	120.505	2.722	0.797	2.17	110.736	125.952	121.036	0.094	
angle	00000001_2	C7 C9 N3	Not unusual (enough hits	37	107.399	106.737	2.199	0.301	0.662	101.643	111.558	106.948	0.082	

angle	00000001_2	C9 C7 S1	Not unusual (enough hits	245	106.577	106.659	2.153	0.038	0.083	100.728	118.537	106.294	0.003	
angle	00000001_2	C4 C10 N3	Not unusual (enough hits	764	116.378	113.088	1.717	1.917	3.291	104.07	122.755	113.045	0.031	
angle	00000001_2	C10 C4 C3	Not unusual (enough hits	155	119.611	121.018	1.641	0.858	1.407	113.768	126.783	120.987	0.017	
angle	00000001_2	C10 C4 C5	Not unusual (enough hits	10997	121.596	120.774	1.905	0.432	0.822	90.622	143.824	120.777	0	
angle	00000001_2	C5 C4 C3	Not unusual (enough hits	495	118.792	117.075	1.499	1.145	1.717	105.829	123.29	116.994	0.032	
angle	00000001_2	C4 C3 N2	Not unusual (enough hits	225	120.572	123.744	1.746	1.817	3.172	117.703	127.597	124.357	0.007	
angle	00000001_2	C6 C5 C4	Not unusual (enough hits	11395	119.769	121.039	1.437	0.884	1.27	93.35	147.791	121.028	0	
angle	00000001_2	C5 C6 C1	Not unusual (enough hits	289	118.893	117.43	0.964	1.518	1.463	114.685	123.178	117.353	0.002	
angle	00000001_2	CL11 C1 N2	Not unusual (enough hits	239	119.394	116.229	2.378	1.331	3.165	106.087	140.591	115.898	0.179	
angle	00000001_2	C6 C1 CL11	Not unusual (enough hits	437	120.775	119.088	2.36	0.715	1.687	96.671	128.568	119.178	0.001	
angle	00000001_2	C11 N21 C8	Unusual (enough hits)	19	124.493	118.367	1.142	5.363	6.126	116.537	121.811	118.22	2.682	
angle	00000001_2	C7 S1 C8	Unusual (enough hits)	103	97.273	91.388	1.578	3.729	5.885	86.226	98.264	91.466	0.991	
angle	00000001_2	C3 N2 C1	Unusual (enough hits)	179	122.143	116.435	1.303	4.381	5.707	112.785	121.37	116.186	0.773	
angle	00000001_2	C6 C1 N2	Unusual (enough hits)	167	119.83	124.711	1.675	2.913	4.881	117.068	127.876	125.155	0.072	
angle	00000001_3	N21 C11 N4	Not unusual (enough hits	229	178.204	172.864	3.874	1.378	5.34	129.202	177.69	173.256	0.513	
angle	00000001_3	S1 C8 N21	Not unusual (enough hits	15	125.848	125.758	0.568	0.158	0.09	124.171	126.665	125.769	0.079	
angle	00000001_3	N3 C8 N21	Not unusual (enough hits	15	123.236	122.137	1.552	0.708	1.099	119.21	125.039	122.189	0.183	
angle	00000001_3	S1 C8 N3	Not unusual (enough hits	17	110.916	112.335	0.891	1.592	1.419	111.047	114.313	112.241	0.131	
angle	00000001_3	C9 N3 C8	Not unusual (enough hits	17	117.759	114.613	1.854	1.697	3.146	111.633	116.76	115.197	0.999	
angle	00000001_3	C10 N3 C8	Not unusual (enough hits	17	123.25	123.878	2.748	0.228	0.627	120.755	131.475	123.652	0.144	
angle	00000001_3	C10 N3 C9	Not unusual (enough hits	109	118.99	120.505	2.722	0.557	1.515	110.736	125.952	121.036	0.03	
angle	00000001_3	C7 C9 N3	Not unusual (enough hits	37	107.447	106.737	2.199	0.323	0.71	101.643	111.558	106.948	0.034	
angle	00000001_3	C9 C7 S1	Not unusual (enough hits	245	106.269	106.659	2.153	0.181	0.391	100.728	118.537	106.294	0.002	
angle	00000001_3	C10 C4 C3	Not unusual (enough hits	155	119.179	121.018	1.641	1.121	1.839	113.768	126.783	120.987	0.096	
angle	00000001_3	C10 C4 C5	Not unusual (enough hits	10997	122.1	120.774	1.905	0.696	1.325	90.622	143.824	120.777	0	
angle	00000001_3	C5 C4 C3	Not unusual (enough hits	495	118.717	117.075	1.499	1.095	1.642	105.829	123.29	116.994	0.028	
angle	00000001_3	C4 C3 N2	Not unusual (enough hits	225	120.546	123.744	1.746	1.832	3.198	117.703	127.597	124.357	0.006	
angle	00000001_3	C6 C5 C4	Not unusual (enough hits	11395	119.698	121.039	1.437	0.934	1.342	93.35	147.791	121.028	0	
angle	00000001_3	C5 C6 C1	Not unusual (enough hits	289	118.859	117.43	0.964	1.482	1.428	114.685	123.178	117.353	0.033	
angle	00000001_3	CL11 C1 N2	Not unusual (enough hits	239	119.374	116.229	2.378	1.323	3.145	106.087	140.591	115.898	0.199	
angle	00000001_3	C6 C1 CL11	Not unusual (enough hits	437	121.065	119.088	2.36	0.838	1.977	96.671	128.568	119.178	0.029	
angle	00000001_3	C11 N21 C8	Unusual (enough hits)	19	125.27	118.367	1.142	6.043	6.903	116.537	121.811	118.22	3.459	
angle	00000001_3	C7 S1 C8	Unusual (enough hits)	103	97.609	91.388	1.578	3.942	6.221	86.226	98.264	91.466	0.655	
angle	00000001_3	C4 C10 N3	Unusual (enough hits)	764	116.978	113.088	1.717	2.266	3.891	104.07	122.755	113.045	0.021	
angle	00000001_3	C3 N2 C1	Unusual (enough hits)	179	122.618	116.435	1.303	4.746	6.183	112.785	121.37	116.186	1.248	
angle	00000001_3	C6 C1 N2	Unusual (enough hits)	167	119.555	124.711	1.675	3.077	5.156	117.068	127.876	125.155	0.336	
angle	00000001_4	N21 C11 N4	Not unusual (enough hits	229	178.861	172.864	3.874	1.548	5.997	129.202	177.69	173.256	1.171	
angle	00000001_4	S1 C8 N21	Not unusual (enough hits	15	125.956	125.758	0.568	0.349	0.199	124.171	126.665	125.769	0.01	
angle	00000001_4	N3 C8 N21	Not unusual (enough hits	15	123.339	122.137	1.552	0.774	1.202	119.21	125.039	122.189	0.167	

angle	00000001_4	S1 C8 N3	Not unusual (enough hits	17	110.704	112.335	0.891	1.829	1.63	111.047	114.313	112.241	0.342	
angle	00000001_4	C9 N3 C8	Not unusual (enough hits	17	117.763	114.613	1.854	1.699	3.15	111.633	116.76	115.197	1.004	
angle	00000001_4	C10 N3 C8	Not unusual (enough hits	17	123.895	123.878	2.748	0.006	0.017	120.755	131.475	123.652	0.004	
angle	00000001_4	C10 N3 C9	Not unusual (enough hits	109	118.341	120.505	2.722	0.795	2.164	110.736	125.952	121.036	0.088	
angle	00000001_4	C7 C9 N3	Not unusual (enough hits	37	107.819	106.737	2.199	0.492	1.081	101.643	111.558	106.948	0.059	
angle	00000001_4	C9 C7 S1	Not unusual (enough hits	245	106.09	106.659	2.153	0.265	0.57	100.728	118.537	106.294	0.001	
angle	00000001_4	C10 C4 C3	Not unusual (enough hits	155	119.431	121.018	1.641	0.967	1.587	113.768	126.783	120.987	0.001	
angle	00000001_4	C10 C4 C5	Not unusual (enough hits	10997	121.49	120.774	1.905	0.376	0.716	90.622	143.824	120.777	0	
angle	00000001_4	C5 C4 C3	Not unusual (enough hits	495	119.068	117.075	1.499	1.329	1.993	105.829	123.29	116.994	0.067	
angle	00000001_4	C6 C5 C4	Not unusual (enough hits	11395	119.535	121.039	1.437	1.047	1.505	93.35	147.791	121.028	0.001	
angle	00000001_4	C5 C6 C1	Not unusual (enough hits	289	118.972	117.43	0.964	1.6	1.542	114.685	123.178	117.353	0.021	
angle	00000001_4	CL11 C1 N2	Not unusual (enough hits	239	119.3	116.229	2.378	1.292	3.071	106.087	140.591	115.898	0.273	
angle	00000001_4	C6 C1 CL11	Not unusual (enough hits	437	121.06	119.088	2.36	0.836	1.972	96.671	128.568	119.178	0.027	
angle	00000001_4	C11 N21 C8	Unusual (enough hits)	19	124.998	118.367	1.142	5.805	6.631	116.537	121.811	118.22	3.187	
angle	00000001_4	C7 S1 C8	Unusual (enough hits)	103	97.624	91.388	1.578	3.952	6.236	86.226	98.264	91.466	0.64	
angle	00000001_4	C4 C10 N3	Unusual (enough hits)	764	118.09	113.088	1.717	2.914	5.003	104.07	122.755	113.045	0.006	
angle	00000001_4	C4 C3 N2	Unusual (enough hits)	225	120.223	123.744	1.746	2.017	3.522	117.703	127.597	124.357	0.065	
angle	00000001_4	C3 N2 C1	Unusual (enough hits)	179	122.564	116.435	1.303	4.704	6.128	112.785	121.37	116.186	1.193	
angle	00000001_4	C6 C1 N2	Unusual (enough hits)	167	119.638	124.711	1.675	3.028	5.073	117.068	127.876	125.155	0.264	
angle	00000001_5	N21 C11 N4	Not unusual (enough hits	229	178.58	172.864	3.874	1.475	5.716	129.202	177.69	173.256	0.89	
angle	00000001_5	S1 C8 N21	Not unusual (enough hits	15	125.59	125.758	0.568	0.295	0.167	124.171	126.665	125.769	0.023	
angle	00000001_5	N3 C8 N21	Not unusual (enough hits	15	123.572	122.137	1.552	0.924	1.435	119.21	125.039	122.189	0.066	
angle	00000001_5	S1 C8 N3	Not unusual (enough hits	17	110.838	112.335	0.891	1.679	1.497	111.047	114.313	112.241	0.209	
angle	00000001_5	C9 N3 C8	Not unusual (enough hits	17	117.8	114.613	1.854	1.719	3.187	111.633	116.76	115.197	1.041	
angle	00000001_5	C10 N3 C8	Not unusual (enough hits	17	123.525	123.878	2.748	0.128	0.352	120.755	131.475	123.652	0.126	
angle	00000001_5	C10 N3 C9	Not unusual (enough hits	109	118.672	120.505	2.722	0.674	1.833	110.736	125.952	121.036	0.049	
angle	00000001_5	C7 C9 N3	Not unusual (enough hits	37	107.611	106.737	2.199	0.398	0.874	101.643	111.558	106.948	0.075	
angle	00000001_5	C9 C7 S1	Not unusual (enough hits	245	105.983	106.659	2.153	0.314	0.676	100.728	118.537	106.294	0.013	
angle	00000001_5	C10 C4 C3	Not unusual (enough hits	155	119.596	121.018	1.641	0.867	1.423	113.768	126.783	120.987	0.033	
angle	00000001_5	C10 C4 C5	Not unusual (enough hits	10997	121.411	120.774	1.905	0.334	0.637	90.622	143.824	120.777	0	
angle	00000001_5	C5 C4 C3	Not unusual (enough hits	495	118.986	117.075	1.499	1.275	1.912	105.829	123.29	116.994	0.015	
angle	00000001_5	C4 C3 N2	Not unusual (enough hits	225	120.259	123.744	1.746	1.997	3.485	117.703	127.597	124.357	0.049	
angle	00000001_5	C6 C5 C4	Not unusual (enough hits	11395	119.688	121.039	1.437	0.94	1.351	93.35	147.791	121.028	0	
angle	00000001_5	C5 C6 C1	Not unusual (enough hits	289	118.835	117.43	0.964	1.457	1.405	114.685	123.178	117.353	0.028	
angle	00000001_5	CL11 C1 N2	Not unusual (enough hits	239	119.664	116.229	2.378	1.445	3.435	106.087	140.591	115.898	0.091	
angle	00000001_5	C6 C1 CL11	Not unusual (enough hits	437	120.491	119.088	2.36	0.594	1.402	96.671	128.568	119.178	0.008	
angle	00000001_5	C11 N21 C8	Unusual (enough hits)	19	124.54	118.367	1.142	5.404	6.173	116.537	121.811	118.22	2.729	
angle	00000001_5	C7 S1 C8	Unusual (enough hits)	103	97.767	91.388	1.578	4.043	6.379	86.226	98.264	91.466	0.497	
angle	00000001_5	C4 C10 N3	Unusual (enough hits)	764	118.049	113.088	1.717	2.89	4.962	104.07	122.755	113.045	0.047	

angle	00000001_5	C3 N2 C1	Unusual (enough hits)	179	122.388	116.435	1.303	4.569	5.953	112.785	121.37	116.186	1.018	
angle	00000001_5	C6 C1 N2	Unusual (enough hits)	167	119.841	124.711	1.675	2.906	4.869	117.068	127.876	125.155	0.061	
torsion	00000001_1	S1 C8 N21 C11	Not unusual (enough hits	42	−0.172								0.037	1
torsion	00000001_1	N3 C8 N21 C11	Not unusual (enough hits	17	−179.986								0.219	1
torsion	00000001_1	C4 C10 N3 C8	Not unusual (enough hits	41	−111.93								0.032	0.22
torsion	00000001_1	C4 C10 N3 C9	Not unusual (enough hits	182	68.49								0.128	0.703
torsion	00000001_1	C3 C4 C10 N3	Not unusual (enough hits	349	−111.832								0.097	0.16
torsion	00000001_1	C5 C4 C10 N3	Not unusual (enough hits	10853	69.214								0.008	0.136
torsion	00000001_1	N4 C11 N21 C8	Unusual (few hits)	4	−54.722								72.927	0
torsion	00000001_2	S1 C8 N21 C11	Not unusual (enough hits	42	−0.12								0.01	1
torsion	00000001_2	N3 C8 N21 C11	Not unusual (enough hits	17	−179.99								0.223	1
torsion	00000001_2	C4 C10 N3 C8	Not unusual (enough hits	41	−116.616								0.203	0.268
torsion	00000001_2	C4 C10 N3 C9	Not unusual (enough hits	182	63.579								0.039	0.566
torsion	00000001_2	C3 C4 C10 N3	Not unusual (enough hits	349	−114.335								0.032	0.158
torsion	00000001_2	C5 C4 C10 N3	Not unusual (enough hits	10853	65.963								0.009	0.142
torsion	00000001_2	N4 C11 N21 C8	Unusual (few hits)	4	−115.928								11.722	0
torsion	00000001_3	S1 C8 N21 C11	Not unusual (enough hits	42	−0.119								0.01	1
torsion	00000001_3	N3 C8 N21 C11	Not unusual (enough hits	17	−179.984								0.217	1
torsion	00000001_3	C4 C10 N3 C8	Not unusual (enough hits	41	−113.006								1.045	0.22
torsion	00000001_3	C4 C10 N3 C9	Not unusual (enough hits	182	67.406								0.148	0.659
torsion	00000001_3	C3 C4 C10 N3	Not unusual (enough hits	349	−114.373								0.005	0.158
torsion	00000001_3	C5 C4 C10 N3	Not unusual (enough hits	10853	66.363								0.004	0.141
torsion	00000001_3	N4 C11 N21 C8	Not unusual (few hits)	4	−159.529								0.994	0.5
torsion	00000001_4	S1 C8 N21 C11	Not unusual (enough hits	42	0.05								0.035	1
torsion	00000001_4	N3 C8 N21 C11	Not unusual (enough hits	17	−179.611								0.102	1
torsion	00000001_4	C4 C10 N3 C8	Not unusual (enough hits	41	−112.436								0.474	0.22
torsion	00000001_4	C4 C10 N3 C9	Not unusual (enough hits	182	68.013								0.121	0.681
torsion	00000001_4	C3 C4 C10 N3	Not unusual (enough hits	349	−106.345								0.055	0.14
torsion	00000001_4	C5 C4 C10 N3	Not unusual (enough hits	10853	74.86								0.001	0.125
torsion	00000001_4	N4 C11 N21 C8	Not unusual (few hits)	4	−158.073								0.461	0.5
torsion	00000001_5	S1 C8 N21 C11	Not unusual (enough hits	42	−0.12								0.011	1
torsion	00000001_5	N3 C8 N21 C11	Not unusual (enough hits	17	−179.889								0.121	1
torsion	00000001_5	C4 C10 N3 C8	Not unusual (enough hits	41	−110.601								1.361	0.22
torsion	00000001_5	C4 C10 N3 C9	Not unusual (enough hits	182	70.006								0.134	0.703
torsion	00000001_5	C3 C4 C10 N3	Not unusual (enough hits	349	−109.855								0.088	0.155
torsion	00000001_5	C5 C4 C10 N3	Not unusual (enough hits	10853	71.113								0.001	0.13
torsion	00000001_5	N4 C11 N21 C8	Unusual (few hits)	4	174.767								16.233	0
ring	00000001_1	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.139	25.6			0.356
ring	00000001_1	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.071	8.05			1

ring	00000001_2	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.134	25.59			0.356
ring	00000001_2	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.024	8.185			1
ring	00000001_3	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.086	25.549			0.356
ring	00000001_3	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.059	7.844			1
ring	00000001_4	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.201	25.596			0.356
ring	00000001_4	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.074	8.232			1
ring	00000001_5	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.112	25.542			0.356
ring	00000001_5	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.057	8.163			1

Table 6. Geometry Analysis by Mogul of Thiacloprid in Complex with Gln55Arg Mutant of *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	| z-score |	| x - mean |	Minimum	Maximum	Median	| d(min) |	Local density
bond	00000001_1	C11 N4	Not unusual (enough hits	24	1.173	1.166	0.024	0.269	0.006	1.112	1.218	1.161	0	
bond	00000001_1	C8 N3	Not unusual (enough hits	18	1.35	1.347	0.012	0.221	0.003	1.315	1.368	1.347	0	
bond	00000001_1	C7 S1	Not unusual (enough hits	1363	1.753	1.803	0.034	1.479	0.05	1.305	1.92	1.808	0.001	
bond	00000001_1	C9 N3	Not unusual (enough hits	103	1.467	1.473	0.022	0.239	0.005	1.363	1.518	1.477	0	
bond	00000001_1	C10 N3	Not unusual (enough hits	29	1.467	1.475	0.019	0.439	0.008	1.439	1.522	1.476	0	
bond	00000001_1	C7 C9	Not unusual (enough hits	279	1.53	1.511	0.034	0.546	0.018	1.351	1.79	1.516	0	
bond	00000001_1	C10 C4	Not unusual (enough hits	940	1.517	1.508	0.024	0.378	0.009	1.294	1.677	1.509	0	
bond	00000001_1	C5 C4	Not unusual (enough hits	14050	1.408	1.384	0.022	1.096	0.024	0.618	1.8	1.386	0	
bond	00000001_1	C3 N2	Not unusual (enough hits	2818	1.363	1.34	0.022	1.031	0.023	1.05	1.584	1.337	0	
bond	00000001_1	C6 C5	Not unusual (enough hits	20000	1.414	1.383	0.019	1.641	0.03	0.882	1.685	1.383	0	
bond	00000001_1	C6 C1	Not unusual (enough hits	479	1.405	1.373	0.022	1.481	0.032	1.267	1.455	1.373	0	
bond	00000001_1	C1 CL11	Not unusual (enough hits	743	1.773	1.738	0.019	1.914	0.035	1.561	1.806	1.74	0	
bond	00000001_1	C11 N21	Unusual (enough hits)	19	1.234	1.314	0.035	2.312	0.08	1.249	1.351	1.326	0.015	
bond	00000001_1	C8 N21	Unusual (enough hits)	72	1.295	1.363	0.018	3.753	0.068	1.302	1.409	1.362	0.007	
bond	00000001_1	C8 S1	Unusual (enough hits)	49	1.668	1.75	0.016	5.242	0.082	1.713	1.782	1.748	0.044	
bond	00000001_1	C3 C4	Unusual (enough hits)	560	1.427	1.381	0.017	2.732	0.046	1.279	1.497	1.382	0.007	
bond	00000001_1	C1 N2	Unusual (enough hits)	245	1.384	1.321	0.025	2.473	0.062	1.254	1.422	1.317	0	
bond	00000001_2	C11 N4	Not unusual (enough hits	24	1.179	1.166	0.024	0.515	0.012	1.112	1.218	1.161	0.005	
bond	00000001_2	C8 N3	Not unusual (enough hits	18	1.353	1.347	0.012	0.505	0.006	1.315	1.368	1.347	0.001	
bond	00000001_2	C7 S1	Not unusual (enough hits	1363	1.756	1.803	0.034	1.381	0.046	1.305	1.92	1.808	0	
bond	00000001_2	C9 N3	Not unusual (enough hits	103	1.463	1.473	0.022	0.431	0.01	1.363	1.518	1.477	0.001	
bond	00000001_2	C10 N3	Not unusual (enough hits	29	1.462	1.475	0.019	0.669	0.013	1.439	1.522	1.476	0	
bond	00000001_2	C7 C9	Not unusual (enough hits	279	1.52	1.511	0.034	0.268	0.009	1.351	1.79	1.516	0	
bond	00000001_2	C10 C4	Not unusual (enough hits	940	1.532	1.508	0.024	0.999	0.024	1.294	1.677	1.509	0	
bond	00000001_2	C5 C4	Not unusual (enough hits	14050	1.41	1.384	0.022	1.206	0.026	0.618	1.8	1.386	0	
bond	00000001_2	C3 N2	Not unusual (enough hits	2818	1.375	1.34	0.022	1.543	0.035	1.05	1.584	1.337	0	
bond	00000001_2	C6 C5	Not unusual (enough hits	20000	1.41	1.383	0.019	1.438	0.027	0.882	1.685	1.383	0	
bond	00000001_2	C6 C1	Not unusual (enough hits	479	1.405	1.373	0.022	1.469	0.032	1.267	1.455	1.373	0	
bond	00000001_2	C1 CL11	Not unusual (enough hits	743	1.77	1.738	0.019	1.732	0.032	1.561	1.806	1.74	0	
bond	00000001_2	C11 N21	Unusual (enough hits)	19	1.242	1.314	0.035	2.071	0.071	1.249	1.351	1.326	0.006	
bond	00000001_2	C8 N21	Unusual (enough hits)	72	1.306	1.363	0.018	3.161	0.057	1.302	1.409	1.362	0.004	
bond	00000001_2	C8 S1	Unusual (enough hits)	49	1.667	1.75	0.016	5.358	0.084	1.713	1.782	1.748	0.046	
bond	00000001_2	C3 C4	Unusual (enough hits)	560	1.432	1.381	0.017	3.028	0.051	1.279	1.497	1.382	0.002	
bond	00000001_2	C1 N2	Unusual (enough hits)	245	1.377	1.321	0.025	2.226	0.056	1.254	1.422	1.317	0.001	
bond	00000001_3	C11 N4	Not unusual (enough hits	24	1.169	1.166	0.024	0.107	0.003	1.112	1.218	1.161	0	
bond	00000001_3	C8 N3	Not unusual (enough hits	18	1.351	1.347	0.012	0.337	0.004	1.315	1.368	1.347	0.001	
bond	00000001_3	C7 S1	Not unusual (enough hits	1363	1.752	1.803	0.034	1.501	0.05	1.305	1.92	1.808	0	

bond	00000001_3	C9 N3	Not unusual (enough hits	103	1.465	1.473	0.022	0.35	0.008	1.363	1.518	1.477	0	
bond	00000001_3	C10 N3	Not unusual (enough hits	29	1.473	1.475	0.019	0.134	0.003	1.439	1.522	1.476	0	
bond	00000001_3	C7 C9	Not unusual (enough hits	279	1.526	1.511	0.034	0.434	0.015	1.351	1.79	1.516	0	
bond	00000001_3	C10 C4	Not unusual (enough hits	940	1.521	1.508	0.024	0.518	0.012	1.294	1.677	1.509	0	
bond	00000001_3	C5 C4	Not unusual (enough hits	14050	1.412	1.384	0.022	1.257	0.028	0.618	1.8	1.386	0	
bond	00000001_3	C3 N2	Not unusual (enough hits	2818	1.365	1.34	0.022	1.108	0.025	1.05	1.584	1.337	0	
bond	00000001_3	C6 C5	Not unusual (enough hits	20000	1.415	1.383	0.019	1.712	0.032	0.882	1.685	1.383	0	
bond	00000001_3	C6 C1	Not unusual (enough hits	479	1.407	1.373	0.022	1.577	0.035	1.267	1.455	1.373	0	
bond	00000001_3	C1 CL11	Not unusual (enough hits	743	1.761	1.738	0.019	1.235	0.023	1.561	1.806	1.74	0	
bond	00000001_3	C11 N21	Unusual (enough hits)	19	1.228	1.314	0.035	2.486	0.086	1.249	1.351	1.326	0.021	
bond	00000001_3	C8 N21	Unusual (enough hits)	72	1.297	1.363	0.018	3.656	0.066	1.302	1.409	1.362	0.005	
bond	00000001_3	C8 S1	Unusual (enough hits)	49	1.669	1.75	0.016	5.225	0.082	1.713	1.782	1.748	0.044	
bond	00000001_3	C3 C4	Unusual (enough hits)	560	1.421	1.381	0.017	2.394	0.04	1.279	1.497	1.382	0.003	
bond	00000001_3	C1 N2	Unusual (enough hits)	245	1.378	1.321	0.025	2.254	0.057	1.254	1.422	1.317	0.001	
bond	00000001_4	C11 N4	Not unusual (enough hits	24	1.165	1.166	0.024	0.046	0.001	1.112	1.218	1.161	0.002	
bond	00000001_4	C7 S1	Not unusual (enough hits	1363	1.767	1.803	0.034	1.049	0.035	1.305	1.92	1.808	0	
bond	00000001_4	C9 N3	Not unusual (enough hits	103	1.464	1.473	0.022	0.372	0.008	1.363	1.518	1.477	0	
bond	00000001_4	C10 N3	Not unusual (enough hits	29	1.452	1.475	0.019	1.219	0.023	1.439	1.522	1.476	0.002	
bond	00000001_4	C7 C9	Not unusual (enough hits	279	1.526	1.511	0.034	0.42	0.014	1.351	1.79	1.516	0	
bond	00000001_4	C10 C4	Not unusual (enough hits	940	1.519	1.508	0.024	0.426	0.01	1.294	1.677	1.509	0	
bond	00000001_4	C5 C4	Not unusual (enough hits	14050	1.412	1.384	0.022	1.255	0.028	0.618	1.8	1.386	0	
bond	00000001_4	C3 N2	Not unusual (enough hits	2818	1.369	1.34	0.022	1.284	0.029	1.05	1.584	1.337	0	
bond	00000001_4	C6 C5	Not unusual (enough hits	20000	1.413	1.383	0.019	1.628	0.03	0.882	1.685	1.383	0	
bond	00000001_4	C6 C1	Not unusual (enough hits	479	1.394	1.373	0.022	0.986	0.022	1.267	1.455	1.373	0	
bond	00000001_4	C1 CL11	Not unusual (enough hits	743	1.765	1.738	0.019	1.48	0.027	1.561	1.806	1.74	0	
bond	00000001_4	C11 N21	Unusual (enough hits)	19	1.224	1.314	0.035	2.602	0.09	1.249	1.351	1.326	0.025	
bond	00000001_4	C8 N21	Unusual (enough hits)	72	1.301	1.363	0.018	3.415	0.062	1.302	1.409	1.362	0.001	
bond	00000001_4	C8 S1	Unusual (enough hits)	49	1.666	1.75	0.016	5.421	0.085	1.713	1.782	1.748	0.047	
bond	00000001_4	C8 N3	Unusual (enough hits)	18	1.373	1.347	0.012	2.111	0.026	1.315	1.368	1.347	0.004	
bond	00000001_4	C3 C4	Unusual (enough hits)	560	1.429	1.381	0.017	2.86	0.048	1.279	1.497	1.382	0.005	
bond	00000001_4	C1 N2	Unusual (enough hits)	245	1.396	1.321	0.025	2.962	0.074	1.254	1.422	1.317	0.001	
bond	00000001_5	C11 N4	Not unusual (enough hits	24	1.167	1.166	0.024	0.017	0	1.112	1.218	1.161	0	
bond	00000001_5	C8 N3	Not unusual (enough hits	18	1.362	1.347	0.012	1.275	0.016	1.315	1.368	1.347	0	
bond	00000001_5	C7 S1	Not unusual (enough hits	1363	1.767	1.803	0.034	1.057	0.035	1.305	1.92	1.808	0	
bond	00000001_5	C9 N3	Not unusual (enough hits	103	1.463	1.473	0.022	0.424	0.009	1.363	1.518	1.477	0.001	
bond	00000001_5	C10 N3	Not unusual (enough hits	29	1.454	1.475	0.019	1.093	0.021	1.439	1.522	1.476	0.001	
bond	00000001_5	C7 C9	Not unusual (enough hits	279	1.527	1.511	0.034	0.45	0.015	1.351	1.79	1.516	0	
bond	00000001_5	C10 C4	Not unusual (enough hits	940	1.519	1.508	0.024	0.454	0.011	1.294	1.677	1.509	0	
bond	00000001_5	C5 C4	Not unusual (enough hits	14050	1.402	1.384	0.022	0.797	0.017	0.618	1.8	1.386	0	

bond	00000001_5	C3 N2	Not unusual (enough hits	2818	1.361	1.34	0.022	0.916	0.021	1.05	1.584	1.337	0	
bond	00000001_5	C6 C5	Not unusual (enough hits	20000	1.4	1.383	0.019	0.911	0.017	0.882	1.685	1.383	0	
bond	00000001_5	C6 C1	Not unusual (enough hits	479	1.399	1.373	0.022	1.194	0.026	1.267	1.455	1.373	0	
bond	00000001_5	C1 CL11	Not unusual (enough hits	743	1.772	1.738	0.019	1.832	0.034	1.561	1.806	1.74	0.001	
bond	00000001_5	C11 N21	Unusual (enough hits)	19	1.232	1.314	0.035	2.371	0.082	1.249	1.351	1.326	0.017	
bond	00000001_5	C8 N21	Unusual (enough hits)	72	1.3	1.363	0.018	3.467	0.063	1.302	1.409	1.362	0.002	
bond	00000001_5	C8 S1	Unusual (enough hits)	49	1.67	1.75	0.016	5.152	0.081	1.713	1.782	1.748	0.043	
bond	00000001_5	C3 C4	Unusual (enough hits)	560	1.431	1.381	0.017	2.952	0.05	1.279	1.497	1.382	0.004	
bond	00000001_5	C1 N2	Unusual (enough hits)	245	1.38	1.321	0.025	2.325	0.058	1.254	1.422	1.317	0.001	
angle	00000001_1	C11 N21 C8	No hits	0	124.74									
angle	00000001_1	S1 C8 N3	No hits	0	110.501									
angle	00000001_1	S1 C8 N21	Not unusual (enough hits	20	125.481	120.612	4.097	1.188	4.869	112.48	127.569	119.504	0.19	
angle	00000001_1	N21 C8 N3	Not unusual (enough hits	12	124.018	122.214	1.748	1.032	1.804	118.888	125.399	122.646	0.185	
angle	00000001_1	C10 N3 C8	Not unusual (enough hits	15	125.099	125.32	2.241	0.099	0.221	121.681	128.396	124.864	0.108	
angle	00000001_1	C7 C9 N3	Not unusual (enough hits	22	107.411	109.022	2.757	0.584	1.611	99.107	111.59	109.508	0.105	
angle	00000001_1	C9 C7 S1	Not unusual (enough hits	252	106.629	106.672	1.963	0.022	0.043	96.401	118.991	106.637	0.001	
angle	00000001_1	C4 C10 N3	Not unusual (enough hits	20	115.065	112.452	1.868	1.399	2.613	107.509	115.688	112.49	0.623	
angle	00000001_1	C10 C4 C3	Not unusual (enough hits	16	121.551	120.264	1.927	0.668	1.287	117.385	124.274	120.474	0.375	
angle	00000001_1	C10 C4 C5	Not unusual (enough hits	1598	119.44	120.601	2.03	0.572	1.161	107.035	130.916	120.592	0.005	
angle	00000001_1	C5 C4 C3	Not unusual (enough hits	495	119.001	117.075	1.499	1.285	1.927	105.829	123.29	116.994	0	
angle	00000001_1	C6 C5 C4	Not unusual (enough hits	11395	119.99	121.039	1.437	0.73	1.049	93.35	147.791	121.028	0	
angle	00000001_1	C5 C6 C1	Not unusual (enough hits	289	119.23	117.43	0.964	1.868	1.8	114.685	123.178	117.353	0.064	
angle	00000001_1	CL11 C1 N2	Not unusual (enough hits	239	119.646	116.229	2.378	1.437	3.417	106.087	140.591	115.898	0.073	
angle	00000001_1	C6 C1 CL11	Not unusual (enough hits	437	120.242	119.088	2.36	0.489	1.154	96.671	128.568	119.178	0.004	
angle	00000001_1	N4 C11 N21	Unusual (enough hits)	19	178.437	173.083	1.486	3.603	5.354	171.407	177.175	173.067	1.262	
angle	00000001_1	C7 S1 C8	Unusual (enough hits)	103	97.476	91.388	1.578	3.858	6.088	86.226	98.264	91.466	0.788	
angle	00000001_1	C9 N3 C8	Unusual (enough hits)	18	117.981	111.69	2.909	2.163	6.291	107.905	117.378	110.821	0.603	
angle	00000001_1	C10 N3 C9	Unusual (enough hits)	26	116.919	122.598	2.502	2.27	5.679	115.726	126.639	123.077	1.193	
angle	00000001_1	C4 C3 N2	Unusual (enough hits)	225	119.899	123.744	1.746	2.203	3.845	117.703	127.597	124.357	0.024	
angle	00000001_1	C3 N2 C1	Unusual (enough hits)	179	121.761	116.435	1.303	4.088	5.326	112.785	121.37	116.186	0.391	
angle	00000001_1	C6 C1 N2	Unusual (enough hits)	167	120.111	124.711	1.675	2.746	4.6	117.068	127.876	125.155	0.064	
angle	00000001_2	C11 N21 C8	No hits	0	125.624									
angle	00000001_2	S1 C8 N3	No hits	0	109.961									
angle	00000001_2	S1 C8 N21	Not unusual (enough hits	20	125.905	120.612	4.097	1.292	5.293	112.48	127.569	119.504	0.234	
angle	00000001_2	N21 C8 N3	Not unusual (enough hits	12	124.133	122.214	1.748	1.097	1.919	118.888	125.399	122.646	0.3	
angle	00000001_2	C10 N3 C8	Not unusual (enough hits	15	125.308	125.32	2.241	0.005	0.012	121.681	128.396	124.864	0.317	
angle	00000001_2	C7 C9 N3	Not unusual (enough hits	22	107.384	109.022	2.757	0.594	1.638	99.107	111.59	109.508	0.077	
angle	00000001_2	C9 C7 S1	Not unusual (enough hits	252	106.722	106.672	1.963	0.026	0.05	96.401	118.991	106.637	0.032	
angle	00000001_2	C4 C10 N3	Not unusual (enough hits	20	116.011	112.452	1.868	1.905	3.558	107.509	115.688	112.49	0.323	

angle	00000001_2	C10 C4 C3	Not unusual (enough hits	16	122.339	120.264	1.927	1.077	2.074	117.385	124.274	120.474	0.219	
angle	00000001_2	C10 C4 C5	Not unusual (enough hits	1598	118.868	120.601	2.03	0.854	1.734	107.035	130.916	120.592	0	
angle	00000001_2	C5 C4 C3	Not unusual (enough hits	495	118.783	117.075	1.499	1.14	1.709	105.829	123.29	116.994	0.024	
angle	00000001_2	C6 C5 C4	Not unusual (enough hits	11395	119.911	121.039	1.437	0.785	1.128	93.35	147.791	121.028	0	
angle	00000001_2	CL11 C1 N2	Not unusual (enough hits	239	120.884	116.229	2.378	1.958	4.655	106.087	140.591	115.898	0.169	
angle	00000001_2	C6 C1 CL11	Not unusual (enough hits	437	119.053	119.088	2.36	0.015	0.035	96.671	128.568	119.178	0.003	
angle	00000001_2	N4 C11 N21	Unusual (enough hits)	19	178.627	173.083	1.486	3.731	5.544	171.407	177.175	173.067	1.452	
angle	00000001_2	C7 S1 C8	Unusual (enough hits)	103	97.521	91.388	1.578	3.886	6.133	86.226	98.264	91.466	0.743	
angle	00000001_2	C9 N3 C8	Unusual (enough hits)	18	118.409	111.69	2.909	2.31	6.719	107.905	117.378	110.821	1.031	
angle	00000001_2	C10 N3 C9	Unusual (enough hits)	26	116.282	122.598	2.502	2.524	6.316	115.726	126.639	123.077	0.556	
angle	00000001_2	C4 C3 N2	Unusual (enough hits)	225	119.803	123.744	1.746	2.258	3.941	117.703	127.597	124.357	0.04	
angle	00000001_2	C3 N2 C1	Unusual (enough hits)	179	121.673	116.435	1.303	4.02	5.237	112.785	121.37	116.186	0.303	
angle	00000001_2	C5 C6 C1	Unusual (enough hits)	289	119.767	117.43	0.964	2.424	2.336	114.685	123.178	117.353	0.125	
angle	00000001_2	C6 C1 N2	Unusual (enough hits)	167	120.058	124.711	1.675	2.777	4.653	117.068	127.876	125.155	0.011	
angle	00000001_3	C11 N21 C8	No hits	0	124.106									
angle	00000001_3	S1 C8 N3	No hits	0	110.585									
angle	00000001_3	S1 C8 N21	Not unusual (enough hits	20	125.05	120.612	4.097	1.083	4.438	112.48	127.569	119.504	0.621	
angle	00000001_3	N21 C8 N3	Not unusual (enough hits	12	124.364	122.214	1.748	1.23	2.15	118.888	125.399	122.646	0.531	
angle	00000001_3	C10 N3 C8	Not unusual (enough hits	15	125.234	125.32	2.241	0.038	0.086	121.681	128.396	124.864	0.243	
angle	00000001_3	C7 C9 N3	Not unusual (enough hits	22	107.755	109.022	2.757	0.46	1.267	99.107	111.59	109.508	0.448	
angle	00000001_3	C9 C7 S1	Not unusual (enough hits	252	106.575	106.672	1.963	0.05	0.097	96.401	118.991	106.637	0	
angle	00000001_3	C4 C10 N3	Not unusual (enough hits	20	113.066	112.452	1.868	0.329	0.614	107.509	115.688	112.49	0.447	
angle	00000001_3	C10 C4 C3	Not unusual (enough hits	16	120.723	120.264	1.927	0.238	0.459	117.385	124.274	120.474	0.02	
angle	00000001_3	C10 C4 C5	Not unusual (enough hits	1598	120.271	120.601	2.03	0.163	0.33	107.035	130.916	120.592	0	
angle	00000001_3	C5 C4 C3	Not unusual (enough hits	495	118.991	117.075	1.499	1.278	1.916	105.829	123.29	116.994	0.01	
angle	00000001_3	C6 C5 C4	Not unusual (enough hits	11395	119.695	121.039	1.437	0.935	1.344	93.35	147.791	121.028	0	
angle	00000001_3	C5 C6 C1	Not unusual (enough hits	289	119.314	117.43	0.964	1.955	1.884	114.685	123.178	117.353	0.077	
angle	00000001_3	CL11 C1 N2	Not unusual (enough hits	239	119.458	116.229	2.378	1.358	3.229	106.087	140.591	115.898	0.115	
angle	00000001_3	C6 C1 CL11	Not unusual (enough hits	437	120.392	119.088	2.36	0.553	1.304	96.671	128.568	119.178	0.034	
angle	00000001_3	N4 C11 N21	Unusual (enough hits)	19	179.171	173.083	1.486	4.098	6.088	171.407	177.175	173.067	1.996	
angle	00000001_3	C7 S1 C8	Unusual (enough hits)	103	97.41	91.388	1.578	3.816	6.021	86.226	98.264	91.466	0.854	
angle	00000001_3	C9 N3 C8	Unusual (enough hits)	18	117.675	111.69	2.909	2.058	5.985	107.905	117.378	110.821	0.297	
angle	00000001_3	C10 N3 C9	Unusual (enough hits)	26	117.09	122.598	2.502	2.201	5.508	115.726	126.639	123.077	1.364	
angle	00000001_3	C4 C3 N2	Unusual (enough hits)	225	120.177	123.744	1.746	2.044	3.567	117.703	127.597	124.357	0.02	
angle	00000001_3	C3 N2 C1	Unusual (enough hits)	179	121.648	116.435	1.303	4.002	5.213	112.785	121.37	116.186	0.278	
angle	00000001_3	C6 C1 N2	Unusual (enough hits)	167	120.143	124.711	1.675	2.727	4.568	117.068	127.876	125.155	0.096	
angle	00000001_4	C11 N21 C8	No hits	0	124.136									
angle	00000001_4	S1 C8 N3	No hits	0	110.459									
angle	00000001_4	S1 C8 N21	Not unusual (enough hits	20	124.918	120.612	4.097	1.051	4.306	112.48	127.569	119.504	0.753	

angle	00000001_4	N21 C8 N3	Not unusual (enough hits	12	124.622	122.214	1.748	1.377	2.408	118.888	125.399	122.646	0.777	
angle	00000001_4	C10 N3 C8	Not unusual (enough hits	15	125.625	125.32	2.241	0.136	0.304	121.681	128.396	124.864	0.379	
angle	00000001_4	C7 C9 N3	Not unusual (enough hits	22	107.247	109.022	2.757	0.644	1.774	99.107	111.59	109.508	0.059	
angle	00000001_4	C9 C7 S1	Not unusual (enough hits	252	107.27	106.672	1.963	0.304	0.598	96.401	118.991	106.637	0.008	
angle	00000001_4	C4 C10 N3	Not unusual (enough hits	20	115.287	112.452	1.868	1.518	2.835	107.509	115.688	112.49	0.401	
angle	00000001_4	C10 C4 C3	Not unusual (enough hits	16	122.482	120.264	1.927	1.151	2.218	117.385	124.274	120.474	0.363	
angle	00000001_4	C10 C4 C5	Not unusual (enough hits	1598	118.367	120.601	2.03	1.101	2.235	107.035	130.916	120.592	0.002	
angle	00000001_4	C5 C4 C3	Not unusual (enough hits	495	119.149	117.075	1.499	1.383	2.074	105.829	123.29	116.994	0.032	
angle	00000001_4	C6 C5 C4	Not unusual (enough hits	11395	120.127	121.039	1.437	0.635	0.912	93.35	147.791	121.028	0	
angle	00000001_4	CL11 C1 N2	Not unusual (enough hits	239	120.724	116.229	2.378	1.89	4.495	106.087	140.591	115.898	0.227	
angle	00000001_4	C6 C1 CL11	Not unusual (enough hits	437	119.286	119.088	2.36	0.084	0.198	96.671	128.568	119.178	0.004	
angle	00000001_4	N4 C11 N21	Unusual (enough hits)	19	178.934	173.083	1.486	3.938	5.851	171.407	177.175	173.067	1.759	
angle	00000001_4	C7 S1 C8	Unusual (enough hits)	103	97.035	91.388	1.578	3.578	5.646	86.226	98.264	91.466	1.229	
angle	00000001_4	C9 N3 C8	Unusual (enough hits)	18	117.989	111.69	2.909	2.166	6.299	107.905	117.378	110.821	0.611	
angle	00000001_4	C10 N3 C9	Unusual (enough hits)	26	116.386	122.598	2.502	2.483	6.212	115.726	126.639	123.077	0.66	
angle	00000001_4	C4 C3 N2	Unusual (enough hits)	225	119.325	123.744	1.746	2.532	4.42	117.703	127.597	124.357	0.121	
angle	00000001_4	C3 N2 C1	Unusual (enough hits)	179	121.933	116.435	1.303	4.22	5.498	112.785	121.37	116.186	0.563	
angle	00000001_4	C5 C6 C1	Unusual (enough hits)	289	119.475	117.43	0.964	2.122	2.045	114.685	123.178	117.353	0.009	
angle	00000001_4	C6 C1 N2	Unusual (enough hits)	167	119.99	124.711	1.675	2.818	4.721	117.068	127.876	125.155	0.057	
angle	00000001_5	C11 N21 C8	No hits	0	125.054									
angle	00000001_5	S1 C8 N3	No hits	0	110.615									
angle	00000001_5	S1 C8 N21	Not unusual (enough hits	20	125.109	120.612	4.097	1.098	4.497	112.48	127.569	119.504	0.562	
angle	00000001_5	N21 C8 N3	Not unusual (enough hits	12	124.276	122.214	1.748	1.179	2.062	118.888	125.399	122.646	0.443	
angle	00000001_5	C10 N3 C8	Not unusual (enough hits	15	125.268	125.32	2.241	0.023	0.052	121.681	128.396	124.864	0.277	
angle	00000001_5	C7 C9 N3	Not unusual (enough hits	22	106.933	109.022	2.757	0.758	2.089	99.107	111.59	109.508	0.218	
angle	00000001_5	C9 C7 S1	Not unusual (enough hits	252	107.455	106.672	1.963	0.399	0.783	96.401	118.991	106.637	0.024	
angle	00000001_5	C4 C10 N3	Not unusual (enough hits	20	115.518	112.452	1.868	1.641	3.066	107.509	115.688	112.49	0.17	
angle	00000001_5	C10 C4 C3	Not unusual (enough hits	16	122.448	120.264	1.927	1.133	2.183	117.385	124.274	120.474	0.328	
angle	00000001_5	C10 C4 C5	Not unusual (enough hits	1598	118.698	120.601	2.03	0.938	1.904	107.035	130.916	120.592	0.001	
angle	00000001_5	C5 C4 C3	Not unusual (enough hits	495	118.852	117.075	1.499	1.186	1.778	105.829	123.29	116.994	0.01	
angle	00000001_5	C6 C5 C4	Not unusual (enough hits	11395	120.305	121.039	1.437	0.511	0.734	93.35	147.791	121.028	0	
angle	00000001_5	C5 C6 C1	Not unusual (enough hits	289	119.252	117.43	0.964	1.89	1.822	114.685	123.178	117.353	0.086	
angle	00000001_5	CL11 C1 N2	Not unusual (enough hits	239	120.476	116.229	2.378	1.786	4.247	106.087	140.591	115.898	0.021	
angle	00000001_5	C6 C1 CL11	Not unusual (enough hits	437	119.124	119.088	2.36	0.015	0.036	96.671	128.568	119.178	0.002	
angle	00000001_5	N4 C11 N21	Unusual (enough hits)	19	178.86	173.083	1.486	3.888	5.777	171.407	177.175	173.067	1.685	
angle	00000001_5	C7 S1 C8	Unusual (enough hits)	103	96.657	91.388	1.578	3.339	5.269	86.226	98.264	91.466	1.607	
angle	00000001_5	C9 N3 C8	Unusual (enough hits)	18	118.34	111.69	2.909	2.286	6.65	107.905	117.378	110.821	0.962	
angle	00000001_5	C10 N3 C9	Unusual (enough hits)	26	116.39	122.598	2.502	2.481	6.208	115.726	126.639	123.077	0.664	
angle	00000001_5	C4 C3 N2	Unusual (enough hits)	225	119.678	123.744	1.746	2.33	4.067	117.703	127.597	124.357	0.067	

angle	00000001_5	C3 N2 C1	Unusual (enough hits)	179	121.498	116.435	1.303	3.886	5.063	112.785	121.37	116.186	0.128	
angle	00000001_5	C6 C1 N2	Unusual (enough hits)	167	120.393	124.711	1.675	2.577	4.318	117.068	127.876	125.155	0.064	
torsion	00000001_1	S1 C8 N21 C11	Not unusual (enough hits	45	−0.239								0.249	0.111
torsion	00000001_1	C4 C10 N3 C8	Not unusual (enough hits	40	82.335								1.203	0.25
torsion	00000001_1	C4 C10 N3 C9	Not unusual (enough hits	50	−97.799								0.063	0.18
torsion	00000001_1	C3 C4 C10 N3	Not unusual (enough hits	670	50.377								0.181	0.112
torsion	00000001_1	C5 C4 C10 N3	Not unusual (enough hits	653	−130.604								0.231	0.104
torsion	00000001_1	N4 C11 N21 C8	Not unusual (few hits)	2	−130.817								9.62	0.5
torsion	00000001_1	N3 C8 N21 C11	Unusual (enough hits)	47	179.672								1.461	0.021
torsion	00000001_2	S1 C8 N21 C11	Not unusual (enough hits	45	−0.409								0.079	0.111
torsion	00000001_2	C4 C10 N3 C8	Not unusual (enough hits	40	76.808								1.164	0.225
torsion	00000001_2	C4 C10 N3 C9	Not unusual (enough hits	50	−103.522								0.589	0.16
torsion	00000001_2	C3 C4 C10 N3	Not unusual (enough hits	670	52.879								0.041	0.11
torsion	00000001_2	C5 C4 C10 N3	Not unusual (enough hits	653	−128.29								0.215	0.107
torsion	00000001_2	N4 C11 N21 C8	Not unusual (few hits)	2	169.622								2.085	0.5
torsion	00000001_2	N3 C8 N21 C11	Unusual (enough hits)	47	179.986								1.775	0.021
torsion	00000001_3	S1 C8 N21 C11	Not unusual (enough hits	45	−0.093								0.395	0.111
torsion	00000001_3	C4 C10 N3 C8	Not unusual (enough hits	40	83.139								0.399	0.25
torsion	00000001_3	C4 C10 N3 C9	Not unusual (enough hits	50	−96.632								0.278	0.18
torsion	00000001_3	C3 C4 C10 N3	Not unusual (enough hits	670	65.341								0.004	0.169
torsion	00000001_3	C5 C4 C10 N3	Not unusual (enough hits	653	−113.264								0.053	0.153
torsion	00000001_3	N3 C8 N21 C11	Unusual (enough hits)	47	179.898								1.687	0.021
torsion	00000001_3	N4 C11 N21 C8	Unusual (few hits)	2	43.055								97.382	0
torsion	00000001_4	S1 C8 N21 C11	Not unusual (enough hits	45	0.08								0.408	0.111
torsion	00000001_4	C4 C10 N3 C8	Not unusual (enough hits	40	85.035								0.912	0.3
torsion	00000001_4	C4 C10 N3 C9	Not unusual (enough hits	50	−95.074								0.161	0.18
torsion	00000001_4	C3 C4 C10 N3	Not unusual (enough hits	670	51.508								0.082	0.112
torsion	00000001_4	C5 C4 C10 N3	Not unusual (enough hits	653	−129.065								0.247	0.109
torsion	00000001_4	N3 C8 N21 C11	Unusual (enough hits)	47	179.861								1.65	0.021
torsion	00000001_4	N4 C11 N21 C8	Unusual (few hits)	2	51.024								89.413	0
torsion	00000001_5	S1 C8 N21 C11	Not unusual (enough hits	45	−0.564								0.076	0.111
torsion	00000001_5	C4 C10 N3 C8	Not unusual (enough hits	40	80.246								0.282	0.25
torsion	00000001_5	C4 C10 N3 C9	Not unusual (enough hits	50	−100.296								0.16	0.18
torsion	00000001_5	C3 C4 C10 N3	Not unusual (enough hits	670	48.114								0.043	0.103
torsion	00000001_5	C5 C4 C10 N3	Not unusual (enough hits	653	−131.327								0.048	0.096
torsion	00000001_5	N3 C8 N21 C11	Unusual (enough hits)	47	179.366								1.155	0.021
torsion	00000001_5	N4 C11 N21 C8	Unusual (few hits)	2	−98.725								41.712	0
ring	00000001_1	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.246	25.617			0.356
ring	00000001_1	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.104	8.131			1

ring	00000001_2	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.348	25.569			0.356
ring	00000001_2	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.117	8.174			1
ring	00000001_3	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.194	25.649			0.356
ring	00000001_3	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.256	8.148			1
ring	00000001_4	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.169	25.629			0.356
ring	00000001_4	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.057	8.268			1
ring	00000001_5	C8 S1 C7 C9 N3	Not unusual (enough hits	45						0.137	25.584			0.356
ring	00000001_5	C4 C3 N2 C1 C6 C5	Not unusual (enough hits	320						0.371	8.101			1

Table 7. Geometry Analysis by Mogul of CH-IMI in Complex with Wild-Type *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	| z-score |	| x - mean |	Minimum	Maximum	Median	| d(min) |	Local density
bond	00000001_1	C1 CL	Not unusual (enough hits	743	1.702	1.738	0.019	1.951	0.036	1.561	1.806	1.74	0.001	
bond	00000001_1	C2 N1	Not unusual (enough hits	2818	1.38	1.34	0.022	1.788	0.04	1.05	1.584	1.337	0	
bond	00000001_1	C4 C3	Not unusual (enough hits	10549	1.528	1.51	0.019	0.952	0.018	1.278	1.842	1.51	0	
bond	00000001_1	C4 N2	Not unusual (enough hits	931	1.464	1.465	0.015	0.058	0.001	1.386	1.561	1.465	0	
bond	00000001_1	C5 C3	Not unusual (enough hits	14050	1.427	1.384	0.022	1.981	0.043	0.618	1.8	1.386	0	
bond	00000001_1	C6 C1	Not unusual (enough hits	479	1.4	1.373	0.022	1.273	0.028	1.267	1.455	1.373	0	
bond	00000001_1	C6 C5	Not unusual (enough hits	20000	1.417	1.383	0.019	1.796	0.033	0.882	1.685	1.383	0	
bond	00000001_1	C8 C7	Not unusual (enough hits	17	1.351	1.404	0.033	1.595	0.053	1.296	1.433	1.409	0.005	
bond	00000001_1	C9 N3	Not unusual (enough hits	1745	1.443	1.457	0.022	0.643	0.014	1.204	1.687	1.458	0	
bond	00000001_1	C10 N2	Not unusual (enough hits	1978	1.478	1.468	0.023	0.424	0.01	1.336	1.699	1.468	0	
bond	00000001_1	C10 C9	Not unusual (enough hits	252	1.547	1.521	0.02	1.344	0.026	1.452	1.629	1.52	0	
bond	00000001_1	C8 N4	Not unusual (enough hits	46	1.45	1.376	0.045	1.662	0.074	1.223	1.481	1.363	0.001	
bond	00000001_1	O1 N4	Not unusual (enough hits	234	1.25	1.236	0.025	0.534	0.013	1.145	1.398	1.233	0	
bond	00000001_1	O2 N4	Not unusual (enough hits	234	1.233	1.236	0.025	0.143	0.004	1.145	1.398	1.233	0	
bond	00000001_1	C1 N1	Unusual (enough hits)	245	1.378	1.321	0.025	2.265	0.057	1.254	1.422	1.317	0.001	
bond	00000001_1	C2 C3	Unusual (enough hits)	560	1.422	1.381	0.017	2.451	0.041	1.279	1.497	1.382	0.004	
bond	00000001_1	C7 N2	Unusual (enough hits)	17	1.4	1.36	0.015	2.608	0.04	1.334	1.38	1.366	0.02	
bond	00000001_1	C7 N3	Unusual (enough hits)	17	1.373	1.335	0.016	2.304	0.037	1.308	1.372	1.331	0.001	
bond	00000001_2	C2 N1	Not unusual (enough hits	2818	1.381	1.34	0.022	1.836	0.041	1.05	1.584	1.337	0	
bond	00000001_2	C4 C3	Not unusual (enough hits	10549	1.522	1.51	0.019	0.666	0.012	1.278	1.842	1.51	0	
bond	00000001_2	C4 N2	Not unusual (enough hits	931	1.455	1.465	0.015	0.661	0.01	1.386	1.561	1.465	0	
bond	00000001_2	C5 C3	Not unusual (enough hits	14050	1.424	1.384	0.022	1.81	0.04	0.618	1.8	1.386	0	
bond	00000001_2	C6 C1	Not unusual (enough hits	479	1.4	1.373	0.022	1.239	0.027	1.267	1.455	1.373	0	
bond	00000001_2	C6 C5	Not unusual (enough hits	20000	1.412	1.383	0.019	1.574	0.029	0.882	1.685	1.383	0	
bond	00000001_2	C8 C7	Not unusual (enough hits	17	1.356	1.404	0.033	1.46	0.048	1.296	1.433	1.409	0.001	
bond	00000001_2	C9 N3	Not unusual (enough hits	1745	1.439	1.457	0.022	0.827	0.018	1.204	1.687	1.458	0	
bond	00000001_2	C10 N2	Not unusual (enough hits	1978	1.478	1.468	0.023	0.428	0.01	1.336	1.699	1.468	0	
bond	00000001_2	C10 C9	Not unusual (enough hits	252	1.543	1.521	0.02	1.142	0.022	1.452	1.629	1.52	0	
bond	00000001_2	C8 N4	Not unusual (enough hits	46	1.463	1.376	0.045	1.951	0.087	1.223	1.481	1.363	0.012	
bond	00000001_2	O1 N4	Not unusual (enough hits	234	1.245	1.236	0.025	0.358	0.009	1.145	1.398	1.233	0	
bond	00000001_2	O2 N4	Not unusual (enough hits	234	1.245	1.236	0.025	0.361	0.009	1.145	1.398	1.233	0	
bond	00000001_2	C1 CL	Unusual (enough hits)	743	1.685	1.738	0.019	2.874	0.053	1.561	1.806	1.74	0.001	
bond	00000001_2	C1 N1	Unusual (enough hits)	245	1.378	1.321	0.025	2.247	0.056	1.254	1.422	1.317	0.001	
bond	00000001_2	C2 C3	Unusual (enough hits)	560	1.427	1.381	0.017	2.738	0.046	1.279	1.497	1.382	0.007	
bond	00000001_2	C7 N2	Unusual (enough hits)	17	1.406	1.36	0.015	2.984	0.046	1.334	1.38	1.366	0.026	
bond	00000001_2	C7 N3	Unusual (enough hits)	17	1.371	1.335	0.016	2.223	0.036	1.308	1.372	1.331	0	
bond	00000001_3	C1 N1	Not unusual (enough hits	245	1.37	1.321	0.025	1.935	0.049	1.254	1.422	1.317	0.004	

bond	00000001_3	C2 N1	Not unusual (enough hits	2818	1.381	1.34	0.022	1.817	0.041	1.05	1.584	1.337	0	
bond	00000001_3	C2 C3	Not unusual (enough hits	560	1.411	1.381	0.017	1.79	0.03	1.279	1.497	1.382	0.001	
bond	00000001_3	C4 C3	Not unusual (enough hits	10549	1.519	1.51	0.019	0.471	0.009	1.278	1.842	1.51	0	
bond	00000001_3	C4 N2	Not unusual (enough hits	931	1.467	1.465	0.015	0.139	0.002	1.386	1.561	1.465	0	
bond	00000001_3	C6 C1	Not unusual (enough hits	479	1.403	1.373	0.022	1.403	0.031	1.267	1.455	1.373	0	
bond	00000001_3	C6 C5	Not unusual (enough hits	20000	1.418	1.383	0.019	1.888	0.035	0.882	1.685	1.383	0	
bond	00000001_3	C8 C7	Not unusual (enough hits	17	1.347	1.404	0.033	1.729	0.057	1.296	1.433	1.409	0.01	
bond	00000001_3	C9 N3	Not unusual (enough hits	1745	1.439	1.457	0.022	0.852	0.019	1.204	1.687	1.458	0	
bond	00000001_3	C10 N2	Not unusual (enough hits	1978	1.473	1.468	0.023	0.209	0.005	1.336	1.699	1.468	0	
bond	00000001_3	C10 C9	Not unusual (enough hits	252	1.546	1.521	0.02	1.304	0.026	1.452	1.629	1.52	0.001	
bond	00000001_3	C8 N4	Not unusual (enough hits	46	1.447	1.376	0.045	1.589	0.071	1.223	1.481	1.363	0.004	
bond	00000001_3	O1 N4	Not unusual (enough hits	234	1.242	1.236	0.025	0.218	0.005	1.145	1.398	1.233	0	
bond	00000001_3	O2 N4	Not unusual (enough hits	234	1.239	1.236	0.025	0.124	0.003	1.145	1.398	1.233	0	
bond	00000001_3	C1 CL	Unusual (enough hits)	743	1.692	1.738	0.019	2.472	0.046	1.561	1.806	1.74	0.002	
bond	00000001_3	C5 C3	Unusual (enough hits)	14050	1.431	1.384	0.022	2.143	0.047	0.618	1.8	1.386	0	
bond	00000001_3	C7 N2	Unusual (enough hits)	17	1.402	1.36	0.015	2.75	0.042	1.334	1.38	1.366	0.022	
bond	00000001_3	C7 N3	Unusual (enough hits)	17	1.369	1.335	0.016	2.079	0.034	1.308	1.372	1.331	0.002	
bond	00000001_4	C2 N1	Not unusual (enough hits	2818	1.382	1.34	0.022	1.853	0.042	1.05	1.584	1.337	0	
bond	00000001_4	C4 C3	Not unusual (enough hits	10549	1.521	1.51	0.019	0.595	0.011	1.278	1.842	1.51	0	
bond	00000001_4	C4 N2	Not unusual (enough hits	931	1.464	1.465	0.015	0.1	0.002	1.386	1.561	1.465	0	
bond	00000001_4	C5 C3	Not unusual (enough hits	14050	1.421	1.384	0.022	1.691	0.037	0.618	1.8	1.386	0	
bond	00000001_4	C6 C1	Not unusual (enough hits	479	1.393	1.373	0.022	0.938	0.021	1.267	1.455	1.373	0	
bond	00000001_4	C6 C5	Not unusual (enough hits	20000	1.418	1.383	0.019	1.855	0.034	0.882	1.685	1.383	0	
bond	00000001_4	C8 C7	Not unusual (enough hits	17	1.343	1.404	0.033	1.847	0.061	1.296	1.433	1.409	0.013	
bond	00000001_4	C7 N3	Not unusual (enough hits	17	1.364	1.335	0.016	1.762	0.029	1.308	1.372	1.331	0.003	
bond	00000001_4	C9 N3	Not unusual (enough hits	1745	1.44	1.457	0.022	0.809	0.018	1.204	1.687	1.458	0	
bond	00000001_4	C10 N2	Not unusual (enough hits	1978	1.471	1.468	0.023	0.13	0.003	1.336	1.699	1.468	0	
bond	00000001_4	C10 C9	Not unusual (enough hits	252	1.544	1.521	0.02	1.172	0.023	1.452	1.629	1.52	0	
bond	00000001_4	C8 N4	Not unusual (enough hits	46	1.453	1.376	0.045	1.725	0.077	1.223	1.481	1.363	0.002	
bond	00000001_4	O1 N4	Not unusual (enough hits	234	1.237	1.236	0.025	0.022	0.001	1.145	1.398	1.233	0	
bond	00000001_4	O2 N4	Not unusual (enough hits	234	1.23	1.236	0.025	0.251	0.006	1.145	1.398	1.233	0	
bond	00000001_4	C1 CL	Unusual (enough hits)	743	1.692	1.738	0.019	2.469	0.046	1.561	1.806	1.74	0.002	
bond	00000001_4	C1 N1	Unusual (enough hits)	245	1.374	1.321	0.025	2.075	0.052	1.254	1.422	1.317	0.001	
bond	00000001_4	C2 C3	Unusual (enough hits)	560	1.416	1.381	0.017	2.09	0.035	1.279	1.497	1.382	0.001	
bond	00000001_4	C7 N2	Unusual (enough hits)	17	1.402	1.36	0.015	2.762	0.043	1.334	1.38	1.366	0.023	
bond	00000001_5	C1 N1	Not unusual (enough hits	245	1.37	1.321	0.025	1.933	0.049	1.254	1.422	1.317	0.004	
bond	00000001_5	C2 N1	Not unusual (enough hits	2818	1.378	1.34	0.022	1.689	0.038	1.05	1.584	1.337	0	
bond	00000001_5	C4 C3	Not unusual (enough hits	10549	1.521	1.51	0.019	0.602	0.011	1.278	1.842	1.51	0	
bond	00000001_5	C4 N2	Not unusual (enough hits	931	1.456	1.465	0.015	0.558	0.009	1.386	1.561	1.465	0	

bond	00000001_5	C5 C3	Not unusual (enough hits	14050	1.427	1.384	0.022	1.96	0.043	0.618	1.8	1.386	0	
bond	00000001_5	C6 C1	Not unusual (enough hits	479	1.406	1.373	0.022	1.538	0.034	1.267	1.455	1.373	0	
bond	00000001_5	C6 C5	Not unusual (enough hits	20000	1.419	1.383	0.019	1.91	0.035	0.882	1.685	1.383	0	
bond	00000001_5	C8 C7	Not unusual (enough hits	17	1.357	1.404	0.033	1.43	0.047	1.296	1.433	1.409	0	
bond	00000001_5	C7 N3	Not unusual (enough hits	17	1.368	1.335	0.016	1.993	0.032	1.308	1.372	1.331	0	
bond	00000001_5	C9 N3	Not unusual (enough hits	1745	1.449	1.457	0.022	0.374	0.008	1.204	1.687	1.458	0	
bond	00000001_5	C10 N2	Not unusual (enough hits	1978	1.475	1.468	0.023	0.314	0.007	1.336	1.699	1.468	0	
bond	00000001_5	C10 C9	Not unusual (enough hits	252	1.544	1.521	0.02	1.204	0.024	1.452	1.629	1.52	0.001	
bond	00000001_5	C8 N4	Not unusual (enough hits	46	1.454	1.376	0.045	1.749	0.078	1.223	1.481	1.363	0.003	
bond	00000001_5	O1 N4	Not unusual (enough hits	234	1.242	1.236	0.025	0.243	0.006	1.145	1.398	1.233	0	
bond	00000001_5	O2 N4	Not unusual (enough hits	234	1.245	1.236	0.025	0.332	0.008	1.145	1.398	1.233	0	
bond	00000001_5	C1 CL	Unusual (enough hits)	743	1.69	1.738	0.019	2.608	0.048	1.561	1.806	1.74	0.001	
bond	00000001_5	C2 C3	Unusual (enough hits)	560	1.423	1.381	0.017	2.506	0.042	1.279	1.497	1.382	0.005	
bond	00000001_5	C7 N2	Unusual (enough hits)	17	1.402	1.36	0.015	2.745	0.042	1.334	1.38	1.366	0.022	
angle	00000001_1	CL C1 N1	Not unusual (enough hits	239	115.272	116.229	2.378	0.402	0.957	106.087	140.591	115.898	0.005	
angle	00000001_1	C6 C1 CL	Not unusual (enough hits	437	120.584	119.088	2.36	0.634	1.495	96.671	128.568	119.178	0.009	
angle	00000001_1	C6 C1 N1	Not unusual (enough hits	167	124.144	124.711	1.675	0.339	0.567	117.068	127.876	125.155	0.089	
angle	00000001_1	C2 N1 C1	Not unusual (enough hits	179	117.03	116.435	1.303	0.456	0.595	112.785	121.37	116.186	0.023	
angle	00000001_1	C3 C2 N1	Not unusual (enough hits	225	123.923	123.744	1.746	0.103	0.179	117.703	127.597	124.357	0.006	
angle	00000001_1	C4 C3 C2	Not unusual (enough hits	155	123.292	121.018	1.641	1.386	2.274	113.768	126.783	120.987	0.024	
angle	00000001_1	C5 C3 C2	Not unusual (enough hits	495	116.29	117.075	1.499	0.524	0.785	105.829	123.29	116.994	0.002	
angle	00000001_1	C4 C3 C5	Not unusual (enough hits	10997	120.416	120.774	1.905	0.188	0.359	90.622	143.824	120.777	0	
angle	00000001_1	C3 C4 N2	Not unusual (enough hits	764	115.849	113.088	1.717	1.608	2.761	104.07	122.755	113.045	0.023	
angle	00000001_1	C4 N2 C7	Not unusual (enough hits	25	130.408	122.65	5.52	1.406	7.758	111.419	127.449	125.38	2.959	
angle	00000001_1	C4 N2 C10	Not unusual (enough hits	109	118.605	120.505	2.722	0.698	1.9	110.736	125.952	121.036	0.018	
angle	00000001_1	C10 N2 C7	Not unusual (enough hits	15	110.987	110.822	0.824	0.2	0.165	109.799	112.489	110.756	0.021	
angle	00000001_1	C6 C5 C3	Not unusual (enough hits	11395	121.228	121.039	1.437	0.131	0.188	93.35	147.791	121.028	0	
angle	00000001_1	C5 C6 C1	Not unusual (enough hits	289	117.385	117.43	0.964	0.047	0.045	114.685	123.178	117.353	0.001	
angle	00000001_1	C8 C7 N2	Not unusual (enough hits	11	125.678	124.573	3.022	0.366	1.105	119.122	129.846	123.452	0.032	
angle	00000001_1	N3 C7 N2	Not unusual (enough hits	15	107.594	109.761	1.606	1.35	2.168	106.878	112.614	110.096	0.009	
angle	00000001_1	C8 C7 N3	Not unusual (enough hits	22	126.728	125.908	1.325	0.619	0.82	122.812	128.392	126.108	0.05	
angle	00000001_1	C7 C8 N4	Not unusual (enough hits	17	124.078	123.744	1.302	0.257	0.334	121.873	127.614	123.627	0.048	
angle	00000001_1	C9 N3 C7	Not unusual (enough hits	51	114.098	111.956	1.974	1.085	2.142	106.231	117.591	112.19	0.228	
angle	00000001_1	C10 C9 N3	Not unusual (enough hits	191	103.254	102.619	1.341	0.473	0.635	94.971	107.419	102.75	0.002	
angle	00000001_1	C9 C10 N2	Not unusual (enough hits	85	104.067	102.951	1.651	0.676	1.115	99.561	108.169	102.882	0.127	
angle	00000001_1	O1 N4 C8	Not unusual (enough hits	92	121.156	119.959	2.943	0.407	1.197	109.341	135.081	119.617	0.055	
angle	00000001_1	O2 N4 C8	Not unusual (enough hits	92	114.461	119.959	2.943	1.868	5.498	109.341	135.081	119.617	1.021	
angle	00000001_1	O2 N4 O1	Not unusual (enough hits	116	124.384	121.724	2.321	1.146	2.659	108.971	128.317	122.551	0.126	
angle	00000001_2	CL C1 N1	Not unusual (enough hits	239	115.568	116.229	2.378	0.278	0.661	106.087	140.591	115.898	0	

angle	00000001_2	C6 C1 CL	Not unusual (enough hits	437	120.107	119.088	2.36	0.432	1.018	96.671	128.568	119.178	0.002	
angle	00000001_2	C6 C1 N1	Not unusual (enough hits	167	124.325	124.711	1.675	0.23	0.386	117.068	127.876	125.155	0.069	
angle	00000001_2	C2 N1 C1	Not unusual (enough hits	179	116.791	116.435	1.303	0.273	0.355	112.785	121.37	116.186	0.008	
angle	00000001_2	C3 C2 N1	Not unusual (enough hits	225	123.823	123.744	1.746	0.045	0.079	117.703	127.597	124.357	0.003	
angle	00000001_2	C4 C3 C2	Not unusual (enough hits	155	123.913	121.018	1.641	1.764	2.895	113.768	126.783	120.987	0.007	
angle	00000001_2	C5 C3 C2	Not unusual (enough hits	495	116.322	117.075	1.499	0.502	0.752	105.829	123.29	116.994	0.006	
angle	00000001_2	C4 C3 C5	Not unusual (enough hits	10997	119.763	120.774	1.905	0.531	1.011	90.622	143.824	120.777	0	
angle	00000001_2	C3 C4 N2	Not unusual (enough hits	764	115.813	113.088	1.717	1.587	2.725	104.07	122.755	113.045	0.007	
angle	00000001_2	C4 N2 C7	Not unusual (enough hits	25	130.974	122.65	5.52	1.508	8.324	111.419	127.449	125.38	3.525	
angle	00000001_2	C4 N2 C10	Not unusual (enough hits	109	118.145	120.505	2.722	0.867	2.36	110.736	125.952	121.036	0.058	
angle	00000001_2	C10 N2 C7	Not unusual (enough hits	15	110.881	110.822	0.824	0.071	0.059	109.799	112.489	110.756	0.07	
angle	00000001_2	C6 C5 C3	Not unusual (enough hits	11395	121.282	121.039	1.437	0.169	0.243	93.35	147.791	121.028	0	
angle	00000001_2	C5 C6 C1	Not unusual (enough hits	289	117.457	117.43	0.964	0.028	0.027	114.685	123.178	117.353	0	
angle	00000001_2	C8 C7 N2	Not unusual (enough hits	11	126.535	124.573	3.022	0.649	1.962	119.122	129.846	123.452	0.123	
angle	00000001_2	N3 C7 N2	Not unusual (enough hits	15	107.3	109.761	1.606	1.533	2.461	106.878	112.614	110.096	0.203	
angle	00000001_2	C8 C7 N3	Not unusual (enough hits	22	126.165	125.908	1.325	0.194	0.257	122.812	128.392	126.108	0.118	
angle	00000001_2	C7 C8 N4	Not unusual (enough hits	17	123.202	123.744	1.302	0.416	0.542	121.873	127.614	123.627	0.049	
angle	00000001_2	C9 N3 C7	Not unusual (enough hits	51	114.325	111.956	1.974	1.2	2.369	106.231	117.591	112.19	0.382	
angle	00000001_2	C10 C9 N3	Not unusual (enough hits	191	103.407	102.619	1.341	0.587	0.788	94.971	107.419	102.75	0.008	
angle	00000001_2	C9 C10 N2	Not unusual (enough hits	85	104.087	102.951	1.651	0.688	1.135	99.561	108.169	102.882	0.106	
angle	00000001_2	O1 N4 C8	Not unusual (enough hits	92	120.632	119.959	2.943	0.229	0.673	109.341	135.081	119.617	0.002	
angle	00000001_2	O2 N4 C8	Not unusual (enough hits	92	115.247	119.959	2.943	1.601	4.712	109.341	135.081	119.617	0.235	
angle	00000001_2	O2 N4 O1	Not unusual (enough hits	116	124.121	121.724	2.321	1.033	2.397	108.971	128.317	122.551	0.035	
angle	00000001_3	CL C1 N1	Not unusual (enough hits	239	114.831	116.229	2.378	0.588	1.398	106.087	140.591	115.898	0.035	
angle	00000001_3	C6 C1 CL	Not unusual (enough hits	437	121.076	119.088	2.36	0.843	1.988	96.671	128.568	119.178	0.017	
angle	00000001_3	C6 C1 N1	Not unusual (enough hits	167	124.092	124.711	1.675	0.369	0.619	117.068	127.876	125.155	0.04	
angle	00000001_3	C2 N1 C1	Not unusual (enough hits	179	117.27	116.435	1.303	0.641	0.835	112.785	121.37	116.186	0.131	
angle	00000001_3	C3 C2 N1	Not unusual (enough hits	225	123.978	123.744	1.746	0.134	0.234	117.703	127.597	124.357	0.005	
angle	00000001_3	C4 C3 C2	Not unusual (enough hits	155	122.389	121.018	1.641	0.836	1.371	113.768	126.783	120.987	0.034	
angle	00000001_3	C5 C3 C2	Not unusual (enough hits	495	116.415	117.075	1.499	0.44	0.659	105.829	123.29	116.994	0.002	
angle	00000001_3	C4 C3 C5	Not unusual (enough hits	10997	121.195	120.774	1.905	0.221	0.42	90.622	143.824	120.777	0	
angle	00000001_3	C3 C4 N2	Not unusual (enough hits	764	111.901	113.088	1.717	0.691	1.187	104.07	122.755	113.045	0.004	
angle	00000001_3	C4 N2 C7	Not unusual (enough hits	25	130.842	122.65	5.52	1.484	8.192	111.419	127.449	125.38	3.393	
angle	00000001_3	C4 N2 C10	Not unusual (enough hits	109	118.541	120.505	2.722	0.721	1.964	110.736	125.952	121.036	0.035	
angle	00000001_3	C10 N2 C7	Not unusual (enough hits	15	110.617	110.822	0.824	0.249	0.205	109.799	112.489	110.756	0.115	
angle	00000001_3	C6 C5 C3	Not unusual (enough hits	11395	121.023	121.039	1.437	0.012	0.017	93.35	147.791	121.028	0	
angle	00000001_3	C5 C6 C1	Not unusual (enough hits	289	117.222	117.43	0.964	0.216	0.208	114.685	123.178	117.353	0.01	
angle	00000001_3	C8 C7 N2	Not unusual (enough hits	11	126.18	124.573	3.022	0.532	1.607	119.122	129.846	123.452	0.123	
angle	00000001_3	N3 C7 N2	Not unusual (enough hits	15	107.712	109.761	1.606	1.276	2.049	106.878	112.614	110.096	0.109	

angle	00000001_3	C8 C7 N3	Not unusual (enough hits	22	126.108	125.908	1.325	0.151	0.2	122.812	128.392	126.108	0.175	
angle	00000001_3	C7 C8 N4	Not unusual (enough hits	17	123.245	123.744	1.302	0.383	0.498	121.873	127.614	123.627	0.006	
angle	00000001_3	C9 N3 C7	Not unusual (enough hits	51	114.208	111.956	1.974	1.141	2.252	106.231	117.591	112.19	0.338	
angle	00000001_3	C10 C9 N3	Not unusual (enough hits	191	103.093	102.619	1.341	0.353	0.473	94.971	107.419	102.75	0.002	
angle	00000001_3	C9 C10 N2	Not unusual (enough hits	85	104.37	102.951	1.651	0.859	1.419	99.561	108.169	102.882	0.177	
angle	00000001_3	O1 N4 C8	Not unusual (enough hits	92	120.864	119.959	2.943	0.307	0.905	109.341	135.081	119.617	0.017	
angle	00000001_3	O2 N4 C8	Not unusual (enough hits	92	114.691	119.959	2.943	1.79	5.268	109.341	135.081	119.617	0.791	
angle	00000001_3	O2 N4 O1	Not unusual (enough hits	116	124.445	121.724	2.321	1.172	2.721	108.971	128.317	122.551	0.188	
angle	00000001_4	CL C1 N1	Not unusual (enough hits	239	115.332	116.229	2.378	0.377	0.897	106.087	140.591	115.898	0.004	
angle	00000001_4	C6 C1 CL	Not unusual (enough hits	437	120.614	119.088	2.36	0.647	1.526	96.671	128.568	119.178	0.005	
angle	00000001_4	C6 C1 N1	Not unusual (enough hits	167	124.054	124.711	1.675	0.392	0.657	117.068	127.876	125.155	0.002	
angle	00000001_4	C2 N1 C1	Not unusual (enough hits	179	117.427	116.435	1.303	0.761	0.992	112.785	121.37	116.186	0.04	
angle	00000001_4	C3 C2 N1	Not unusual (enough hits	225	123.488	123.744	1.746	0.147	0.257	117.703	127.597	124.357	0.019	
angle	00000001_4	C4 C3 C2	Not unusual (enough hits	155	123.753	121.018	1.641	1.667	2.735	113.768	126.783	120.987	0.167	
angle	00000001_4	C5 C3 C2	Not unusual (enough hits	495	116.377	117.075	1.499	0.465	0.697	105.829	123.29	116.994	0.001	
angle	00000001_4	C4 C3 C5	Not unusual (enough hits	10997	119.864	120.774	1.905	0.478	0.91	90.622	143.824	120.777	0	
angle	00000001_4	C4 N2 C7	Not unusual (enough hits	25	130.902	122.65	5.52	1.495	8.252	111.419	127.449	125.38	3.453	
angle	00000001_4	C4 N2 C10	Not unusual (enough hits	109	118.36	120.505	2.722	0.788	2.145	110.736	125.952	121.036	0.069	
angle	00000001_4	C10 N2 C7	Not unusual (enough hits	15	110.734	110.822	0.824	0.106	0.088	109.799	112.489	110.756	0.003	
angle	00000001_4	C6 C5 C3	Not unusual (enough hits	11395	121.472	121.039	1.437	0.301	0.433	93.35	147.791	121.028	0	
angle	00000001_4	C5 C6 C1	Not unusual (enough hits	289	117.182	117.43	0.964	0.258	0.249	114.685	123.178	117.353	0.001	
angle	00000001_4	C8 C7 N2	Not unusual (enough hits	11	126.478	124.573	3.022	0.63	1.905	119.122	129.846	123.452	0.176	
angle	00000001_4	N3 C7 N2	Not unusual (enough hits	15	107.713	109.761	1.606	1.276	2.048	106.878	112.614	110.096	0.11	
angle	00000001_4	C8 C7 N3	Not unusual (enough hits	22	125.808	125.908	1.325	0.076	0.1	122.812	128.392	126.108	0.096	
angle	00000001_4	C7 C8 N4	Not unusual (enough hits	17	122.736	123.744	1.302	0.774	1.008	121.873	127.614	123.627	0.12	
angle	00000001_4	C9 N3 C7	Not unusual (enough hits	51	114.132	111.956	1.974	1.103	2.176	106.231	117.591	112.19	0.262	
angle	00000001_4	C10 C9 N3	Not unusual (enough hits	191	103.232	102.619	1.341	0.457	0.613	94.971	107.419	102.75	0.002	
angle	00000001_4	C9 C10 N2	Not unusual (enough hits	85	104.188	102.951	1.651	0.749	1.236	99.561	108.169	102.882	0.005	
angle	00000001_4	O1 N4 C8	Not unusual (enough hits	92	120.919	119.959	2.943	0.326	0.96	109.341	135.081	119.617	0.001	
angle	00000001_4	O2 N4 C8	Not unusual (enough hits	92	115.13	119.959	2.943	1.641	4.829	109.341	135.081	119.617	0.351	
angle	00000001_4	O2 N4 O1	Not unusual (enough hits	116	123.95	121.724	2.321	0.959	2.226	108.971	128.317	122.551	0.068	
angle	00000001_4	C3 C4 N2	Unusual (enough hits)	764	118.053	113.088	1.717	2.892	4.966	104.07	122.755	113.045	0.043	
angle	00000001_5	CL C1 N1	Not unusual (enough hits	239	114.659	116.229	2.378	0.66	1.57	106.087	140.591	115.898	0.017	
angle	00000001_5	C6 C1 CL	Not unusual (enough hits	437	120.972	119.088	2.36	0.798	1.884	96.671	128.568	119.178	0.002	
angle	00000001_5	C6 C1 N1	Not unusual (enough hits	167	124.368	124.711	1.675	0.205	0.343	117.068	127.876	125.155	0.027	
angle	00000001_5	C2 N1 C1	Not unusual (enough hits	179	117.109	116.435	1.303	0.517	0.674	112.785	121.37	116.186	0.029	
angle	00000001_5	C3 C2 N1	Not unusual (enough hits	225	123.813	123.744	1.746	0.039	0.068	117.703	127.597	124.357	0.007	
angle	00000001_5	C4 C3 C2	Not unusual (enough hits	155	122.78	121.018	1.641	1.074	1.761	113.768	126.783	120.987	0.019	
angle	00000001_5	C5 C3 C2	Not unusual (enough hits	495	116.6	117.075	1.499	0.316	0.474	105.829	123.29	116.994	0.001	

angle	00000001_5	C4 C3 C5	Not unusual (enough hits	10997	120.618	120.774	1.905	0.082	0.156	90.622	143.824	120.777	0	
angle	00000001_5	C3 C4 N2	Not unusual (enough hits	764	114.833	113.088	1.717	1.017	1.746	104.07	122.755	113.045	0.002	
angle	00000001_5	C4 N2 C7	Not unusual (enough hits	25	130.429	122.65	5.52	1.409	7.779	111.419	127.449	125.38	2.98	
angle	00000001_5	C4 N2 C10	Not unusual (enough hits	109	118.348	120.505	2.722	0.793	2.157	110.736	125.952	121.036	0.081	
angle	00000001_5	C10 N2 C7	Not unusual (enough hits	15	111.223	110.822	0.824	0.487	0.401	109.799	112.489	110.756	0.085	
angle	00000001_5	C6 C5 C3	Not unusual (enough hits	11395	120.865	121.039	1.437	0.122	0.175	93.35	147.791	121.028	0	
angle	00000001_5	C5 C6 C1	Not unusual (enough hits	289	117.245	117.43	0.964	0.192	0.185	114.685	123.178	117.353	0.001	
angle	00000001_5	C8 C7 N2	Not unusual (enough hits	11	125.912	124.573	3.022	0.443	1.339	119.122	129.846	123.452	0.202	
angle	00000001_5	N3 C7 N2	Not unusual (enough hits	15	107.322	109.761	1.606	1.519	2.439	106.878	112.614	110.096	0.182	
angle	00000001_5	C8 C7 N3	Not unusual (enough hits	22	126.766	125.908	1.325	0.647	0.858	122.812	128.392	126.108	0.02	
angle	00000001_5	C7 C8 N4	Not unusual (enough hits	17	124.476	123.744	1.302	0.562	0.732	121.873	127.614	123.627	0.013	
angle	00000001_5	C9 N3 C7	Not unusual (enough hits	51	114.302	111.956	1.974	1.189	2.346	106.231	117.591	112.19	0.405	
angle	00000001_5	C10 C9 N3	Not unusual (enough hits	191	103.054	102.619	1.341	0.324	0.434	94.971	107.419	102.75	0.005	
angle	00000001_5	C9 C10 N2	Not unusual (enough hits	85	104.099	102.951	1.651	0.695	1.148	99.561	108.169	102.882	0.094	
angle	00000001_5	O1 N4 C8	Not unusual (enough hits	92	121.008	119.959	2.943	0.356	1.049	109.341	135.081	119.617	0	
angle	00000001_5	O2 N4 C8	Not unusual (enough hits	92	114.796	119.959	2.943	1.754	5.163	109.341	135.081	119.617	0.685	
angle	00000001_5	O2 N4 O1	Not unusual (enough hits	116	124.195	121.724	2.321	1.065	2.471	108.971	128.317	122.551	0.039	
torsion	00000001_1	C2 C3 C4 N2	Not unusual (enough hits	349	58.746								0.408	0.16
torsion	00000001_1	C5 C3 C4 N2	Not unusual (enough hits	10853	−121.852								0.008	0.134
torsion	00000001_1	C3 C4 N2 C10	Not unusual (enough hits	182	−103.344								0.039	0.055
torsion	00000001_1	C7 C8 N4 O1	Not unusual (enough hits	40	−0.036								0.035	0.475
torsion	00000001_1	C7 C8 N4 O2	Not unusual (enough hits	40	179.887								0.199	0.475
torsion	00000001_1	N4 C8 C7 N2	Not unusual (few hits)	6	−179.933								0.25	0.667
torsion	00000001_1	N4 C8 C7 N3	Not unusual (few hits)	7	0.01								0.743	0.571
torsion	00000001_1	C3 C4 N2 C7	Unusual (enough hits)	49	76.843								3.171	0.02
torsion	00000001_2	C2 C3 C4 N2	Not unusual (enough hits	349	32.842								0.532	0.092
torsion	00000001_2	C5 C3 C4 N2	Not unusual (enough hits	10853	−147.646								0.011	0.114
torsion	00000001_2	C3 C4 N2 C7	Not unusual (enough hits	49	78.317								1.697	0.061
torsion	00000001_2	C3 C4 N2 C10	Not unusual (enough hits	182	−102.034								0.87	0.055
torsion	00000001_2	C7 C8 N4 O1	Not unusual (enough hits	40	0.229								0.024	0.475
torsion	00000001_2	C7 C8 N4 O2	Not unusual (enough hits	40	−179.658								0.03	0.475
torsion	00000001_2	N4 C8 C7 N2	Not unusual (few hits)	6	179.883								0.2	0.667
torsion	00000001_2	N4 C8 C7 N3	Not unusual (few hits)	7	−0.024								0.73	0.571
torsion	00000001_3	C2 C3 C4 N2	Not unusual (enough hits	349	75.942								0.139	0.117
torsion	00000001_3	C5 C3 C4 N2	Not unusual (enough hits	10853	−103.803								0.002	0.117
torsion	00000001_3	C3 C4 N2 C7	Not unusual (enough hits	49	81.772								1.758	0.102
torsion	00000001_3	C3 C4 N2 C10	Not unusual (enough hits	182	−98.144								1.932	0.077
torsion	00000001_3	C7 C8 N4 O1	Not unusual (enough hits	40	0.438								0.002	0.475
torsion	00000001_3	C7 C8 N4 O2	Not unusual (enough hits	40	−179.703								0.015	0.475

torsion	00000001_3	N4 C8 C7 N2	Not unusual (few hits)	6	−179.705								0.022	0.667
torsion	00000001_3	N4 C8 C7 N3	Not unusual (few hits)	7	0.165								0.588	0.571
torsion	00000001_4	C2 C3 C4 N2	Not unusual (enough hits	349	47.063								0.426	0.103
torsion	00000001_4	C5 C3 C4 N2	Not unusual (enough hits	10853	−133.813								0.012	0.128
torsion	00000001_4	C7 C8 N4 O1	Not unusual (enough hits	40	0.035								0.037	0.475
torsion	00000001_4	C7 C8 N4 O2	Not unusual (enough hits	40	−179.634								0.05	0.475
torsion	00000001_4	N4 C8 C7 N2	Not unusual (few hits)	6	179.585								0.098	0.667
torsion	00000001_4	N4 C8 C7 N3	Not unusual (few hits)	7	−0.147								0.606	0.571
torsion	00000001_4	C3 C4 N2 C7	Unusual (enough hits)	49	75.645								4.369	0.02
torsion	00000001_4	C3 C4 N2 C10	Unusual (enough hits)	182	−105.174								1.11	0.038
torsion	00000001_5	C2 C3 C4 N2	Not unusual (enough hits	349	54.091								0.1	0.138
torsion	00000001_5	C5 C3 C4 N2	Not unusual (enough hits	10853	−126.434								0.002	0.134
torsion	00000001_5	C7 C8 N4 O1	Not unusual (enough hits	40	0.233								0.028	0.475
torsion	00000001_5	C7 C8 N4 O2	Not unusual (enough hits	40	−179.613								0.029	0.475
torsion	00000001_5	N4 C8 C7 N2	Not unusual (few hits)	6	−179.935								0.253	0.667
torsion	00000001_5	N4 C8 C7 N3	Not unusual (few hits)	7	0.171								0.582	0.571
torsion	00000001_5	C3 C4 N2 C7	Unusual (enough hits)	49	75.477								4.537	0.02
torsion	00000001_5	C3 C4 N2 C10	Unusual (enough hits)	182	−104.87								0.806	0.038
ring	00000001_1	C1 N1 C2 C3 C5 C	Not unusual (enough hits	320						0.074	8.246			1
ring	00000001_1	N2 C7 N3 C9 C10	Not unusual (enough hits	35						0.682	16.343			0.771
ring	00000001_2	C1 N1 C2 C3 C5 C	Not unusual (enough hits	320						0.036	8.337			1
ring	00000001_2	N2 C7 N3 C9 C10	Not unusual (enough hits	35						0.641	16.351			0.771
ring	00000001_3	C1 N1 C2 C3 C5 C	Not unusual (enough hits	320						0.079	8.297			1
ring	00000001_3	N2 C7 N3 C9 C10	Not unusual (enough hits	35						0.657	16.33			0.771
ring	00000001_4	C1 N1 C2 C3 C5 C	Not unusual (enough hits	320						0.074	8.302			1
ring	00000001_4	N2 C7 N3 C9 C10	Not unusual (enough hits	35						0.702	16.392			0.771
ring	00000001_5	C1 N1 C2 C3 C5 C	Not unusual (enough hits	320						0.057	8.252			1
ring	00000001_5	N2 C7 N3 C9 C10	Not unusual (enough hits	35						0.685	16.347			0.771

Table 8. Geometry Analysis by Mogul of CH-IMI in Complex withGln55Arg Mutant of *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	| z-score |	| x - mean |	Minimum	Maximum	Median	| d(min) |	Local density
bond	00000001_1	C6 C1	Not unusual (enough hits)	479	1.396	1.373	0.022	1.056	0.023	1.267	1.455	1.373	0	
bond	00000001_1	C4 C3	Not unusual (enough hits)	10549	1.524	1.51	0.019	0.742	0.014	1.278	1.842	1.51	0	
bond	00000001_1	C5 C3	Not unusual (enough hits)	14050	1.424	1.384	0.022	1.817	0.04	0.618	1.8	1.386	0	
bond	00000001_1	C4 N2	Not unusual (enough hits)	931	1.458	1.465	0.015	0.482	0.007	1.386	1.561	1.465	0	
bond	00000001_1	C10 N2	Not unusual (enough hits)	1978	1.481	1.468	0.023	0.576	0.013	1.336	1.699	1.468	0	
bond	00000001_1	C6 C5	Not unusual (enough hits)	20000	1.417	1.383	0.019	1.8	0.033	0.882	1.685	1.383	0	
bond	00000001_1	C8 C7	Not unusual (enough hits)	17	1.341	1.404	0.033	1.913	0.064	1.296	1.433	1.409	0.016	
bond	00000001_1	C8 N4	Not unusual (enough hits)	46	1.446	1.376	0.045	1.573	0.07	1.223	1.481	1.363	0.004	
bond	00000001_1	C9 N3	Not unusual (enough hits)	1745	1.443	1.457	0.022	0.67	0.015	1.204	1.687	1.458	0	
bond	00000001_1	C10 C9	Not unusual (enough hits)	252	1.541	1.521	0.02	1.053	0.021	1.452	1.629	1.52	0	
bond	00000001_1	O1 N4	Not unusual (enough hits)	234	1.246	1.236	0.025	0.37	0.009	1.145	1.398	1.233	0	
bond	00000001_1	O2 N4	Not unusual (enough hits)	234	1.232	1.236	0.025	0.173	0.004	1.145	1.398	1.233	0	
bond	00000001_1	C1 CL	Unusual (enough hits)	743	1.697	1.738	0.019	2.193	0.041	1.561	1.806	1.74	0	
bond	00000001_1	C1 N1	Unusual (enough hits)	245	1.377	1.321	0.025	2.197	0.055	1.254	1.422	1.317	0.001	
bond	00000001_1	C2 N1	Unusual (enough hits)	2818	1.387	1.34	0.022	2.093	0.047	1.05	1.584	1.337	0	
bond	00000001_1	C2 C3	Unusual (enough hits)	560	1.423	1.381	0.017	2.52	0.042	1.279	1.497	1.382	0.006	
bond	00000001_1	C7 N2	Unusual (enough hits)	17	1.391	1.36	0.015	2.057	0.032	1.334	1.38	1.366	0.012	
bond	00000001_1	C7 N3	Unusual (enough hits)	17	1.369	1.335	0.016	2.1	0.034	1.308	1.372	1.331	0.002	
bond	00000001_2	C6 C1	Not unusual (enough hits)	479	1.401	1.373	0.022	1.278	0.028	1.267	1.455	1.373	0	
bond	00000001_2	C4 C3	Not unusual (enough hits)	10549	1.533	1.51	0.019	1.233	0.023	1.278	1.842	1.51	0	
bond	00000001_2	C5 C3	Not unusual (enough hits)	14050	1.427	1.384	0.022	1.956	0.043	0.618	1.8	1.386	0	
bond	00000001_2	C4 N2	Not unusual (enough hits)	931	1.457	1.465	0.015	0.519	0.008	1.386	1.561	1.465	0	
bond	00000001_2	C10 N2	Not unusual (enough hits)	1978	1.475	1.468	0.023	0.274	0.006	1.336	1.699	1.468	0	
bond	00000001_2	C8 C7	Not unusual (enough hits)	17	1.358	1.404	0.033	1.384	0.046	1.296	1.433	1.409	0.002	
bond	00000001_2	C8 N4	Not unusual (enough hits)	46	1.459	1.376	0.045	1.867	0.084	1.223	1.481	1.363	0.008	
bond	00000001_2	C9 N3	Not unusual (enough hits)	1745	1.443	1.457	0.022	0.643	0.014	1.204	1.687	1.458	0	
bond	00000001_2	C10 C9	Not unusual (enough hits)	252	1.547	1.521	0.02	1.369	0.027	1.452	1.629	1.52	0	
bond	00000001_2	O1 N4	Not unusual (enough hits)	234	1.25	1.236	0.025	0.553	0.014	1.145	1.398	1.233	0	
bond	00000001_2	O2 N4	Not unusual (enough hits)	234	1.246	1.236	0.025	0.378	0.009	1.145	1.398	1.233	0	
bond	00000001_2	C1 CL	Unusual (enough hits)	743	1.687	1.738	0.019	2.766	0.051	1.561	1.806	1.74	0	
bond	00000001_2	C1 N1	Unusual (enough hits)	245	1.381	1.321	0.025	2.357	0.059	1.254	1.422	1.317	0	
bond	00000001_2	C2 N1	Unusual (enough hits)	2818	1.387	1.34	0.022	2.086	0.047	1.05	1.584	1.337	0	
bond	00000001_2	C2 C3	Unusual (enough hits)	560	1.42	1.381	0.017	2.346	0.04	1.279	1.497	1.382	0.003	
bond	00000001_2	C7 N2	Unusual (enough hits)	17	1.407	1.36	0.015	3.095	0.048	1.334	1.38	1.366	0.028	
bond	00000001_2	C6 C5	Unusual (enough hits)	20000	1.42	1.383	0.019	2.009	0.037	0.882	1.685	1.383	0	
bond	00000001_2	C7 N3	Unusual (enough hits)	17	1.375	1.335	0.016	2.48	0.04	1.308	1.372	1.331	0.004	
bond	00000001_3	C6 C1	Not unusual (enough hits)	479	1.402	1.373	0.022	1.346	0.029	1.267	1.455	1.373	0	

bond	00000001_3	C2 N1	Not unusual (enough hits)	2818	1.38	1.34	0.022	1.781	0.04	1.05	1.584	1.337	0	
bond	00000001_3	C2 C3	Not unusual (enough hits)	560	1.412	1.381	0.017	1.837	0.031	1.279	1.497	1.382	0.002	
bond	00000001_3	C4 C3	Not unusual (enough hits)	10549	1.511	1.51	0.019	0.077	0.001	1.278	1.842	1.51	0	
bond	00000001_3	C5 C3	Not unusual (enough hits)	14050	1.424	1.384	0.022	1.842	0.04	0.618	1.8	1.386	0	
bond	00000001_3	C4 N2	Not unusual (enough hits)	931	1.468	1.465	0.015	0.176	0.003	1.386	1.561	1.465	0	
bond	00000001_3	C10 N2	Not unusual (enough hits)	1978	1.479	1.468	0.023	0.485	0.011	1.336	1.699	1.468	0	
bond	00000001_3	C8 C7	Not unusual (enough hits)	17	1.351	1.404	0.033	1.598	0.053	1.296	1.433	1.409	0.005	
bond	00000001_3	C8 N4	Not unusual (enough hits)	46	1.454	1.376	0.045	1.753	0.078	1.223	1.481	1.363	0.003	
bond	00000001_3	C9 N3	Not unusual (enough hits)	1745	1.444	1.457	0.022	0.626	0.014	1.204	1.687	1.458	0	
bond	00000001_3	C10 C9	Not unusual (enough hits)	252	1.539	1.521	0.02	0.943	0.018	1.452	1.629	1.52	0	
bond	00000001_3	O1 N4	Not unusual (enough hits)	234	1.245	1.236	0.025	0.341	0.008	1.145	1.398	1.233	0	
bond	00000001_3	O2 N4	Not unusual (enough hits)	234	1.238	1.236	0.025	0.082	0.002	1.145	1.398	1.233	0	
bond	00000001_3	C1 CL	Unusual (enough hits)	743	1.69	1.738	0.019	2.587	0.048	1.561	1.806	1.74	0	
bond	00000001_3	C1 N1	Unusual (enough hits)	245	1.375	1.321	0.025	2.144	0.054	1.254	1.422	1.317	0.001	
bond	00000001_3	C7 N2	Unusual (enough hits)	17	1.401	1.36	0.015	2.675	0.041	1.334	1.38	1.366	0.021	
bond	00000001_3	C6 C5	Unusual (enough hits)	20000	1.423	1.383	0.019	2.138	0.04	0.882	1.685	1.383	0	
bond	00000001_3	C7 N3	Unusual (enough hits)	17	1.368	1.335	0.016	2.034	0.033	1.308	1.372	1.331	0.001	
bond	00000001_4	C6 C1	Not unusual (enough hits)	479	1.39	1.373	0.022	0.784	0.017	1.267	1.455	1.373	0	
bond	00000001_4	C2 N1	Not unusual (enough hits)	2818	1.378	1.34	0.022	1.666	0.037	1.05	1.584	1.337	0	
bond	00000001_4	C2 C3	Not unusual (enough hits)	560	1.41	1.381	0.017	1.702	0.029	1.279	1.497	1.382	0	
bond	00000001_4	C4 C3	Not unusual (enough hits)	10549	1.52	1.51	0.019	0.549	0.01	1.278	1.842	1.51	0	
bond	00000001_4	C5 C3	Not unusual (enough hits)	14050	1.427	1.384	0.022	1.964	0.043	0.618	1.8	1.386	0	
bond	00000001_4	C4 N2	Not unusual (enough hits)	931	1.449	1.465	0.015	1.037	0.016	1.386	1.561	1.465	0	
bond	00000001_4	C10 N2	Not unusual (enough hits)	1978	1.473	1.468	0.023	0.186	0.004	1.336	1.699	1.468	0	
bond	00000001_4	C6 C5	Not unusual (enough hits)	20000	1.42	1.383	0.019	1.975	0.037	0.882	1.685	1.383	0	
bond	00000001_4	C8 C7	Not unusual (enough hits)	17	1.339	1.404	0.033	1.958	0.065	1.296	1.433	1.409	0.017	
bond	00000001_4	C7 N3	Not unusual (enough hits)	17	1.362	1.335	0.016	1.654	0.027	1.308	1.372	1.331	0.005	
bond	00000001_4	C8 N4	Not unusual (enough hits)	46	1.436	1.376	0.045	1.344	0.06	1.223	1.481	1.363	0.001	
bond	00000001_4	C9 N3	Not unusual (enough hits)	1745	1.444	1.457	0.022	0.609	0.013	1.204	1.687	1.458	0	
bond	00000001_4	C10 C9	Not unusual (enough hits)	252	1.545	1.521	0.02	1.266	0.025	1.452	1.629	1.52	0	
bond	00000001_4	O1 N4	Not unusual (enough hits)	234	1.237	1.236	0.025	0.009	0	1.145	1.398	1.233	0	
bond	00000001_4	O2 N4	Not unusual (enough hits)	234	1.232	1.236	0.025	0.166	0.004	1.145	1.398	1.233	0	
bond	00000001_4	C1 CL	Unusual (enough hits)	743	1.694	1.738	0.019	2.366	0.044	1.561	1.806	1.74	0	
bond	00000001_4	C1 N1	Unusual (enough hits)	245	1.376	1.321	0.025	2.181	0.055	1.254	1.422	1.317	0	
bond	00000001_4	C7 N2	Unusual (enough hits)	17	1.395	1.36	0.015	2.314	0.036	1.334	1.38	1.366	0.016	
bond	00000001_5	C1 N1	Not unusual (enough hits)	245	1.371	1.321	0.025	1.97	0.049	1.254	1.422	1.317	0.004	
bond	00000001_5	C6 C1	Not unusual (enough hits)	479	1.406	1.373	0.022	1.516	0.033	1.267	1.455	1.373	0.001	
bond	00000001_5	C2 N1	Not unusual (enough hits)	2818	1.371	1.34	0.022	1.384	0.031	1.05	1.584	1.337	0	
bond	00000001_5	C4 C3	Not unusual (enough hits)	10549	1.523	1.51	0.019	0.697	0.013	1.278	1.842	1.51	0	

bond	00000001_5	C5 C3	Not unusual (enough hits)	14050	1.426	1.384	0.022	1.926	0.042	0.618	1.8	1.386	0	
bond	00000001_5	C4 N2	Not unusual (enough hits)	931	1.46	1.465	0.015	0.304	0.005	1.386	1.561	1.465	0	
bond	00000001_5	C10 N2	Not unusual (enough hits)	1978	1.479	1.468	0.023	0.451	0.01	1.336	1.699	1.468	0	
bond	00000001_5	C6 C5	Not unusual (enough hits)	20000	1.417	1.383	0.019	1.835	0.034	0.882	1.685	1.383	0	
bond	00000001_5	C8 C7	Not unusual (enough hits)	17	1.353	1.404	0.033	1.53	0.051	1.296	1.433	1.409	0.003	
bond	00000001_5	C8 N4	Not unusual (enough hits)	46	1.452	1.376	0.045	1.701	0.076	1.223	1.481	1.363	0.001	
bond	00000001_5	C9 N3	Not unusual (enough hits)	1745	1.446	1.457	0.022	0.506	0.011	1.204	1.687	1.458	0	
bond	00000001_5	C10 C9	Not unusual (enough hits)	252	1.547	1.521	0.02	1.366	0.027	1.452	1.629	1.52	0	
bond	00000001_5	O1 N4	Not unusual (enough hits)	234	1.246	1.236	0.025	0.376	0.009	1.145	1.398	1.233	0	
bond	00000001_5	O2 N4	Not unusual (enough hits)	234	1.239	1.236	0.025	0.105	0.003	1.145	1.398	1.233	0	
bond	00000001_5	C1 CL	Unusual (enough hits)	743	1.69	1.738	0.019	2.566	0.048	1.561	1.806	1.74	0	
bond	00000001_5	C2 C3	Unusual (enough hits)	560	1.421	1.381	0.017	2.348	0.04	1.279	1.497	1.382	0.003	
bond	00000001_5	C7 N2	Unusual (enough hits)	17	1.407	1.36	0.015	3.069	0.047	1.334	1.38	1.366	0.027	
bond	00000001_5	C7 N3	Unusual (enough hits)	17	1.369	1.335	0.016	2.104	0.034	1.308	1.372	1.331	0.002	
angle	00000001_1	CL C1 N1	Not unusual (enough hits)	239	115.563	116.229	2.378	0.28	0.666	106.087	140.591	115.898	0.001	
angle	00000001_1	C6 C1 CL	Not unusual (enough hits)	437	120.308	119.088	2.36	0.517	1.22	96.671	128.568	119.178	0.009	
angle	00000001_1	C6 C1 N1	Not unusual (enough hits)	167	124.128	124.711	1.675	0.348	0.583	117.068	127.876	125.155	0.075	
angle	00000001_1	C2 N1 C1	Not unusual (enough hits)	179	117.081	116.435	1.303	0.496	0.646	112.785	121.37	116.186	0	
angle	00000001_1	C3 C2 N1	Not unusual (enough hits)	225	123.593	123.744	1.746	0.087	0.152	117.703	127.597	124.357	0.003	
angle	00000001_1	C4 C3 C2	Not unusual (enough hits)	155	123.665	121.018	1.641	1.613	2.647	113.768	126.783	120.987	0.17	
angle	00000001_1	C5 C3 C2	Not unusual (enough hits)	495	116.359	117.075	1.499	0.477	0.715	105.829	123.29	116.994	0.003	
angle	00000001_1	C4 C3 C5	Not unusual (enough hits)	10997	119.974	120.774	1.905	0.42	0.8	90.622	143.824	120.777	0	
angle	00000001_1	C3 C4 N2	Not unusual (enough hits)	764	115.761	113.088	1.717	1.557	2.674	104.07	122.755	113.045	0.003	
angle	00000001_1	C4 N2 C7	Not unusual (enough hits)	25	130.307	122.65	5.52	1.387	7.657	111.419	127.449	125.38	2.858	
angle	00000001_1	C4 N2 C10	Not unusual (enough hits)	109	118.854	120.505	2.722	0.606	1.651	110.736	125.952	121.036	0.016	
angle	00000001_1	C10 N2 C7	Not unusual (enough hits)	15	110.839	110.822	0.824	0.02	0.017	109.799	112.489	110.756	0.082	
angle	00000001_1	C6 C5 C3	Not unusual (enough hits)	11395	121.286	121.039	1.437	0.172	0.247	93.35	147.791	121.028	0	
angle	00000001_1	C5 C6 C1	Not unusual (enough hits)	289	117.553	117.43	0.964	0.127	0.123	114.685	123.178	117.353	0.008	
angle	00000001_1	C8 C7 N2	Not unusual (enough hits)	11	126.036	124.573	3.022	0.484	1.464	119.122	129.846	123.452	0.266	
angle	00000001_1	N3 C7 N2	Not unusual (enough hits)	15	107.767	109.761	1.606	1.242	1.994	106.878	112.614	110.096	0.164	
angle	00000001_1	C8 C7 N3	Not unusual (enough hits)	22	126.196	125.908	1.325	0.218	0.288	122.812	128.392	126.108	0.087	
angle	00000001_1	C7 C8 N4	Not unusual (enough hits)	17	122.519	123.744	1.302	0.94	1.224	121.873	127.614	123.627	0.083	
angle	00000001_1	C9 N3 C7	Not unusual (enough hits)	51	114.161	111.956	1.974	1.117	2.205	106.231	117.591	112.19	0.291	
angle	00000001_1	C10 C9 N3	Not unusual (enough hits)	191	103.096	102.619	1.341	0.355	0.476	94.971	107.419	102.75	0	
angle	00000001_1	C9 C10 N2	Not unusual (enough hits)	85	104.137	102.951	1.651	0.718	1.186	99.561	108.169	102.882	0.056	
angle	00000001_1	O1 N4 C8	Not unusual (enough hits)	92	120.611	119.959	2.943	0.222	0.653	109.341	135.081	119.617	0.009	
angle	00000001_1	O2 N4 C8	Not unusual (enough hits)	92	114.899	119.959	2.943	1.719	5.06	109.341	135.081	119.617	0.583	
angle	00000001_1	O2 N4 O1	Not unusual (enough hits)	116	124.489	121.724	2.321	1.191	2.765	108.971	128.317	122.551	0.232	
angle	00000001_2	CL C1 N1	Not unusual (enough hits)	239	115.494	116.229	2.378	0.309	0.736	106.087	140.591	115.898	0.003	

angle	00000001_2	C6 C1 CL	Not unusual (enough hits)	437	120.432	119.088	2.36	0.57	1.344	96.671	128.568	119.178	0.005	
angle	00000001_2	C6 C1 N1	Not unusual (enough hits)	167	124.074	124.711	1.675	0.38	0.637	117.068	127.876	125.155	0.021	
angle	00000001_2	C2 N1 C1	Not unusual (enough hits)	179	117.114	116.435	1.303	0.521	0.679	112.785	121.37	116.186	0.025	
angle	00000001_2	C3 C2 N1	Not unusual (enough hits)	225	123.807	123.744	1.746	0.036	0.063	117.703	127.597	124.357	0.013	
angle	00000001_2	C4 C3 C2	Not unusual (enough hits)	155	123.817	121.018	1.641	1.706	2.798	113.768	126.783	120.987	0.103	
angle	00000001_2	C5 C3 C2	Not unusual (enough hits)	495	116.275	117.075	1.499	0.533	0.8	105.829	123.29	116.994	0.007	
angle	00000001_2	C4 C3 C5	Not unusual (enough hits)	10997	119.905	120.774	1.905	0.456	0.869	90.622	143.824	120.777	0	
angle	00000001_2	C4 N2 C7	Not unusual (enough hits)	25	130.736	122.65	5.52	1.465	8.087	111.419	127.449	125.38	3.288	
angle	00000001_2	C4 N2 C10	Not unusual (enough hits)	109	118.354	120.505	2.722	0.79	2.151	110.736	125.952	121.036	0.074	
angle	00000001_2	C10 N2 C7	Not unusual (enough hits)	15	110.909	110.822	0.824	0.106	0.087	109.799	112.489	110.756	0.041	
angle	00000001_2	C6 C5 C3	Not unusual (enough hits)	11395	121.491	121.039	1.437	0.314	0.451	93.35	147.791	121.028	0	
angle	00000001_2	C5 C6 C1	Not unusual (enough hits)	289	117.239	117.43	0.964	0.198	0.191	114.685	123.178	117.353	0.001	
angle	00000001_2	C8 C7 N2	Not unusual (enough hits)	11	125.985	124.573	3.022	0.467	1.412	119.122	129.846	123.452	0.275	
angle	00000001_2	N3 C7 N2	Not unusual (enough hits)	15	107.49	109.761	1.606	1.415	2.272	106.878	112.614	110.096	0.014	
angle	00000001_2	C8 C7 N3	Not unusual (enough hits)	22	126.526	125.908	1.325	0.466	0.618	122.812	128.392	126.108	0.025	
angle	00000001_2	C7 C8 N4	Not unusual (enough hits)	17	123.917	123.744	1.302	0.133	0.173	121.873	127.614	123.627	0.072	
angle	00000001_2	C9 N3 C7	Not unusual (enough hits)	51	113.987	111.956	1.974	1.029	2.031	106.231	117.591	112.19	0.116	
angle	00000001_2	C10 C9 N3	Not unusual (enough hits)	191	103.397	102.619	1.341	0.58	0.777	94.971	107.419	102.75	0.003	
angle	00000001_2	C9 C10 N2	Not unusual (enough hits)	85	104.218	102.951	1.651	0.767	1.266	99.561	108.169	102.882	0.024	
angle	00000001_2	O1 N4 C8	Not unusual (enough hits)	92	120.862	119.959	2.943	0.307	0.903	109.341	135.081	119.617	0.019	
angle	00000001_2	O2 N4 C8	Not unusual (enough hits)	92	114.763	119.959	2.943	1.765	5.195	109.341	135.081	119.617	0.718	
angle	00000001_2	O2 N4 O1	Not unusual (enough hits)	116	124.374	121.724	2.321	1.142	2.65	108.971	128.317	122.551	0.117	
angle	00000001_2	C3 C4 N2	Unusual (enough hits)	764	116.615	113.088	1.717	2.055	3.528	104.07	122.755	113.045	0.186	
angle	00000001_3	CL C1 N1	Not unusual (enough hits)	239	114.952	116.229	2.378	0.537	1.278	106.087	140.591	115.898	0.009	
angle	00000001_3	C6 C1 CL	Not unusual (enough hits)	437	121.051	119.088	2.36	0.832	1.962	96.671	128.568	119.178	0.017	
angle	00000001_3	C6 C1 N1	Not unusual (enough hits)	167	123.998	124.711	1.675	0.426	0.713	117.068	127.876	125.155	0.055	
angle	00000001_3	C2 N1 C1	Not unusual (enough hits)	179	117.3	116.435	1.303	0.664	0.865	112.785	121.37	116.186	0.161	
angle	00000001_3	C3 C2 N1	Not unusual (enough hits)	225	123.801	123.744	1.746	0.032	0.056	117.703	127.597	124.357	0.019	
angle	00000001_3	C4 C3 C2	Not unusual (enough hits)	155	122.236	121.018	1.641	0.742	1.218	113.768	126.783	120.987	0.023	
angle	00000001_3	C5 C3 C2	Not unusual (enough hits)	495	116.733	117.075	1.499	0.228	0.342	105.829	123.29	116.994	0.002	
angle	00000001_3	C4 C3 C5	Not unusual (enough hits)	10997	121.03	120.774	1.905	0.134	0.256	90.622	143.824	120.777	0	
angle	00000001_3	C3 C4 N2	Not unusual (enough hits)	764	112.465	113.088	1.717	0.363	0.623	104.07	122.755	113.045	0.004	
angle	00000001_3	C4 N2 C7	Not unusual (enough hits)	25	130.728	122.65	5.52	1.464	8.078	111.419	127.449	125.38	3.279	
angle	00000001_3	C4 N2 C10	Not unusual (enough hits)	109	118.647	120.505	2.722	0.683	1.858	110.736	125.952	121.036	0.024	
angle	00000001_3	C10 N2 C7	Not unusual (enough hits)	15	110.626	110.822	0.824	0.238	0.196	109.799	112.489	110.756	0.106	
angle	00000001_3	C6 C5 C3	Not unusual (enough hits)	11395	121.015	121.039	1.437	0.017	0.024	93.35	147.791	121.028	0	
angle	00000001_3	C5 C6 C1	Not unusual (enough hits)	289	117.154	117.43	0.964	0.286	0.276	114.685	123.178	117.353	0.002	
angle	00000001_3	C8 C7 N2	Not unusual (enough hits)	11	126.17	124.573	3.022	0.529	1.597	119.122	129.846	123.452	0.132	
angle	00000001_3	N3 C7 N2	Not unusual (enough hits)	15	107.453	109.761	1.606	1.438	2.309	106.878	112.614	110.096	0.051	

angle	00000001_3	C8 C7 N3	Not unusual (enough hits)	22	126.377	125.908	1.325	0.354	0.469	122.812	128.392	126.108	0.002	
angle	00000001_3	C7 C8 N4	Not unusual (enough hits)	17	123.774	123.744	1.302	0.023	0.03	121.873	127.614	123.627	0.034	
angle	00000001_3	C9 N3 C7	Not unusual (enough hits)	51	114.495	111.956	1.974	1.287	2.539	106.231	117.591	112.19	0.212	
angle	00000001_3	C10 C9 N3	Not unusual (enough hits)	191	102.916	102.619	1.341	0.221	0.297	94.971	107.419	102.75	0.008	
angle	00000001_3	C9 C10 N2	Not unusual (enough hits)	85	104.51	102.951	1.651	0.944	1.559	99.561	108.169	102.882	0.041	
angle	00000001_3	O1 N4 C8	Not unusual (enough hits)	92	121.18	119.959	2.943	0.415	1.222	109.341	135.081	119.617	0.08	
angle	00000001_3	O2 N4 C8	Not unusual (enough hits)	92	114.57	119.959	2.943	1.831	5.389	109.341	135.081	119.617	0.912	
angle	00000001_3	O2 N4 O1	Not unusual (enough hits)	116	124.25	121.724	2.321	1.088	2.525	108.971	128.317	122.551	0.008	
angle	00000001_4	CL C1 N1	Not unusual (enough hits)	239	115.154	116.229	2.378	0.452	1.075	106.087	140.591	115.898	0.008	
angle	00000001_4	C6 C1 CL	Not unusual (enough hits)	437	120.736	119.088	2.36	0.698	1.647	96.671	128.568	119.178	0.01	
angle	00000001_4	C6 C1 N1	Not unusual (enough hits)	167	124.111	124.711	1.675	0.358	0.6	117.068	127.876	125.155	0.058	
angle	00000001_4	C2 N1 C1	Not unusual (enough hits)	179	117.715	116.435	1.303	0.983	1.28	112.785	121.37	116.186	0.111	
angle	00000001_4	C3 C2 N1	Not unusual (enough hits)	225	123.357	123.744	1.746	0.222	0.388	117.703	127.597	124.357	0.006	
angle	00000001_4	C4 C3 C2	Not unusual (enough hits)	155	123.187	121.018	1.641	1.322	2.169	113.768	126.783	120.987	0.107	
angle	00000001_4	C5 C3 C2	Not unusual (enough hits)	495	116.48	117.075	1.499	0.397	0.595	105.829	123.29	116.994	0.001	
angle	00000001_4	C4 C3 C5	Not unusual (enough hits)	10997	120.327	120.774	1.905	0.235	0.447	90.622	143.824	120.777	0	
angle	00000001_4	C3 C4 N2	Not unusual (enough hits)	764	116.041	113.088	1.717	1.72	2.953	104.07	122.755	113.045	0.02	
angle	00000001_4	C4 N2 C7	Not unusual (enough hits)	25	130.042	122.65	5.52	1.339	7.393	111.419	127.449	125.38	2.594	
angle	00000001_4	C4 N2 C10	Not unusual (enough hits)	109	118.91	120.505	2.722	0.586	1.595	110.736	125.952	121.036	0.04	
angle	00000001_4	C10 N2 C7	Not unusual (enough hits)	15	111.047	110.822	0.824	0.273	0.225	109.799	112.489	110.756	0.039	
angle	00000001_4	C6 C5 C3	Not unusual (enough hits)	11395	121.459	121.039	1.437	0.292	0.42	93.35	147.791	121.028	0	
angle	00000001_4	C5 C6 C1	Not unusual (enough hits)	289	116.877	117.43	0.964	0.574	0.553	114.685	123.178	117.353	0.015	
angle	00000001_4	C8 C7 N2	Not unusual (enough hits)	11	125.388	124.573	3.022	0.27	0.815	119.122	129.846	123.452	0.321	
angle	00000001_4	N3 C7 N2	Not unusual (enough hits)	15	107.941	109.761	1.606	1.134	1.82	106.878	112.614	110.096	0.338	
angle	00000001_4	C8 C7 N3	Not unusual (enough hits)	22	126.67	125.908	1.325	0.575	0.762	122.812	128.392	126.108	0.008	
angle	00000001_4	C7 C8 N4	Not unusual (enough hits)	17	123.693	123.744	1.302	0.039	0.051	121.873	127.614	123.627	0.048	
angle	00000001_4	C9 N3 C7	Not unusual (enough hits)	51	113.869	111.956	1.974	0.969	1.913	106.231	117.591	112.19	0.001	
angle	00000001_4	C10 C9 N3	Not unusual (enough hits)	191	103.286	102.619	1.341	0.497	0.666	94.971	107.419	102.75	0.03	
angle	00000001_4	C9 C10 N2	Not unusual (enough hits)	85	103.857	102.951	1.651	0.548	0.905	99.561	108.169	102.882	0.002	
angle	00000001_4	O1 N4 C8	Not unusual (enough hits)	92	121.021	119.959	2.943	0.361	1.062	109.341	135.081	119.617	0.007	
angle	00000001_4	O2 N4 C8	Not unusual (enough hits)	92	114.302	119.959	2.943	1.922	5.657	109.341	135.081	119.617	1.18	
angle	00000001_4	O2 N4 O1	Not unusual (enough hits)	116	124.676	121.724	2.321	1.272	2.952	108.971	128.317	122.551	0.271	
angle	00000001_5	CL C1 N1	Not unusual (enough hits)	239	114.73	116.229	2.378	0.63	1.499	106.087	140.591	115.898	0.019	
angle	00000001_5	C6 C1 CL	Not unusual (enough hits)	437	120.945	119.088	2.36	0.787	1.856	96.671	128.568	119.178	0.006	
angle	00000001_5	C6 C1 N1	Not unusual (enough hits)	167	124.325	124.711	1.675	0.23	0.386	117.068	127.876	125.155	0.069	
angle	00000001_5	C2 N1 C1	Not unusual (enough hits)	179	117.195	116.435	1.303	0.583	0.76	112.785	121.37	116.186	0.056	
angle	00000001_5	C3 C2 N1	Not unusual (enough hits)	225	123.813	123.744	1.746	0.04	0.069	117.703	127.597	124.357	0.007	
angle	00000001_5	C4 C3 C2	Not unusual (enough hits)	155	122.533	121.018	1.641	0.923	1.515	113.768	126.783	120.987	0.013	
angle	00000001_5	C5 C3 C2	Not unusual (enough hits)	495	116.744	117.075	1.499	0.221	0.331	105.829	123.29	116.994	0.001	

angle	00000001_5	C4 C3 C5	Not unusual (enough hits)	10997	120.721	120.774	1.905	0.028	0.054	90.622	143.824	120.777	0	
angle	00000001_5	C3 C4 N2	Not unusual (enough hits)	764	115.056	113.088	1.717	1.146	1.968	104.07	122.755	113.045	0.001	
angle	00000001_5	C4 N2 C7	Not unusual (enough hits)	25	130.68	122.65	5.52	1.455	8.03	111.419	127.449	125.38	3.231	
angle	00000001_5	C4 N2 C10	Not unusual (enough hits)	109	118.284	120.505	2.722	0.816	2.221	110.736	125.952	121.036	0.052	
angle	00000001_5	C10 N2 C7	Not unusual (enough hits)	15	111.036	110.822	0.824	0.26	0.214	109.799	112.489	110.756	0.028	
angle	00000001_5	C6 C5 C3	Not unusual (enough hits)	11395	120.765	121.039	1.437	0.191	0.274	93.35	147.791	121.028	0	
angle	00000001_5	C5 C6 C1	Not unusual (enough hits)	289	117.157	117.43	0.964	0.284	0.274	114.685	123.178	117.353	0.004	
angle	00000001_5	C8 C7 N2	Not unusual (enough hits)	11	125.761	124.573	3.022	0.393	1.188	119.122	129.846	123.452	0.052	
angle	00000001_5	N3 C7 N2	Not unusual (enough hits)	15	107.422	109.761	1.606	1.457	2.34	106.878	112.614	110.096	0.082	
angle	00000001_5	C8 C7 N3	Not unusual (enough hits)	22	126.817	125.908	1.325	0.686	0.909	122.812	128.392	126.108	0.031	
angle	00000001_5	C7 C8 N4	Not unusual (enough hits)	17	124.919	123.744	1.302	0.903	1.176	121.873	127.614	123.627	0.008	
angle	00000001_5	C9 N3 C7	Not unusual (enough hits)	51	114.242	111.956	1.974	1.158	2.286	106.231	117.591	112.19	0.372	
angle	00000001_5	C10 C9 N3	Not unusual (enough hits)	191	103.316	102.619	1.341	0.519	0.696	94.971	107.419	102.75	0.011	
angle	00000001_5	C9 C10 N2	Not unusual (enough hits)	85	103.984	102.951	1.651	0.626	1.033	99.561	108.169	102.882	0.103	
angle	00000001_5	O1 N4 C8	Not unusual (enough hits)	92	121.473	119.959	2.943	0.515	1.515	109.341	135.081	119.617	0.013	
angle	00000001_5	O2 N4 C8	Not unusual (enough hits)	92	114.326	119.959	2.943	1.914	5.632	109.341	135.081	119.617	1.155	
angle	00000001_5	O2 N4 O1	Not unusual (enough hits)	116	124.2	121.724	2.321	1.067	2.476	108.971	128.317	122.551	0.044	
torsion	00000001_1	C2 C3 C4 N2	Not unusual (enough hits)	349	47.206								0.284	0.103
torsion	00000001_1	C5 C3 C4 N2	Not unusual (enough hits)	10853	−133.267								0.002	0.128
torsion	00000001_1	C3 C4 N2 C7	Not unusual (enough hits)	49	80.983								0.969	0.102
torsion	00000001_1	C3 C4 N2 C10	Not unusual (enough hits)	182	−99.335								1.829	0.071
torsion	00000001_1	C7 C8 N4 O1	Not unusual (enough hits)	40	−0.43								0.006	0.475
torsion	00000001_1	C7 C8 N4 O2	Not unusual (enough hits)	40	179.758								0.07	0.475
torsion	00000001_1	N4 C8 C7 N2	Not unusual (few hits)	6	179.7								0.017	0.667
torsion	00000001_1	N4 C8 C7 N3	Not unusual (few hits)	7	−0.162								0.592	0.571
torsion	00000001_2	C2 C3 C4 N2	Not unusual (enough hits)	349	40.475								0.322	0.08
torsion	00000001_2	C5 C3 C4 N2	Not unusual (enough hits)	10853	−140.156								0.001	0.119
torsion	00000001_2	C3 C4 N2 C10	Not unusual (enough hits)	182	−103.432								0.049	0.055
torsion	00000001_2	C7 C8 N4 O1	Not unusual (enough hits)	40	−0.086								0.014	0.475
torsion	00000001_2	C7 C8 N4 O2	Not unusual (enough hits)	40	179.863								0.175	0.475
torsion	00000001_2	N4 C8 C7 N2	Not unusual (few hits)	6	179.742								0.059	0.667
torsion	00000001_2	N4 C8 C7 N3	Not unusual (few hits)	7	−0.139								0.614	0.571
torsion	00000001_2	C3 C4 N2 C7	Unusual (enough hits)	49	76.892								3.122	0.02
torsion	00000001_3	C2 C3 C4 N2	Not unusual (enough hits)	349	72.155								0.604	0.132
torsion	00000001_3	C5 C3 C4 N2	Not unusual (enough hits)	10853	−107.536								0.001	0.121
torsion	00000001_3	C3 C4 N2 C7	Not unusual (enough hits)	49	82.205								2.191	0.122
torsion	00000001_3	C3 C4 N2 C10	Not unusual (enough hits)	182	−97.785								1.573	0.082
torsion	00000001_3	C7 C8 N4 O1	Not unusual (enough hits)	40	0.318								0.112	0.475
torsion	00000001_3	C7 C8 N4 O2	Not unusual (enough hits)	40	−179.746								0.058	0.475

torsion	00000001_3	N4 C8 C7 N2	Not unusual (few hits)	6	−179.854								0.172	0.667
torsion	00000001_3	N4 C8 C7 N3	Not unusual (few hits)	7	0.273								0.48	0.571
torsion	00000001_4	C2 C3 C4 N2	Not unusual (enough hits)	349	50.745								0.042	0.123
torsion	00000001_4	C5 C3 C4 N2	Not unusual (enough hits)	10853	−130.166								0.001	0.131
torsion	00000001_4	C3 C4 N2 C7	Not unusual (enough hits)	49	78.518								1.496	0.061
torsion	00000001_4	C3 C4 N2 C10	Not unusual (enough hits)	182	−101.892								0.728	0.055
torsion	00000001_4	C7 C8 N4 O1	Not unusual (enough hits)	40	−0.078								0.007	0.475
torsion	00000001_4	C7 C8 N4 O2	Not unusual (enough hits)	40	−179.79								0.102	0.475
torsion	00000001_4	N4 C8 C7 N2	Not unusual (few hits)	6	179.486								0.197	0.667
torsion	00000001_4	N4 C8 C7 N3	Not unusual (few hits)	7	−0.273								0.48	0.571
torsion	00000001_5	C2 C3 C4 N2	Not unusual (enough hits)	349	63.819								0.008	0.155
torsion	00000001_5	C5 C3 C4 N2	Not unusual (enough hits)	10853	−116.755								0	0.133
torsion	00000001_5	C7 C8 N4 O1	Not unusual (enough hits)	40	0.39								0.046	0.475
torsion	00000001_5	C7 C8 N4 O2	Not unusual (enough hits)	40	−179.74								0.052	0.475
torsion	00000001_5	N4 C8 C7 N2	Not unusual (few hits)	6	−179.744								0.062	0.667
torsion	00000001_5	N4 C8 C7 N3	Not unusual (few hits)	7	0.502								0.252	0.571
torsion	00000001_5	C3 C4 N2 C7	Unusual (enough hits)	49	75.866								4.148	0.02
torsion	00000001_5	C3 C4 N2 C10	Unusual (enough hits)	182	−104.292								0.228	0.049
ring	00000001_1	C1 N1 C2 C3 C5 C6	Not unusual (enough hits)	320						0.048	8.244			1
ring	00000001_1	N2 C7 N3 C9 C10	Not unusual (enough hits)	35						0.64	16.304			0.771
ring	00000001_2	C1 N1 C2 C3 C5 C6	Not unusual (enough hits)	320						0.083	8.323			1
ring	00000001_2	N2 C7 N3 C9 C10	Not unusual (enough hits)	35						0.67	16.355			0.771
ring	00000001_3	C1 N1 C2 C3 C5 C6	Not unusual (enough hits)	320						0.088	8.304			1
ring	00000001_3	N2 C7 N3 C9 C10	Not unusual (enough hits)	35						0.746	16.406			0.771
ring	00000001_4	C1 N1 C2 C3 C5 C6	Not unusual (enough hits)	320						0.056	8.264			1
ring	00000001_4	N2 C7 N3 C9 C10	Not unusual (enough hits)	35						0.683	16.381			0.771
ring	00000001_5	C1 N1 C2 C3 C5 C6	Not unusual (enough hits)	320						0.068	8.298			1
ring	00000001_5	N2 C7 N3 C9 C10	Not unusual (enough hits)	35						0.706	16.366			0.771

Table 9. Geometry Analysis by Mogul of DN-IMI in Complex with Wild-Type *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	| z-score |	| x - mean |	Minimum	Maximum	Median	| d(min) |	Local density
bond	00000001_1	C2 N4	Not unusual (enough hits)	1745	1.458	1.457	0.022	0.04	0.001	1.204	1.687	1.458	0	
bond	00000001_1	C3 N3	Not unusual (enough hits)	1978	1.47	1.468	0.023	0.094	0.002	1.336	1.699	1.468	0	
bond	00000001_1	C3 C2	Not unusual (enough hits)	252	1.534	1.521	0.02	0.665	0.013	1.452	1.629	1.52	0	
bond	00000001_1	C4 CL1	Not unusual (enough hits)	743	1.73	1.738	0.019	0.436	0.008	1.561	1.806	1.74	0	
bond	00000001_1	C4 N6	Not unusual (enough hits)	245	1.353	1.321	0.025	1.246	0.031	1.254	1.422	1.317	0	
bond	00000001_1	C5 N6	Not unusual (enough hits)	2818	1.347	1.34	0.022	0.322	0.007	1.05	1.584	1.337	0	
bond	00000001_1	C7 C6	Not unusual (enough hits)	14050	1.423	1.384	0.022	1.76	0.039	0.618	1.8	1.386	0	
bond	00000001_1	C8 C7	Not unusual (enough hits)	20000	1.409	1.383	0.019	1.414	0.026	0.882	1.685	1.383	0	
bond	00000001_1	C9 N3	Not unusual (enough hits)	931	1.482	1.465	0.015	1.073	0.017	1.386	1.561	1.465	0	
bond	00000001_1	C9 C6	Not unusual (enough hits)	10549	1.541	1.51	0.019	1.658	0.031	1.278	1.842	1.51	0	
bond	00000001_1	C1 N2	Unusual (enough hits)	18	1.274	1.329	0.015	3.706	0.055	1.303	1.358	1.329	0.03	
bond	00000001_1	C1 N3	Unusual (enough hits)	27	1.422	1.352	0.022	3.212	0.071	1.327	1.394	1.344	0.028	
bond	00000001_1	C1 N4	Unusual (enough hits)	41	1.403	1.345	0.016	3.559	0.058	1.287	1.39	1.343	0.013	
bond	00000001_1	C5 C6	Unusual (enough hits)	560	1.437	1.381	0.017	3.312	0.056	1.279	1.497	1.382	0.002	
bond	00000001_1	C8 C4	Unusual (enough hits)	479	1.423	1.373	0.022	2.297	0.05	1.267	1.455	1.373	0.004	
bond	00000001_10	C2 N4	Not unusual (enough hits)	1745	1.461	1.457	0.022	0.166	0.004	1.204	1.687	1.458	0	
bond	00000001_10	C3 N3	Not unusual (enough hits)	1978	1.475	1.468	0.023	0.308	0.007	1.336	1.699	1.468	0	
bond	00000001_10	C3 C2	Not unusual (enough hits)	252	1.538	1.521	0.02	0.88	0.017	1.452	1.629	1.52	0	
bond	00000001_10	C4 CL1	Not unusual (enough hits)	743	1.751	1.738	0.019	0.722	0.013	1.561	1.806	1.74	0	
bond	00000001_10	C4 N6	Not unusual (enough hits)	245	1.349	1.321	0.025	1.093	0.027	1.254	1.422	1.317	0.003	
bond	00000001_10	C5 N6	Not unusual (enough hits)	2818	1.342	1.34	0.022	0.087	0.002	1.05	1.584	1.337	0	
bond	00000001_10	C7 C6	Not unusual (enough hits)	14050	1.422	1.384	0.022	1.727	0.038	0.618	1.8	1.386	0	
bond	00000001_10	C8 C7	Not unusual (enough hits)	20000	1.41	1.383	0.019	1.462	0.027	0.882	1.685	1.383	0	
bond	00000001_10	C9 N3	Not unusual (enough hits)	931	1.483	1.465	0.015	1.14	0.018	1.386	1.561	1.465	0	
bond	00000001_10	C9 C6	Not unusual (enough hits)	10549	1.541	1.51	0.019	1.671	0.031	1.278	1.842	1.51	0	
bond	00000001_10	C1 N2	Unusual (enough hits)	18	1.279	1.329	0.015	3.329	0.049	1.303	1.358	1.329	0.024	
bond	00000001_10	C1 N3	Unusual (enough hits)	27	1.426	1.352	0.022	3.402	0.075	1.327	1.394	1.344	0.032	
bond	00000001_10	C1 N4	Unusual (enough hits)	41	1.409	1.345	0.016	3.913	0.064	1.287	1.39	1.343	0.019	
bond	00000001_10	C5 C6	Unusual (enough hits)	560	1.431	1.381	0.017	2.959	0.05	1.279	1.497	1.382	0.004	
bond	00000001_10	C8 C4	Unusual (enough hits)	479	1.422	1.373	0.022	2.279	0.05	1.267	1.455	1.373	0.003	
bond	00000001_2	C2 N4	Not unusual (enough hits)	1745	1.463	1.457	0.022	0.248	0.005	1.204	1.687	1.458	0	
bond	00000001_2	C3 N3	Not unusual (enough hits)	1978	1.466	1.468	0.023	0.104	0.002	1.336	1.699	1.468	0	
bond	00000001_2	C3 C2	Not unusual (enough hits)	252	1.527	1.521	0.02	0.345	0.007	1.452	1.629	1.52	0	
bond	00000001_2	C4 CL1	Not unusual (enough hits)	743	1.745	1.738	0.019	0.401	0.007	1.561	1.806	1.74	0	
bond	00000001_2	C4 N6	Not unusual (enough hits)	245	1.339	1.321	0.025	0.716	0.018	1.254	1.422	1.317	0.001	
bond	00000001_2	C5 N6	Not unusual (enough hits)	2818	1.328	1.34	0.022	0.564	0.013	1.05	1.584	1.337	0	
bond	00000001_2	C8 C7	Not unusual (enough hits)	20000	1.415	1.383	0.019	1.702	0.032	0.882	1.685	1.383	0	

bond	00000001_2	C9 N3	Not unusual (enough hits)	931	1.463	1.465	0.015	0.102	0.002	1.386	1.561	1.465	0	
bond	00000001_2	C9 C6	Not unusual (enough hits)	10549	1.532	1.51	0.019	1.209	0.022	1.278	1.842	1.51	0	
bond	00000001_2	C1 N2	Unusual (enough hits)	18	1.28	1.329	0.015	3.269	0.048	1.303	1.358	1.329	0.023	
bond	00000001_2	C1 N3	Unusual (enough hits)	27	1.416	1.352	0.022	2.952	0.065	1.327	1.394	1.344	0.023	
bond	00000001_2	C1 N4	Unusual (enough hits)	41	1.405	1.345	0.016	3.697	0.06	1.287	1.39	1.343	0.016	
bond	00000001_2	C5 C6	Unusual (enough hits)	560	1.416	1.381	0.017	2.067	0.035	1.279	1.497	1.382	0	
bond	00000001_2	C7 C6	Unusual (enough hits)	14050	1.429	1.384	0.022	2.037	0.045	0.618	1.8	1.386	0	
bond	00000001_2	C8 C4	Unusual (enough hits)	479	1.429	1.373	0.022	2.582	0.057	1.267	1.455	1.373	0.01	
bond	00000001_3	C2 N4	Not unusual (enough hits)	1745	1.462	1.457	0.022	0.19	0.004	1.204	1.687	1.458	0	
bond	00000001_3	C3 N3	Not unusual (enough hits)	1978	1.473	1.468	0.023	0.219	0.005	1.336	1.699	1.468	0	
bond	00000001_3	C3 C2	Not unusual (enough hits)	252	1.535	1.521	0.02	0.757	0.015	1.452	1.629	1.52	0	
bond	00000001_3	C4 CL1	Not unusual (enough hits)	743	1.746	1.738	0.019	0.409	0.008	1.561	1.806	1.74	0	
bond	00000001_3	C4 N6	Not unusual (enough hits)	245	1.353	1.321	0.025	1.271	0.032	1.254	1.422	1.317	0	
bond	00000001_3	C5 N6	Not unusual (enough hits)	2818	1.34	1.34	0.022	0.011	0	1.05	1.584	1.337	0	
bond	00000001_3	C7 C6	Not unusual (enough hits)	14050	1.421	1.384	0.022	1.678	0.037	0.618	1.8	1.386	0	
bond	00000001_3	C8 C7	Not unusual (enough hits)	20000	1.409	1.383	0.019	1.412	0.026	0.882	1.685	1.383	0	
bond	00000001_3	C9 N3	Not unusual (enough hits)	931	1.479	1.465	0.015	0.91	0.014	1.386	1.561	1.465	0	
bond	00000001_3	C9 C6	Not unusual (enough hits)	10549	1.538	1.51	0.019	1.531	0.028	1.278	1.842	1.51	0	
bond	00000001_3	C1 N2	Unusual (enough hits)	18	1.284	1.329	0.015	3	0.044	1.303	1.358	1.329	0.019	
bond	00000001_3	C1 N3	Unusual (enough hits)	27	1.423	1.352	0.022	3.229	0.071	1.327	1.394	1.344	0.029	
bond	00000001_3	C1 N4	Unusual (enough hits)	41	1.408	1.345	0.016	3.851	0.063	1.287	1.39	1.343	0.018	
bond	00000001_3	C5 C6	Unusual (enough hits)	560	1.434	1.381	0.017	3.141	0.053	1.279	1.497	1.382	0	
bond	00000001_3	C8 C4	Unusual (enough hits)	479	1.421	1.373	0.022	2.191	0.048	1.267	1.455	1.373	0.002	
bond	00000001_4	C2 N4	Not unusual (enough hits)	1745	1.46	1.457	0.022	0.117	0.003	1.204	1.687	1.458	0	
bond	00000001_4	C3 N3	Not unusual (enough hits)	1978	1.472	1.468	0.023	0.178	0.004	1.336	1.699	1.468	0	
bond	00000001_4	C3 C2	Not unusual (enough hits)	252	1.537	1.521	0.02	0.835	0.016	1.452	1.629	1.52	0	
bond	00000001_4	C4 CL1	Not unusual (enough hits)	743	1.74	1.738	0.019	0.121	0.002	1.561	1.806	1.74	0	
bond	00000001_4	C4 N6	Not unusual (enough hits)	245	1.348	1.321	0.025	1.078	0.027	1.254	1.422	1.317	0.003	
bond	00000001_4	C5 N6	Not unusual (enough hits)	2818	1.352	1.34	0.022	0.505	0.011	1.05	1.584	1.337	0	
bond	00000001_4	C7 C6	Not unusual (enough hits)	14050	1.42	1.384	0.022	1.645	0.036	0.618	1.8	1.386	0	
bond	00000001_4	C8 C4	Not unusual (enough hits)	479	1.408	1.373	0.022	1.621	0.035	1.267	1.455	1.373	0	
bond	00000001_4	C8 C7	Not unusual (enough hits)	20000	1.412	1.383	0.019	1.528	0.028	0.882	1.685	1.383	0	
bond	00000001_4	C9 N3	Not unusual (enough hits)	931	1.485	1.465	0.015	1.26	0.019	1.386	1.561	1.465	0	
bond	00000001_4	C1 N2	Unusual (enough hits)	18	1.291	1.329	0.015	2.517	0.037	1.303	1.358	1.329	0.012	
bond	00000001_4	C1 N3	Unusual (enough hits)	27	1.433	1.352	0.022	3.7	0.081	1.327	1.394	1.344	0.039	
bond	00000001_4	C1 N4	Unusual (enough hits)	41	1.403	1.345	0.016	3.559	0.058	1.287	1.39	1.343	0.013	
bond	00000001_4	C5 C6	Unusual (enough hits)	560	1.433	1.381	0.017	3.068	0.052	1.279	1.497	1.382	0.002	
bond	00000001_4	C9 C6	Unusual (enough hits)	10549	1.549	1.51	0.019	2.075	0.039	1.278	1.842	1.51	0	
bond	00000001_5	C2 N4	Not unusual (enough hits)	1745	1.46	1.457	0.022	0.101	0.002	1.204	1.687	1.458	0	

bond	00000001_5	C3 N3	Not unusual (enough hits)	1978	1.473	1.468	0.023	0.193	0.004	1.336	1.699	1.468	0	
bond	00000001_5	C3 C2	Not unusual (enough hits)	252	1.539	1.521	0.02	0.914	0.018	1.452	1.629	1.52	0	
bond	00000001_5	C4 CL1	Not unusual (enough hits)	743	1.755	1.738	0.019	0.931	0.017	1.561	1.806	1.74	0	
bond	00000001_5	C4 N6	Not unusual (enough hits)	245	1.357	1.321	0.025	1.406	0.035	1.254	1.422	1.317	0.001	
bond	00000001_5	C5 N6	Not unusual (enough hits)	2818	1.355	1.34	0.022	0.647	0.015	1.05	1.584	1.337	0	
bond	00000001_5	C7 C6	Not unusual (enough hits)	14050	1.423	1.384	0.022	1.77	0.039	0.618	1.8	1.386	0	
bond	00000001_5	C8 C4	Not unusual (enough hits)	479	1.416	1.373	0.022	1.999	0.044	1.267	1.455	1.373	0.002	
bond	00000001_5	C8 C7	Not unusual (enough hits)	20000	1.413	1.383	0.019	1.617	0.03	0.882	1.685	1.383	0	
bond	00000001_5	C9 N3	Not unusual (enough hits)	931	1.483	1.465	0.015	1.148	0.018	1.386	1.561	1.465	0	
bond	00000001_5	C9 C6	Not unusual (enough hits)	10549	1.545	1.51	0.019	1.898	0.035	1.278	1.842	1.51	0	
bond	00000001_5	C1 N2	Unusual (enough hits)	18	1.28	1.329	0.015	3.284	0.049	1.303	1.358	1.329	0.023	
bond	00000001_5	C1 N3	Unusual (enough hits)	27	1.427	1.352	0.022	3.447	0.076	1.327	1.394	1.344	0.033	
bond	00000001_5	C1 N4	Unusual (enough hits)	41	1.403	1.345	0.016	3.59	0.058	1.287	1.39	1.343	0.014	
bond	00000001_5	C5 C6	Unusual (enough hits)	560	1.434	1.381	0.017	3.158	0.053	1.279	1.497	1.382	0	
bond	00000001_6	C2 N4	Not unusual (enough hits)	1745	1.46	1.457	0.022	0.135	0.003	1.204	1.687	1.458	0	
bond	00000001_6	C3 N3	Not unusual (enough hits)	1978	1.475	1.468	0.023	0.29	0.007	1.336	1.699	1.468	0	
bond	00000001_6	C3 C2	Not unusual (enough hits)	252	1.539	1.521	0.02	0.922	0.018	1.452	1.629	1.52	0	
bond	00000001_6	C4 CL1	Not unusual (enough hits)	743	1.761	1.738	0.019	1.245	0.023	1.561	1.806	1.74	0	
bond	00000001_6	C4 N6	Not unusual (enough hits)	245	1.35	1.321	0.025	1.157	0.029	1.254	1.422	1.317	0.001	
bond	00000001_6	C5 N6	Not unusual (enough hits)	2818	1.346	1.34	0.022	0.274	0.006	1.05	1.584	1.337	0	
bond	00000001_6	C7 C6	Not unusual (enough hits)	14050	1.423	1.384	0.022	1.773	0.039	0.618	1.8	1.386	0	
bond	00000001_6	C8 C7	Not unusual (enough hits)	20000	1.414	1.383	0.019	1.661	0.031	0.882	1.685	1.383	0	
bond	00000001_6	C9 N3	Not unusual (enough hits)	931	1.485	1.465	0.015	1.297	0.02	1.386	1.561	1.465	0	
bond	00000001_6	C9 C6	Not unusual (enough hits)	10549	1.544	1.51	0.019	1.818	0.034	1.278	1.842	1.51	0	
bond	00000001_6	C1 N2	Unusual (enough hits)	18	1.283	1.329	0.015	3.111	0.046	1.303	1.358	1.329	0.021	
bond	00000001_6	C1 N3	Unusual (enough hits)	27	1.428	1.352	0.022	3.486	0.077	1.327	1.394	1.344	0.034	
bond	00000001_6	C1 N4	Unusual (enough hits)	41	1.408	1.345	0.016	3.88	0.063	1.287	1.39	1.343	0.019	
bond	00000001_6	C5 C6	Unusual (enough hits)	560	1.432	1.381	0.017	3.035	0.051	1.279	1.497	1.382	0.002	
bond	00000001_6	C8 C4	Unusual (enough hits)	479	1.419	1.373	0.022	2.133	0.047	1.267	1.455	1.373	0	
bond	00000001_7	C2 N4	Not unusual (enough hits)	1745	1.464	1.457	0.022	0.273	0.006	1.204	1.687	1.458	0	
bond	00000001_7	C3 N3	Not unusual (enough hits)	1978	1.478	1.468	0.023	0.43	0.01	1.336	1.699	1.468	0	
bond	00000001_7	C3 C2	Not unusual (enough hits)	252	1.54	1.521	0.02	1.007	0.02	1.452	1.629	1.52	0	
bond	00000001_7	C4 CL1	Not unusual (enough hits)	743	1.728	1.738	0.019	0.513	0.01	1.561	1.806	1.74	0	
bond	00000001_7	C4 N6	Not unusual (enough hits)	245	1.351	1.321	0.025	1.161	0.029	1.254	1.422	1.317	0.001	
bond	00000001_7	C5 N6	Not unusual (enough hits)	2818	1.348	1.34	0.022	0.337	0.008	1.05	1.584	1.337	0	
bond	00000001_7	C7 C6	Not unusual (enough hits)	14050	1.418	1.384	0.022	1.558	0.034	0.618	1.8	1.386	0	
bond	00000001_7	C8 C7	Not unusual (enough hits)	20000	1.412	1.383	0.019	1.534	0.028	0.882	1.685	1.383	0	
bond	00000001_7	C9 N3	Not unusual (enough hits)	931	1.486	1.465	0.015	1.347	0.021	1.386	1.561	1.465	0	
bond	00000001_7	C9 C6	Not unusual (enough hits)	10549	1.542	1.51	0.019	1.744	0.032	1.278	1.842	1.51	0	

bond	00000001_7	C1 N2	Unusual (enough hits)	18	1.29	1.329	0.015	2.624	0.039	1.303	1.358	1.329	0.014	
bond	00000001_7	C1 N3	Unusual (enough hits)	27	1.42	1.352	0.022	3.104	0.068	1.327	1.394	1.344	0.026	
bond	00000001_7	C1 N4	Unusual (enough hits)	41	1.412	1.345	0.016	4.141	0.067	1.287	1.39	1.343	0.023	
bond	00000001_7	C5 C6	Unusual (enough hits)	560	1.439	1.381	0.017	3.459	0.058	1.279	1.497	1.382	0.005	
bond	00000001_7	C8 C4	Unusual (enough hits)	479	1.423	1.373	0.022	2.28	0.05	1.267	1.455	1.373	0.004	
bond	00000001_8	C2 N4	Not unusual (enough hits)	1745	1.46	1.457	0.022	0.132	0.003	1.204	1.687	1.458	0	
bond	00000001_8	C3 N3	Not unusual (enough hits)	1978	1.476	1.468	0.023	0.34	0.008	1.336	1.699	1.468	0	
bond	00000001_8	C3 C2	Not unusual (enough hits)	252	1.539	1.521	0.02	0.929	0.018	1.452	1.629	1.52	0	
bond	00000001_8	C4 CL1	Not unusual (enough hits)	743	1.759	1.738	0.019	1.154	0.021	1.561	1.806	1.74	0	
bond	00000001_8	C4 N6	Not unusual (enough hits)	245	1.35	1.321	0.025	1.157	0.029	1.254	1.422	1.317	0.001	
bond	00000001_8	C5 N6	Not unusual (enough hits)	2818	1.347	1.34	0.022	0.282	0.006	1.05	1.584	1.337	0	
bond	00000001_8	C7 C6	Not unusual (enough hits)	14050	1.424	1.384	0.022	1.818	0.04	0.618	1.8	1.386	0	
bond	00000001_8	C8 C7	Not unusual (enough hits)	20000	1.415	1.383	0.019	1.689	0.031	0.882	1.685	1.383	0	
bond	00000001_8	C9 N3	Not unusual (enough hits)	931	1.488	1.465	0.015	1.463	0.023	1.386	1.561	1.465	0	
bond	00000001_8	C9 C6	Not unusual (enough hits)	10549	1.545	1.51	0.019	1.864	0.035	1.278	1.842	1.51	0	
bond	00000001_8	C1 N2	Unusual (enough hits)	18	1.282	1.329	0.015	3.156	0.047	1.303	1.358	1.329	0.022	
bond	00000001_8	C1 N3	Unusual (enough hits)	27	1.425	1.352	0.022	3.327	0.073	1.327	1.394	1.344	0.031	
bond	00000001_8	C1 N4	Unusual (enough hits)	41	1.409	1.345	0.016	3.928	0.064	1.287	1.39	1.343	0.019	
bond	00000001_8	C5 C6	Unusual (enough hits)	560	1.433	1.381	0.017	3.108	0.052	1.279	1.497	1.382	0.001	
bond	00000001_8	C8 C4	Unusual (enough hits)	479	1.421	1.373	0.022	2.231	0.049	1.267	1.455	1.373	0.002	
bond	00000001_9	C1 N2	Not unusual (enough hits)	48	1.287	1.312	0.014	1.801	0.025	1.286	1.351	1.31	0.002	
bond	00000001_9	C2 N4	Not unusual (enough hits)	1745	1.466	1.457	0.022	0.377	0.008	1.204	1.687	1.458	0	
bond	00000001_9	C3 N3	Not unusual (enough hits)	1978	1.476	1.468	0.023	0.319	0.007	1.336	1.699	1.468	0	
bond	00000001_9	C3 C2	Not unusual (enough hits)	252	1.545	1.521	0.02	1.244	0.024	1.452	1.629	1.52	0	
bond	00000001_9	C4 CL1	Not unusual (enough hits)	743	1.747	1.738	0.019	0.504	0.009	1.561	1.806	1.74	0	
bond	00000001_9	C4 N6	Not unusual (enough hits)	245	1.355	1.321	0.025	1.328	0.033	1.254	1.422	1.317	0.002	
bond	00000001_9	C5 N6	Not unusual (enough hits)	2818	1.349	1.34	0.022	0.397	0.009	1.05	1.584	1.337	0	
bond	00000001_9	C7 C6	Not unusual (enough hits)	14050	1.421	1.384	0.022	1.694	0.037	0.618	1.8	1.386	0	
bond	00000001_9	C8 C7	Not unusual (enough hits)	20000	1.411	1.383	0.019	1.522	0.028	0.882	1.685	1.383	0	
bond	00000001_9	C9 N3	Not unusual (enough hits)	931	1.488	1.465	0.015	1.458	0.023	1.386	1.561	1.465	0	
bond	00000001_9	C9 C6	Not unusual (enough hits)	10549	1.54	1.51	0.019	1.635	0.03	1.278	1.842	1.51	0	
bond	00000001_9	C1 N3	Unusual (enough hits)	29	1.426	1.322	0.007	14.079	0.104	1.307	1.336	1.321	0.09	
bond	00000001_9	C1 N4	Unusual (enough hits)	16	1.41	1.327	0.013	6.659	0.084	1.294	1.339	1.329	0.071	
bond	00000001_9	C5 C6	Unusual (enough hits)	560	1.44	1.381	0.017	3.502	0.059	1.279	1.497	1.382	0.006	
bond	00000001_9	C8 C4	Unusual (enough hits)	479	1.417	1.373	0.022	2.026	0.044	1.267	1.455	1.373	0.002	
angle	00000001_1	C3 N3 C1	Not unusual (enough hits)	23	108.37	109.675	2.799	0.467	1.306	104.343	112.076	111.094	1.026	
angle	00000001_1	C9 N3 C3	Not unusual (enough hits)	109	123.543	120.505	2.722	1.116	3.038	110.736	125.952	121.036	0.147	
angle	00000001_1	N3 C1 N2	Not unusual (enough hits)	16	123.938	125.746	3.213	0.563	1.808	120.039	133.881	124.868	0.02	
angle	00000001_1	N4 C1 N2	Not unusual (enough hits)	5	125.305	122.569	2.404	1.138	2.736	120.265	126.041	122.711	0.736	

angle	00000001_1	N4 C1 N3	Not unusual (enough hits)	19	110.757	109.894	0.771	1.119	0.863	107.953	111.238	110.048	0.039	
angle	00000001_1	C2 N4 C1	Not unusual (enough hits)	53	109.532	110.972	2.593	0.555	1.44	105.927	114.592	111.774	0.009	
angle	00000001_1	C2 C3 N3	Not unusual (enough hits)	85	105.71	102.951	1.651	1.671	2.758	99.561	108.169	102.882	0.01	
angle	00000001_1	CL1 C4 N6	Not unusual (enough hits)	239	119.693	116.229	2.378	1.457	3.464	106.087	140.591	115.898	0.12	
angle	00000001_1	C8 C4 CL1	Not unusual (enough hits)	437	118.998	119.088	2.36	0.038	0.09	96.671	128.568	119.178	0.004	
angle	00000001_1	C6 C5 N6	Not unusual (enough hits)	225	120.963	123.744	1.746	1.593	2.781	117.703	127.597	124.357	0.048	
angle	00000001_1	C7 C6 C5	Not unusual (enough hits)	495	117.531	117.075	1.499	0.304	0.456	105.829	123.29	116.994	0.001	
angle	00000001_1	C9 C6 C5	Not unusual (enough hits)	155	122.674	121.018	1.641	1.009	1.656	113.768	126.783	120.987	0.055	
angle	00000001_1	C9 C6 C7	Not unusual (enough hits)	10997	119.795	120.774	1.905	0.514	0.98	90.622	143.824	120.777	0	
angle	00000001_1	C8 C7 C6	Not unusual (enough hits)	11395	120.442	121.039	1.437	0.416	0.597	93.35	147.791	121.028	0	
angle	00000001_1	C7 C8 C4	Not unusual (enough hits)	289	118.031	117.43	0.964	0.623	0.601	114.685	123.178	117.353	0.008	
angle	00000001_1	C9 N3 C1	Unusual (enough hits)	15	128.086	124.917	0.706	4.489	3.169	123.364	126.201	124.859	1.885	
angle	00000001_1	C3 C2 N4	Unusual (enough hits)	191	105.631	102.619	1.341	2.246	3.012	94.971	107.419	102.75	0.036	
angle	00000001_1	C8 C4 N6	Unusual (enough hits)	167	121.308	124.711	1.675	2.031	3.403	117.068	127.876	125.155	0	
angle	00000001_1	C5 N6 C4	Unusual (enough hits)	179	121.724	116.435	1.303	4.06	5.289	112.785	121.37	116.186	0.354	
angle	00000001_1	C6 C9 N3	Unusual (enough hits)	764	118.227	113.088	1.717	2.993	5.139	104.07	122.755	113.045	0.131	
angle	00000001_10	C3 N3 C1	Not unusual (enough hits)	23	108.351	109.675	2.799	0.473	1.324	104.343	112.076	111.094	1.007	
angle	00000001_10	C9 N3 C3	Not unusual (enough hits)	109	123.122	120.505	2.722	0.962	2.617	110.736	125.952	121.036	0.019	
angle	00000001_10	N3 C1 N2	Not unusual (enough hits)	16	124.253	125.746	3.213	0.465	1.493	120.039	133.881	124.868	0.205	
angle	00000001_10	N4 C1 N2	Not unusual (enough hits)	5	125.125	122.569	2.404	1.064	2.557	120.265	126.041	122.711	0.915	
angle	00000001_10	N4 C1 N3	Not unusual (enough hits)	19	110.622	109.894	0.771	0.943	0.728	107.953	111.238	110.048	0.058	
angle	00000001_10	C2 N4 C1	Not unusual (enough hits)	53	109.688	110.972	2.593	0.495	1.284	105.927	114.592	111.774	0.085	
angle	00000001_10	C2 C3 N3	Not unusual (enough hits)	85	105.799	102.951	1.651	1.725	2.848	99.561	108.169	102.882	0.02	
angle	00000001_10	CL1 C4 N6	Not unusual (enough hits)	239	119.708	116.229	2.378	1.463	3.479	106.087	140.591	115.898	0.135	
angle	00000001_10	C8 C4 CL1	Not unusual (enough hits)	437	119.159	119.088	2.36	0.03	0.071	96.671	128.568	119.178	0.003	
angle	00000001_10	C6 C5 N6	Not unusual (enough hits)	225	120.978	123.744	1.746	1.585	2.766	117.703	127.597	124.357	0.033	
angle	00000001_10	C7 C6 C5	Not unusual (enough hits)	495	117.487	117.075	1.499	0.275	0.413	105.829	123.29	116.994	0	
angle	00000001_10	C9 C6 C5	Not unusual (enough hits)	155	122.705	121.018	1.641	1.028	1.686	113.768	126.783	120.987	0.025	
angle	00000001_10	C9 C6 C7	Not unusual (enough hits)	10997	119.808	120.774	1.905	0.507	0.967	90.622	143.824	120.777	0.001	
angle	00000001_10	C8 C7 C6	Not unusual (enough hits)	11395	120.483	121.039	1.437	0.387	0.556	93.35	147.791	121.028	0	
angle	00000001_10	C7 C8 C4	Not unusual (enough hits)	289	117.842	117.43	0.964	0.427	0.411	114.685	123.178	117.353	0.012	
angle	00000001_10	C9 N3 C1	Unusual (enough hits)	15	128.526	124.917	0.706	5.112	3.608	123.364	126.201	124.859	2.324	
angle	00000001_10	C3 C2 N4	Unusual (enough hits)	191	105.54	102.619	1.341	2.178	2.92	94.971	107.419	102.75	0.055	
angle	00000001_10	C8 C4 N6	Unusual (enough hits)	167	121.133	124.711	1.675	2.136	3.578	117.068	127.876	125.155	0.175	
angle	00000001_10	C5 N6 C4	Unusual (enough hits)	179	122.077	116.435	1.303	4.331	5.642	112.785	121.37	116.186	0.707	
angle	00000001_10	C6 C9 N3	Unusual (enough hits)	764	118.831	113.088	1.717	3.345	5.743	104.07	122.755	113.045	0.347	
angle	00000001_2	C3 N3 C1	Not unusual (enough hits)	23	108.916	109.675	2.799	0.271	0.759	104.343	112.076	111.094	1.341	
angle	00000001_2	C9 N3 C3	Not unusual (enough hits)	109	123.154	120.505	2.722	0.973	2.649	110.736	125.952	121.036	0.013	
angle	00000001_2	N3 C1 N2	Not unusual (enough hits)	16	123.658	125.746	3.213	0.65	2.089	120.039	133.881	124.868	0.117	

angle	00000001_2	N4 C1 N2	Not unusual (enough hits)	5	125.834	122.569	2.404	1.358	3.265	120.265	126.041	122.711	0.207	
angle	00000001_2	N4 C1 N3	Not unusual (enough hits)	19	110.508	109.894	0.771	0.797	0.614	107.953	111.238	110.048	0.021	
angle	00000001_2	C2 N4 C1	Not unusual (enough hits)	53	109.236	110.972	2.593	0.669	1.735	105.927	114.592	111.774	0.056	
angle	00000001_2	C2 C3 N3	Not unusual (enough hits)	85	105.566	102.951	1.651	1.584	2.614	99.561	108.169	102.882	0.014	
angle	00000001_2	CL1 C4 N6	Not unusual (enough hits)	239	118.435	116.229	2.378	0.928	2.206	106.087	140.591	115.898	0.161	
angle	00000001_2	C8 C4 CL1	Not unusual (enough hits)	437	120.355	119.088	2.36	0.537	1.267	96.671	128.568	119.178	0.035	
angle	00000001_2	C6 C5 N6	Not unusual (enough hits)	225	121.767	123.744	1.746	1.132	1.977	117.703	127.597	124.357	0.002	
angle	00000001_2	C7 C6 C5	Not unusual (enough hits)	495	117.639	117.075	1.499	0.376	0.564	105.829	123.29	116.994	0.001	
angle	00000001_2	C9 C6 C5	Not unusual (enough hits)	155	119.103	121.018	1.641	1.167	1.915	113.768	126.783	120.987	0.045	
angle	00000001_2	C9 C6 C7	Not unusual (enough hits)	10997	123.258	120.774	1.905	1.304	2.484	90.622	143.824	120.777	0	
angle	00000001_2	C8 C7 C6	Not unusual (enough hits)	11395	119.703	121.039	1.437	0.93	1.336	93.35	147.791	121.028	0	
angle	00000001_2	C7 C8 C4	Not unusual (enough hits)	289	117.605	117.43	0.964	0.181	0.174	114.685	123.178	117.353	0.004	
angle	00000001_2	C9 N3 C1	Unusual (enough hits)	15	127.93	124.917	0.706	4.267	3.012	123.364	126.201	124.859	1.728	
angle	00000001_2	C3 C2 N4	Unusual (enough hits)	191	105.773	102.619	1.341	2.352	3.154	94.971	107.419	102.75	0.178	
angle	00000001_2	C8 C4 N6	Unusual (enough hits)	167	121.21	124.711	1.675	2.09	3.501	117.068	127.876	125.155	0.098	
angle	00000001_2	C5 N6 C4	Unusual (enough hits)	179	122.076	116.435	1.303	4.33	5.641	112.785	121.37	116.186	0.706	
angle	00000001_2	C6 C9 N3	Unusual (enough hits)	764	119.274	113.088	1.717	3.604	6.187	104.07	122.755	113.045	0.06	
angle	00000001_3	C3 N3 C1	Not unusual (enough hits)	23	108.544	109.675	2.799	0.404	1.131	104.343	112.076	111.094	1.2	
angle	00000001_3	C9 N3 C3	Not unusual (enough hits)	109	123.332	120.505	2.722	1.039	2.827	110.736	125.952	121.036	0.014	
angle	00000001_3	N3 C1 N2	Not unusual (enough hits)	16	123.847	125.746	3.213	0.591	1.9	120.039	133.881	124.868	0.111	
angle	00000001_3	N4 C1 N2	Not unusual (enough hits)	5	125.545	122.569	2.404	1.238	2.976	120.265	126.041	122.711	0.496	
angle	00000001_3	N4 C1 N3	Not unusual (enough hits)	19	110.609	109.894	0.771	0.927	0.715	107.953	111.238	110.048	0.045	
angle	00000001_3	C2 N4 C1	Not unusual (enough hits)	53	109.56	110.972	2.593	0.544	1.411	105.927	114.592	111.774	0.014	
angle	00000001_3	C2 C3 N3	Not unusual (enough hits)	85	105.68	102.951	1.651	1.653	2.729	99.561	108.169	102.882	0.019	
angle	00000001_3	CL1 C4 N6	Not unusual (enough hits)	239	119.606	116.229	2.378	1.42	3.377	106.087	140.591	115.898	0.034	
angle	00000001_3	C8 C4 CL1	Not unusual (enough hits)	437	119.067	119.088	2.36	0.009	0.021	96.671	128.568	119.178	0.001	
angle	00000001_3	C6 C5 N6	Not unusual (enough hits)	225	120.879	123.744	1.746	1.641	2.865	117.703	127.597	124.357	0.131	
angle	00000001_3	C7 C6 C5	Not unusual (enough hits)	495	117.621	117.075	1.499	0.365	0.547	105.829	123.29	116.994	0.004	
angle	00000001_3	C9 C6 C5	Not unusual (enough hits)	155	122.556	121.018	1.641	0.937	1.538	113.768	126.783	120.987	0.023	
angle	00000001_3	C9 C6 C7	Not unusual (enough hits)	10997	119.822	120.774	1.905	0.5	0.952	90.622	143.824	120.777	0	
angle	00000001_3	C8 C7 C6	Not unusual (enough hits)	11395	120.488	121.039	1.437	0.384	0.551	93.35	147.791	121.028	0	
angle	00000001_3	C7 C8 C4	Not unusual (enough hits)	289	117.785	117.43	0.964	0.368	0.355	114.685	123.178	117.353	0.004	
angle	00000001_3	C9 N3 C1	Unusual (enough hits)	15	128.124	124.917	0.706	4.542	3.206	123.364	126.201	124.859	1.922	
angle	00000001_3	C3 C2 N4	Unusual (enough hits)	191	105.607	102.619	1.341	2.228	2.987	94.971	107.419	102.75	0.011	
angle	00000001_3	C8 C4 N6	Unusual (enough hits)	167	121.326	124.711	1.675	2.02	3.385	117.068	127.876	125.155	0.018	
angle	00000001_3	C5 N6 C4	Unusual (enough hits)	179	121.9	116.435	1.303	4.195	5.465	112.785	121.37	116.186	0.53	
angle	00000001_3	C6 C9 N3	Unusual (enough hits)	764	118.097	113.088	1.717	2.918	5.009	104.07	122.755	113.045	0.001	
angle	00000001_4	C3 N3 C1	Not unusual (enough hits)	23	108.299	109.675	2.799	0.492	1.376	104.343	112.076	111.094	0.955	
angle	00000001_4	C9 N3 C3	Not unusual (enough hits)	109	122.808	120.505	2.722	0.846	2.303	110.736	125.952	121.036	0.002	

angle	00000001_4	N3 C1 N2	Not unusual (enough hits)	16	124.492	125.746	3.213	0.39	1.254	120.039	133.881	124.868	0.109	
angle	00000001_4	N4 C1 N2	Not unusual (enough hits)	5	125.141	122.569	2.404	1.07	2.572	120.265	126.041	122.711	0.9	
angle	00000001_4	N4 C1 N3	Not unusual (enough hits)	19	110.367	109.894	0.771	0.613	0.473	107.953	111.238	110.048	0.115	
angle	00000001_4	C2 N4 C1	Not unusual (enough hits)	53	110.031	110.972	2.593	0.363	0.94	105.927	114.592	111.774	0.211	
angle	00000001_4	C2 C3 N3	Not unusual (enough hits)	85	105.885	102.951	1.651	1.777	2.933	99.561	108.169	102.882	0.065	
angle	00000001_4	CL1 C4 N6	Not unusual (enough hits)	239	120.051	116.229	2.378	1.607	3.822	106.087	140.591	115.898	0.077	
angle	00000001_4	C8 C4 CL1	Not unusual (enough hits)	437	118.75	119.088	2.36	0.143	0.338	96.671	128.568	119.178	0	
angle	00000001_4	C6 C5 N6	Not unusual (enough hits)	225	120.853	123.744	1.746	1.656	2.891	117.703	127.597	124.357	0.128	
angle	00000001_4	C7 C6 C5	Not unusual (enough hits)	495	117.165	117.075	1.499	0.06	0.09	105.829	123.29	116.994	0.002	
angle	00000001_4	C9 C6 C5	Not unusual (enough hits)	155	123.089	121.018	1.641	1.262	2.071	113.768	126.783	120.987	0.009	
angle	00000001_4	C9 C6 C7	Not unusual (enough hits)	10997	119.746	120.774	1.905	0.54	1.029	90.622	143.824	120.777	0.001	
angle	00000001_4	C8 C7 C6	Not unusual (enough hits)	11395	120.604	121.039	1.437	0.303	0.436	93.35	147.791	121.028	0	
angle	00000001_4	C7 C8 C4	Not unusual (enough hits)	289	118.242	117.43	0.964	0.842	0.812	114.685	123.178	117.353	0.007	
angle	00000001_4	C9 N3 C1	Unusual (enough hits)	15	128.892	124.917	0.706	5.63	3.974	123.364	126.201	124.859	2.69	
angle	00000001_4	C3 C2 N4	Unusual (enough hits)	191	105.418	102.619	1.341	2.087	2.798	94.971	107.419	102.75	0.005	
angle	00000001_4	C8 C4 N6	Unusual (enough hits)	167	121.199	124.711	1.675	2.096	3.512	117.068	127.876	125.155	0.109	
angle	00000001_4	C5 N6 C4	Unusual (enough hits)	179	121.937	116.435	1.303	4.223	5.502	112.785	121.37	116.186	0.567	
angle	00000001_4	C6 C9 N3	Unusual (enough hits)	764	119.207	113.088	1.717	3.564	6.119	104.07	122.755	113.045	0.028	
angle	00000001_5	C3 N3 C1	Not unusual (enough hits)	23	108.3	109.675	2.799	0.491	1.375	104.343	112.076	111.094	0.956	
angle	00000001_5	C9 N3 C3	Not unusual (enough hits)	109	123.111	120.505	2.722	0.958	2.606	110.736	125.952	121.036	0.023	
angle	00000001_5	N3 C1 N2	Not unusual (enough hits)	16	124.091	125.746	3.213	0.515	1.656	120.039	133.881	124.868	0.043	
angle	00000001_5	N4 C1 N2	Not unusual (enough hits)	5	125.245	122.569	2.404	1.114	2.677	120.265	126.041	122.711	0.795	
angle	00000001_5	N4 C1 N3	Not unusual (enough hits)	19	110.664	109.894	0.771	0.998	0.77	107.953	111.238	110.048	0.1	
angle	00000001_5	C2 N4 C1	Not unusual (enough hits)	53	109.796	110.972	2.593	0.454	1.176	105.927	114.592	111.774	0.007	
angle	00000001_5	C2 C3 N3	Not unusual (enough hits)	85	105.781	102.951	1.651	1.714	2.829	99.561	108.169	102.882	0.038	
angle	00000001_5	CL1 C4 N6	Not unusual (enough hits)	239	120.072	116.229	2.378	1.616	3.843	106.087	140.591	115.898	0.098	
angle	00000001_5	C8 C4 CL1	Not unusual (enough hits)	437	118.865	119.088	2.36	0.094	0.223	96.671	128.568	119.178	0.004	
angle	00000001_5	C6 C5 N6	Not unusual (enough hits)	225	120.746	123.744	1.746	1.718	2.998	117.703	127.597	124.357	0.021	
angle	00000001_5	C7 C6 C5	Not unusual (enough hits)	495	117.319	117.075	1.499	0.163	0.244	105.829	123.29	116.994	0.001	
angle	00000001_5	C9 C6 C5	Not unusual (enough hits)	155	123.29	121.018	1.641	1.384	2.272	113.768	126.783	120.987	0.026	
angle	00000001_5	C9 C6 C7	Not unusual (enough hits)	10997	119.391	120.774	1.905	0.726	1.383	90.622	143.824	120.777	0	
angle	00000001_5	C8 C7 C6	Not unusual (enough hits)	11395	120.847	121.039	1.437	0.134	0.192	93.35	147.791	121.028	0	
angle	00000001_5	C7 C8 C4	Not unusual (enough hits)	289	118.017	117.43	0.964	0.609	0.587	114.685	123.178	117.353	0.005	
angle	00000001_5	C9 N3 C1	Unusual (enough hits)	15	128.587	124.917	0.706	5.199	3.67	123.364	126.201	124.859	2.386	
angle	00000001_5	C3 C2 N4	Unusual (enough hits)	191	105.459	102.619	1.341	2.118	2.84	94.971	107.419	102.75	0.047	
angle	00000001_5	C8 C4 N6	Unusual (enough hits)	167	121.063	124.711	1.675	2.178	3.648	117.068	127.876	125.155	0.24	
angle	00000001_5	C5 N6 C4	Unusual (enough hits)	179	122.009	116.435	1.303	4.278	5.573	112.785	121.37	116.186	0.638	
angle	00000001_5	C6 C9 N3	Unusual (enough hits)	764	119.725	113.088	1.717	3.866	6.638	104.07	122.755	113.045	0.037	
angle	00000001_6	C3 N3 C1	Not unusual (enough hits)	23	108.293	109.675	2.799	0.494	1.383	104.343	112.076	111.094	0.949	

angle	00000001_6	C9 N3 C3	Not unusual (enough hits)	109	123.165	120.505	2.722	0.978	2.661	110.736	125.952	121.036	0.025	
angle	00000001_6	N3 C1 N2	Not unusual (enough hits)	16	124.118	125.746	3.213	0.507	1.629	120.039	133.881	124.868	0.07	
angle	00000001_6	N4 C1 N2	Not unusual (enough hits)	5	125.262	122.569	2.404	1.12	2.693	120.265	126.041	122.711	0.779	
angle	00000001_6	N4 C1 N3	Not unusual (enough hits)	19	110.62	109.894	0.771	0.942	0.726	107.953	111.238	110.048	0.057	
angle	00000001_6	C2 N4 C1	Not unusual (enough hits)	53	109.726	110.972	2.593	0.481	1.246	105.927	114.592	111.774	0.047	
angle	00000001_6	C2 C3 N3	Not unusual (enough hits)	85	105.824	102.951	1.651	1.74	2.873	99.561	108.169	102.882	0.005	
angle	00000001_6	CL1 C4 N6	Not unusual (enough hits)	239	119.811	116.229	2.378	1.506	3.582	106.087	140.591	115.898	0.163	
angle	00000001_6	C8 C4 CL1	Not unusual (enough hits)	437	119.24	119.088	2.36	0.064	0.151	96.671	128.568	119.178	0.007	
angle	00000001_6	C6 C5 N6	Not unusual (enough hits)	225	121.018	123.744	1.746	1.562	2.726	117.703	127.597	124.357	0.007	
angle	00000001_6	C7 C6 C5	Not unusual (enough hits)	495	117.285	117.075	1.499	0.14	0.21	105.829	123.29	116.994	0.001	
angle	00000001_6	C9 C6 C5	Not unusual (enough hits)	155	122.692	121.018	1.641	1.02	1.674	113.768	126.783	120.987	0.037	
angle	00000001_6	C9 C6 C7	Not unusual (enough hits)	10997	120.023	120.774	1.905	0.395	0.752	90.622	143.824	120.777	0	
angle	00000001_6	C8 C7 C6	Not unusual (enough hits)	11395	120.526	121.039	1.437	0.357	0.513	93.35	147.791	121.028	0	
angle	00000001_6	C7 C8 C4	Not unusual (enough hits)	289	118.058	117.43	0.964	0.651	0.628	114.685	123.178	117.353	0.019	
angle	00000001_6	C9 N3 C1	Unusual (enough hits)	15	128.541	124.917	0.706	5.133	3.624	123.364	126.201	124.859	2.34	
angle	00000001_6	C3 C2 N4	Unusual (enough hits)	191	105.537	102.619	1.341	2.175	2.917	94.971	107.419	102.75	0.059	
angle	00000001_6	C8 C4 N6	Unusual (enough hits)	167	120.949	124.711	1.675	2.245	3.762	117.068	127.876	125.155	0.126	
angle	00000001_6	C5 N6 C4	Unusual (enough hits)	179	122.164	116.435	1.303	4.397	5.729	112.785	121.37	116.186	0.794	
angle	00000001_6	C6 C9 N3	Unusual (enough hits)	764	118.405	113.088	1.717	3.097	5.317	104.07	122.755	113.045	0.309	
angle	00000001_7	C3 N3 C1	Not unusual (enough hits)	23	108.503	109.675	2.799	0.419	1.172	104.343	112.076	111.094	1.159	
angle	00000001_7	C9 N3 C3	Not unusual (enough hits)	109	123.592	120.505	2.722	1.134	3.087	110.736	125.952	121.036	0.098	
angle	00000001_7	N3 C1 N2	Not unusual (enough hits)	16	123.742	125.746	3.213	0.624	2.005	120.039	133.881	124.868	0.202	
angle	00000001_7	N4 C1 N2	Not unusual (enough hits)	5	125.613	122.569	2.404	1.266	3.044	120.265	126.041	122.711	0.428	
angle	00000001_7	N4 C1 N3	Not unusual (enough hits)	19	110.646	109.894	0.771	0.974	0.752	107.953	111.238	110.048	0.082	
angle	00000001_7	C2 N4 C1	Not unusual (enough hits)	53	109.751	110.972	2.593	0.471	1.22	105.927	114.592	111.774	0.021	
angle	00000001_7	C3 C2 N4	Not unusual (enough hits)	191	105.287	102.619	1.341	1.989	2.667	94.971	107.419	102.75	0.069	
angle	00000001_7	C2 C3 N3	Not unusual (enough hits)	85	105.813	102.951	1.651	1.734	2.862	99.561	108.169	102.882	0.006	
angle	00000001_7	CL1 C4 N6	Not unusual (enough hits)	239	119.495	116.229	2.378	1.373	3.266	106.087	140.591	115.898	0.078	
angle	00000001_7	C8 C4 CL1	Not unusual (enough hits)	437	119.045	119.088	2.36	0.018	0.043	96.671	128.568	119.178	0.003	
angle	00000001_7	C8 C4 N6	Not unusual (enough hits)	167	121.46	124.711	1.675	1.941	3.251	117.068	127.876	125.155	0.095	
angle	00000001_7	C6 C5 N6	Not unusual (enough hits)	225	121.038	123.744	1.746	1.55	2.706	117.703	127.597	124.357	0.006	
angle	00000001_7	C7 C6 C5	Not unusual (enough hits)	495	117.511	117.075	1.499	0.291	0.437	105.829	123.29	116.994	0.001	
angle	00000001_7	C9 C6 C5	Not unusual (enough hits)	155	122.616	121.018	1.641	0.973	1.597	113.768	126.783	120.987	0.036	
angle	00000001_7	C9 C6 C7	Not unusual (enough hits)	10997	119.873	120.774	1.905	0.473	0.901	90.622	143.824	120.777	0	
angle	00000001_7	C8 C7 C6	Not unusual (enough hits)	11395	120.456	121.039	1.437	0.406	0.584	93.35	147.791	121.028	0	
angle	00000001_7	C7 C8 C4	Not unusual (enough hits)	289	117.973	117.43	0.964	0.563	0.543	114.685	123.178	117.353	0.003	
angle	00000001_7	C9 N3 C1	Unusual (enough hits)	15	127.904	124.917	0.706	4.231	2.987	123.364	126.201	124.859	1.703	
angle	00000001_7	C5 N6 C4	Unusual (enough hits)	179	121.562	116.435	1.303	3.935	5.127	112.785	121.37	116.186	0.192	
angle	00000001_7	C6 C9 N3	Unusual (enough hits)	764	118.008	113.088	1.717	2.866	4.921	104.07	122.755	113.045	0.064	

angle	00000001_8	C3 N3 C1	Not unusual (enough hits)	23	108.202	109.675	2.799	0.526	1.473	104.343	112.076	111.094	0.858	
angle	00000001_8	C9 N3 C3	Not unusual (enough hits)	109	123.525	120.505	2.722	1.11	3.021	110.736	125.952	121.036	0.165	
angle	00000001_8	N3 C1 N2	Not unusual (enough hits)	16	123.876	125.746	3.213	0.582	1.871	120.039	133.881	124.868	0.082	
angle	00000001_8	N4 C1 N2	Not unusual (enough hits)	5	125.338	122.569	2.404	1.152	2.769	120.265	126.041	122.711	0.703	
angle	00000001_8	N4 C1 N3	Not unusual (enough hits)	19	110.787	109.894	0.771	1.157	0.893	107.953	111.238	110.048	0.009	
angle	00000001_8	C2 N4 C1	Not unusual (enough hits)	53	109.664	110.972	2.593	0.504	1.308	105.927	114.592	111.774	0.061	
angle	00000001_8	C2 C3 N3	Not unusual (enough hits)	85	105.886	102.951	1.651	1.778	2.935	99.561	108.169	102.882	0.067	
angle	00000001_8	CL1 C4 N6	Not unusual (enough hits)	239	119.685	116.229	2.378	1.453	3.456	106.087	140.591	115.898	0.112	
angle	00000001_8	C8 C4 CL1	Not unusual (enough hits)	437	119.276	119.088	2.36	0.08	0.188	96.671	128.568	119.178	0.003	
angle	00000001_8	C6 C5 N6	Not unusual (enough hits)	225	120.974	123.744	1.746	1.587	2.77	117.703	127.597	124.357	0.037	
angle	00000001_8	C7 C6 C5	Not unusual (enough hits)	495	117.361	117.075	1.499	0.191	0.287	105.829	123.29	116.994	0.003	
angle	00000001_8	C9 C6 C5	Not unusual (enough hits)	155	122.775	121.018	1.641	1.071	1.757	113.768	126.783	120.987	0.024	
angle	00000001_8	C9 C6 C7	Not unusual (enough hits)	10997	119.864	120.774	1.905	0.478	0.911	90.622	143.824	120.777	0	
angle	00000001_8	C8 C7 C6	Not unusual (enough hits)	11395	120.497	121.039	1.437	0.378	0.542	93.35	147.791	121.028	0	
angle	00000001_8	C7 C8 C4	Not unusual (enough hits)	289	117.978	117.43	0.964	0.568	0.547	114.685	123.178	117.353	0.001	
angle	00000001_8	C9 N3 C1	Unusual (enough hits)	15	128.27	124.917	0.706	4.749	3.353	123.364	126.201	124.859	2.069	
angle	00000001_8	C3 C2 N4	Unusual (enough hits)	191	105.461	102.619	1.341	2.119	2.842	94.971	107.419	102.75	0.048	
angle	00000001_8	C8 C4 N6	Unusual (enough hits)	167	121.039	124.711	1.675	2.192	3.672	117.068	127.876	125.155	0.216	
angle	00000001_8	C5 N6 C4	Unusual (enough hits)	179	122.151	116.435	1.303	4.387	5.716	112.785	121.37	116.186	0.781	
angle	00000001_8	C6 C9 N3	Unusual (enough hits)	764	118.988	113.088	1.717	3.437	5.901	104.07	122.755	113.045	0.19	
angle	00000001_9	C3 N3 C1	Not unusual (enough hits)	47	108.533	107.481	2.754	0.382	1.052	101.087	112.593	107.642	0.043	
angle	00000001_9	C9 N3 C3	Not unusual (enough hits)	109	123.281	120.505	2.722	1.02	2.776	110.736	125.952	121.036	0.004	
angle	00000001_9	N4 C1 N2	Not unusual (enough hits)	18	125.413	124.34	1.033	1.039	1.074	122.959	126.3	124.227	0.209	
angle	00000001_9	N4 C1 N3	Not unusual (enough hits)	23	110.621	109.522	1.992	0.552	1.098	105.05	111.894	109.815	0.317	
angle	00000001_9	C2 N4 C1	Not unusual (enough hits)	30	109.815	110.448	2.422	0.261	0.632	106.025	117.223	110.226	0.013	
angle	00000001_9	C3 C2 N4	Not unusual (enough hits)	191	105.222	102.619	1.341	1.941	2.603	94.971	107.419	102.75	0.005	
angle	00000001_9	C2 C3 N3	Not unusual (enough hits)	85	105.808	102.951	1.651	1.731	2.857	99.561	108.169	102.882	0.011	
angle	00000001_9	CL1 C4 N6	Not unusual (enough hits)	239	119.936	116.229	2.378	1.559	3.707	106.087	140.591	115.898	0.038	
angle	00000001_9	C8 C4 CL1	Not unusual (enough hits)	437	118.847	119.088	2.36	0.102	0.241	96.671	128.568	119.178	0	
angle	00000001_9	C6 C5 N6	Not unusual (enough hits)	225	120.752	123.744	1.746	1.714	2.992	117.703	127.597	124.357	0.027	
angle	00000001_9	C7 C6 C5	Not unusual (enough hits)	495	117.486	117.075	1.499	0.274	0.411	105.829	123.29	116.994	0	
angle	00000001_9	C9 C6 C5	Not unusual (enough hits)	155	122.65	121.018	1.641	0.994	1.632	113.768	126.783	120.987	0.071	
angle	00000001_9	C9 C6 C7	Not unusual (enough hits)	10997	119.864	120.774	1.905	0.478	0.91	90.622	143.824	120.777	0	
angle	00000001_9	C8 C7 C6	Not unusual (enough hits)	11395	120.471	121.039	1.437	0.395	0.568	93.35	147.791	121.028	0	
angle	00000001_9	C7 C8 C4	Not unusual (enough hits)	289	118.207	117.43	0.964	0.806	0.777	114.685	123.178	117.353	0.024	
angle	00000001_9	C9 N3 C1	Unusual (enough hits)	17	128.184	124.963	0.849	3.792	3.221	123.364	126.773	124.859	1.411	
angle	00000001_9	N3 C1 N2	Unusual (enough hits)	21	123.966	126.65	0.877	3.059	2.684	124.996	128.069	126.406	1.03	
angle	00000001_9	C8 C4 N6	Unusual (enough hits)	167	121.216	124.711	1.675	2.086	3.495	117.068	127.876	125.155	0.092	
angle	00000001_9	C5 N6 C4	Unusual (enough hits)	179	121.867	116.435	1.303	4.17	5.432	112.785	121.37	116.186	0.497	

angle	00000001_9	C6 C9 N3	Unusual (enough hits)	764	118.301	113.088	1.717	3.036	5.213	104.07	122.755	113.045	0.205	
torsion	00000001_1	C6 C9 N3 C1	Not unusual (enough hits)	48	−114.525								0.547	0.271
torsion	00000001_1	C6 C9 N3 C3	Not unusual (enough hits)	182	65.898								0.06	0.599
torsion	00000001_1	C5 C6 C9 N3	Not unusual (enough hits)	349	21.124								0.209	0.109
torsion	00000001_1	C7 C6 C9 N3	Not unusual (enough hits)	10853	−158.894								0.002	0.095
torsion	00000001_10	C6 C9 N3 C1	Not unusual (enough hits)	48	−106.37								0.099	0.188
torsion	00000001_10	C6 C9 N3 C3	Not unusual (enough hits)	182	74.105								0.098	0.632
torsion	00000001_10	C5 C6 C9 N3	Not unusual (enough hits)	349	11.612								0.32	0.083
torsion	00000001_10	C7 C6 C9 N3	Not unusual (enough hits)	10853	−168.543								0.008	0.078
torsion	00000001_2	C6 C9 N3 C1	Not unusual (enough hits)	48	108.237								0.686	0.188
torsion	00000001_2	C6 C9 N3 C3	Not unusual (enough hits)	182	−71.972								0.006	0.687
torsion	00000001_2	C5 C6 C9 N3	Not unusual (enough hits)	349	158.876								0.858	0.074
torsion	00000001_2	C7 C6 C9 N3	Not unusual (enough hits)	10853	−21.285								0.017	0.086
torsion	00000001_3	C6 C9 N3 C1	Not unusual (enough hits)	48	−106.897								0.103	0.208
torsion	00000001_3	C6 C9 N3 C3	Not unusual (enough hits)	182	73.314								0.065	0.665
torsion	00000001_3	C5 C6 C9 N3	Not unusual (enough hits)	349	18.079								0.228	0.103
torsion	00000001_3	C7 C6 C9 N3	Not unusual (enough hits)	10853	−162.082								0.001	0.09
torsion	00000001_4	C6 C9 N3 C1	Not unusual (enough hits)	48	−105.116								0.095	0.188
torsion	00000001_4	C6 C9 N3 C3	Not unusual (enough hits)	182	75.331								0.14	0.615
torsion	00000001_4	C5 C6 C9 N3	Not unusual (enough hits)	349	13.292								0.385	0.1
torsion	00000001_4	C7 C6 C9 N3	Not unusual (enough hits)	10853	−166.919								0.001	0.081
torsion	00000001_5	C6 C9 N3 C1	Not unusual (enough hits)	48	−94.952								0.207	0.229
torsion	00000001_5	C6 C9 N3 C3	Not unusual (enough hits)	182	85.619								0.5	0.297
torsion	00000001_5	C5 C6 C9 N3	Not unusual (enough hits)	349	−6.46								0.008	0.072
torsion	00000001_5	C7 C6 C9 N3	Not unusual (enough hits)	10853	173.687								0.006	0.061
torsion	00000001_6	C6 C9 N3 C1	Not unusual (enough hits)	48	−99.661								0.171	0.229
torsion	00000001_6	C6 C9 N3 C3	Not unusual (enough hits)	182	80.689								0.237	0.445
torsion	00000001_6	C5 C6 C9 N3	Not unusual (enough hits)	349	5.753								0.699	0.063
torsion	00000001_6	C7 C6 C9 N3	Not unusual (enough hits)	10853	−174.241								0.001	0.058
torsion	00000001_7	C6 C9 N3 C1	Not unusual (enough hits)	48	−113.808								1.265	0.229
torsion	00000001_7	C6 C9 N3 C3	Not unusual (enough hits)	182	66.442								0.021	0.615
torsion	00000001_7	C5 C6 C9 N3	Not unusual (enough hits)	349	15.353								0.582	0.092
torsion	00000001_7	C7 C6 C9 N3	Not unusual (enough hits)	10853	−164.785								0.011	0.085
torsion	00000001_8	C6 C9 N3 C1	Not unusual (enough hits)	48	−104.134								0.14	0.208
torsion	00000001_8	C6 C9 N3 C3	Not unusual (enough hits)	182	76.442								0.026	0.577
torsion	00000001_8	C5 C6 C9 N3	Not unusual (enough hits)	349	3.055								0.331	0.054
torsion	00000001_8	C7 C6 C9 N3	Unusual (enough hits)	10853	−176.876								0.039	0.049
torsion	00000001_9	C6 C9 N3 C1	Not unusual (enough hits)	48	−108.232								0.681	0.188
torsion	00000001_9	C6 C9 N3 C3	Not unusual (enough hits)	182	72.235								0.082	0.687

torsion	00000001_9	C5 C6 C9 N3	Not unusual (enough hits)	349	17.789								0.057	0.097
torsion	00000001_9	C7 C6 C9 N3	Not unusual (enough hits)	10853	−162.359								0.017	0.089
ring	00000001_1	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.671	16.292			0.771
ring	00000001_1	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.032	8.354			1
ring	00000001_10	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.619	16.263			0.771
ring	00000001_10	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.033	8.358			1
ring	00000001_2	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.725	16.348			0.771
ring	00000001_2	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.06	8.319			1
ring	00000001_3	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.723	16.368			0.771
ring	00000001_3	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.031	8.366			1
ring	00000001_4	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.684	16.328			0.771
ring	00000001_4	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.041	8.269			1
ring	00000001_5	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.629	16.334			0.771
ring	00000001_5	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.028	8.368			1
ring	00000001_6	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.696	16.34			0.771
ring	00000001_6	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.046	8.326			1
ring	00000001_7	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.676	16.346			0.771
ring	00000001_7	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.021	8.37			1
ring	00000001_8	N3 C1 N4 C2 C3	Not unusual (enough hits)	35						0.681	16.31			0.771
ring	00000001_8	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.01	8.359			1
ring	00000001_9	N3 C1 N4 C2 C3	Not unusual (enough hits)	41						1.151	19.614			0.415
ring	00000001_9	C4 N6 C5 C6 C7 C8	Not unusual (enough hits)	320						0.038	8.373			1

Table 10. Geometry Analysis by Mogul of DN-IMI in Complex withGln55Arg Mutant of *Ls*-AChBP

Type	Molecule	Fragment	Classification	No. of hits	Query value	Mean	Std. dev.	|z-score|	|x - mean|	Minimum	Maximum	Median	|d(min)|	Local density
bond	00000001_1	C3 N3	Not unusual (enough hits	1978	1.469	1.468	0.023	0.025	0.001	1.336	1.699	1.468	0	
bond	00000001_1	C9 N3	Not unusual (enough hits	931	1.488	1.465	0.015	1.484	0.023	1.386	1.561	1.465	0	
bond	00000001_1	C2 N4	Not unusual (enough hits	1745	1.46	1.457	0.022	0.103	0.002	1.204	1.687	1.458	0	
bond	00000001_1	C3 C2	Not unusual (enough hits	252	1.544	1.521	0.02	1.198	0.023	1.452	1.629	1.52	0.001	
bond	00000001_1	C4 CL1	Not unusual (enough hits	743	1.746	1.738	0.019	0.457	0.008	1.561	1.806	1.74	0	
bond	00000001_1	C4 N6	Not unusual (enough hits	245	1.326	1.321	0.025	0.178	0.004	1.254	1.422	1.317	0	
bond	00000001_1	C5 N6	Not unusual (enough hits	2818	1.333	1.34	0.022	0.338	0.008	1.05	1.584	1.337	0	
bond	00000001_1	C9 C6	Not unusual (enough hits	10549	1.543	1.51	0.019	1.79	0.033	1.278	1.842	1.51	0	
bond	00000001_1	C1 N2	Unusual (enough hits)	18	1.281	1.329	0.015	3.232	0.048	1.303	1.358	1.329	0.023	
bond	00000001_1	C1 N3	Unusual (enough hits)	27	1.419	1.352	0.022	3.089	0.068	1.327	1.394	1.344	0.026	
bond	00000001_1	C1 N4	Unusual (enough hits)	41	1.411	1.345	0.016	4.033	0.066	1.287	1.39	1.343	0.021	
bond	00000001_1	C8 C4	Unusual (enough hits)	479	1.438	1.373	0.022	2.991	0.065	1.267	1.455	1.373	0.001	
bond	00000001_1	C5 C6	Unusual (enough hits)	560	1.423	1.381	0.017	2.526	0.043	1.279	1.497	1.382	0.006	
bond	00000001_1	C7 C6	Unusual (enough hits)	14050	1.433	1.384	0.022	2.218	0.049	0.618	1.8	1.386	0	
bond	00000001_1	C8 C7	Unusual (enough hits)	20000	1.43	1.383	0.019	2.549	0.047	0.882	1.685	1.383	0	
bond	00000001_2	C3 N3	Not unusual (enough hits	1978	1.466	1.468	0.023	0.094	0.002	1.336	1.699	1.468	0	
bond	00000001_2	C9 N3	Not unusual (enough hits	931	1.472	1.465	0.015	0.468	0.007	1.386	1.561	1.465	0	
bond	00000001_2	C2 N4	Not unusual (enough hits	1745	1.467	1.457	0.022	0.435	0.01	1.204	1.687	1.458	0	
bond	00000001_2	C3 C2	Not unusual (enough hits	252	1.543	1.521	0.02	1.119	0.022	1.452	1.629	1.52	0.001	
bond	00000001_2	C4 CL1	Not unusual (enough hits	743	1.744	1.738	0.019	0.349	0.006	1.561	1.806	1.74	0	
bond	00000001_2	C4 N6	Not unusual (enough hits	245	1.33	1.321	0.025	0.333	0.008	1.254	1.422	1.317	0	
bond	00000001_2	C5 N6	Not unusual (enough hits	2818	1.331	1.34	0.022	0.421	0.009	1.05	1.584	1.337	0	
bond	00000001_2	C9 C6	Not unusual (enough hits	10549	1.542	1.51	0.019	1.75	0.033	1.278	1.842	1.51	0	
bond	00000001_2	C1 N2	Unusual (enough hits)	18	1.282	1.329	0.015	3.126	0.046	1.303	1.358	1.329	0.021	
bond	00000001_2	C1 N3	Unusual (enough hits)	27	1.424	1.352	0.022	3.281	0.072	1.327	1.394	1.344	0.03	
bond	00000001_2	C1 N4	Unusual (enough hits)	41	1.404	1.345	0.016	3.65	0.059	1.287	1.39	1.343	0.015	
bond	00000001_2	C8 C4	Unusual (enough hits)	479	1.436	1.373	0.022	2.91	0.064	1.267	1.455	1.373	0.003	
bond	00000001_2	C5 C6	Unusual (enough hits)	560	1.417	1.381	0.017	2.162	0.036	1.279	1.497	1.382	0.001	
bond	00000001_2	C7 C6	Unusual (enough hits)	14050	1.436	1.384	0.022	2.373	0.052	0.618	1.8	1.386	0	
bond	00000001_2	C8 C7	Unusual (enough hits)	20000	1.439	1.383	0.019	3.013	0.056	0.882	1.685	1.383	0	
bond	00000001_3	C3 N3	Not unusual (enough hits	1978	1.477	1.468	0.023	0.404	0.009	1.336	1.699	1.468	0	
bond	00000001_3	C9 N3	Not unusual (enough hits	931	1.486	1.465	0.015	1.362	0.021	1.386	1.561	1.465	0	
bond	00000001_3	C2 N4	Not unusual (enough hits	1745	1.467	1.457	0.022	0.452	0.01	1.204	1.687	1.458	0	
bond	00000001_3	C3 C2	Not unusual (enough hits	252	1.545	1.521	0.02	1.235	0.024	1.452	1.629	1.52	0	
bond	00000001_3	C4 CL1	Not unusual (enough hits	743	1.734	1.738	0.019	0.199	0.004	1.561	1.806	1.74	0	
bond	00000001_3	C4 N6	Not unusual (enough hits	245	1.325	1.321	0.025	0.124	0.003	1.254	1.422	1.317	0	
bond	00000001_3	C5 N6	Not unusual (enough hits	2818	1.329	1.34	0.022	0.479	0.011	1.05	1.584	1.337	0	
bond	00000001_3	C7 C6	Not unusual (enough hits	14050	1.426	1.384	0.022	1.906	0.042	0.618	1.8	1.386	0	
bond	00000001_3	C9 C6	Not unusual (enough hits	10549	1.542	1.51	0.019	1.737	0.032	1.278	1.842	1.51	0	
bond	00000001_3	C1 N2	Unusual (enough hits)	18	1.291	1.329	0.015	2.511	0.037	1.303	1.358	1.329	0.012	
bond	00000001_3	C1 N3	Unusual (enough hits)	27	1.425	1.352	0.022	3.348	0.074	1.327	1.394	1.344	0.031	
bond	00000001_3	C1 N4	Unusual (enough hits)	41	1.412	1.345	0.016	4.103	0.067	1.287	1.39	1.343	0.022	
bond	00000001_3	C8 C4	Unusual (enough hits)	479	1.428	1.373	0.022	2.536	0.056	1.267	1.455	1.373	0.009	

bond	00000001_3	C5 C6	Unusual (enough hits)	560	1.423	1.381	0.017	2.479	0.042	1.279	1.497	1.382	0.005	
bond	00000001_3	C8 C7	Unusual (enough hits)	20000	1.428	1.383	0.019	2.395	0.044	0.882	1.685	1.383	0	
bond	00000001_4	C3 N3	Not unusual (enough hits	1978	1.475	1.468	0.023	0.305	0.007	1.336	1.699	1.468	0	
bond	00000001_4	C9 N3	Not unusual (enough hits	931	1.482	1.465	0.015	1.125	0.017	1.386	1.561	1.465	0	
bond	00000001_4	C2 N4	Not unusual (enough hits	1745	1.472	1.457	0.022	0.676	0.015	1.204	1.687	1.458	0	
bond	00000001_4	C3 C2	Not unusual (enough hits	252	1.541	1.521	0.02	1.021	0.02	1.452	1.629	1.52	0	
bond	00000001_4	C4 CL1	Not unusual (enough hits	743	1.727	1.738	0.019	0.612	0.011	1.561	1.806	1.74	0	
bond	00000001_4	C4 N6	Not unusual (enough hits	245	1.346	1.321	0.025	0.969	0.024	1.254	1.422	1.317	0.003	
bond	00000001_4	C8 C4	Not unusual (enough hits	479	1.414	1.373	0.022	1.88	0.041	1.267	1.455	1.373	0	
bond	00000001_4	C5 N6	Not unusual (enough hits	2818	1.344	1.34	0.022	0.171	0.004	1.05	1.584	1.337	0	
bond	00000001_4	C9 C6	Not unusual (enough hits	10549	1.541	1.51	0.019	1.66	0.031	1.278	1.842	1.51	0	
bond	00000001_4	C8 C7	Not unusual (enough hits	20000	1.412	1.383	0.019	1.579	0.029	0.882	1.685	1.383	0	
bond	00000001_4	C1 N2	Unusual (enough hits)	18	1.284	1.329	0.015	3.017	0.045	1.303	1.358	1.329	0.02	
bond	00000001_4	C1 N3	Unusual (enough hits)	27	1.434	1.352	0.022	3.732	0.082	1.327	1.394	1.344	0.04	
bond	00000001_4	C1 N4	Unusual (enough hits)	41	1.402	1.345	0.016	3.501	0.057	1.287	1.39	1.343	0.012	
bond	00000001_4	C5 C6	Unusual (enough hits)	560	1.425	1.381	0.017	2.589	0.044	1.279	1.497	1.382	0.007	
bond	00000001_4	C7 C6	Unusual (enough hits)	14050	1.428	1.384	0.022	2.006	0.044	0.618	1.8	1.386	0	
bond	00000001_5	C3 N3	Not unusual (enough hits	1978	1.468	1.468	0.023	0.009	0	1.336	1.699	1.468	0	
bond	00000001_5	C9 N3	Not unusual (enough hits	931	1.485	1.465	0.015	1.272	0.02	1.386	1.561	1.465	0	
bond	00000001_5	C2 N4	Not unusual (enough hits	1745	1.458	1.457	0.022	0.04	0.001	1.204	1.687	1.458	0	
bond	00000001_5	C3 C2	Not unusual (enough hits	252	1.539	1.521	0.02	0.951	0.019	1.452	1.629	1.52	0	
bond	00000001_5	C4 CL1	Not unusual (enough hits	743	1.752	1.738	0.019	0.737	0.014	1.561	1.806	1.74	0	
bond	00000001_5	C4 N6	Not unusual (enough hits	245	1.355	1.321	0.025	1.343	0.034	1.254	1.422	1.317	0.002	
bond	00000001_5	C8 C4	Not unusual (enough hits	479	1.414	1.373	0.022	1.896	0.042	1.267	1.455	1.373	0	
bond	00000001_5	C5 N6	Not unusual (enough hits	2818	1.347	1.34	0.022	0.31	0.007	1.05	1.584	1.337	0	
bond	00000001_5	C7 C6	Not unusual (enough hits	14050	1.427	1.384	0.022	1.958	0.043	0.618	1.8	1.386	0	
bond	00000001_5	C9 C6	Not unusual (enough hits	10549	1.535	1.51	0.019	1.371	0.025	1.278	1.842	1.51	0	
bond	00000001_5	C8 C7	Not unusual (enough hits	20000	1.416	1.383	0.019	1.773	0.033	0.882	1.685	1.383	0	
bond	00000001_5	C1 N2	Unusual (enough hits)	18	1.281	1.329	0.015	3.191	0.047	1.303	1.358	1.329	0.022	
bond	00000001_5	C1 N3	Unusual (enough hits)	27	1.423	1.352	0.022	3.271	0.072	1.327	1.394	1.344	0.03	
bond	00000001_5	C1 N4	Unusual (enough hits)	41	1.408	1.345	0.016	3.879	0.063	1.287	1.39	1.343	0.019	
bond	00000001_5	C5 C6	Unusual (enough hits)	560	1.427	1.381	0.017	2.748	0.046	1.279	1.497	1.382	0.007	
angle	00000001_1	C3 N3 C1	Not unusual (enough hits	23	108.49	109.675	2.799	0.423	1.185	104.343	112.076	111.094	1.146	
angle	00000001_1	C9 N3 C3	Not unusual (enough hits	109	123.488	120.505	2.722	1.096	2.983	110.736	125.952	121.036	0.169	
angle	00000001_1	N3 C1 N2	Not unusual (enough hits	16	123.635	125.746	3.213	0.657	2.112	120.039	133.881	124.868	0.095	
angle	00000001_1	N4 C1 N2	Not unusual (enough hits	5	125.548	122.569	2.404	1.239	2.979	120.265	126.041	122.711	0.493	
angle	00000001_1	N4 C1 N3	Not unusual (enough hits	19	110.817	109.894	0.771	1.197	0.923	107.953	111.238	110.048	0.021	
angle	00000001_1	C2 N4 C1	Not unusual (enough hits	53	109.573	110.972	2.593	0.54	1.399	105.927	114.592	111.774	0.024	
angle	00000001_1	C3 C2 N4	Not unusual (enough hits	191	105.254	102.619	1.341	1.965	2.635	94.971	107.419	102.75	0.037	
angle	00000001_1	C2 C3 N3	Not unusual (enough hits	85	105.865	102.951	1.651	1.765	2.914	99.561	108.169	102.882	0.046	
angle	00000001_1	CL1 C4 N6	Not unusual (enough hits	239	117.212	116.229	2.378	0.413	0.983	106.087	140.591	115.898	0.001	
angle	00000001_1	C8 C4 CL1	Not unusual (enough hits	437	121.849	119.088	2.36	1.17	2.761	96.671	128.568	119.178	0.017	
angle	00000001_1	C6 C5 N6	Not unusual (enough hits	225	122.227	123.744	1.746	0.869	1.517	117.703	127.597	124.357	0.039	
angle	00000001_1	C7 C6 C5	Not unusual (enough hits	495	117.068	117.075	1.499	0.004	0.007	105.829	123.29	116.994	0.001	
angle	00000001_1	C9 C6 C5	Not unusual (enough hits	155	117.98	121.018	1.641	1.852	3.038	113.768	126.783	120.987	0.032	

angle	00000001_1	C8 C7 C6	Not unusual (enough hits	11395	119.444	121.039	1.437	1.11	1.595	93.35	147.791	121.028	0	
angle	00000001_1	C7 C8 C4	Not unusual (enough hits	289	117.808	117.43	0.964	0.392	0.377	114.685	123.178	117.353	0	
angle	00000001_1	C9 N3 C1	Unusual (enough hits)	15	128.017	124.917	0.706	4.391	3.1	123.364	126.201	124.859	1.816	
angle	00000001_1	C8 C4 N6	Unusual (enough hits)	167	120.939	124.711	1.675	2.251	3.772	117.068	127.876	125.155	0.116	
angle	00000001_1	C5 N6 C4	Unusual (enough hits)	179	122.514	116.435	1.303	4.666	6.079	112.785	121.37	116.186	1.144	
angle	00000001_1	C9 C6 C7	Unusual (enough hits)	10997	124.95	120.774	1.905	2.192	4.176	90.622	143.824	120.777	0.005	
angle	00000001_1	C6 C9 N3	Unusual (enough hits)	764	122.602	113.088	1.717	5.542	9.514	104.07	122.755	113.045	0.153	
angle	00000001_2	C3 N3 C1	Not unusual (enough hits	23	108.751	109.675	2.799	0.33	0.925	104.343	112.076	111.094	1.407	
angle	00000001_2	C9 N3 C3	Not unusual (enough hits	109	123.35	120.505	2.722	1.046	2.846	110.736	125.952	121.036	0.032	
angle	00000001_2	N3 C1 N2	Not unusual (enough hits	16	124.014	125.746	3.213	0.539	1.732	120.039	133.881	124.868	0.033	
angle	00000001_2	N4 C1 N2	Not unusual (enough hits	5	125.351	122.569	2.404	1.158	2.782	120.265	126.041	122.711	0.69	
angle	00000001_2	N4 C1 N3	Not unusual (enough hits	19	110.634	109.894	0.771	0.96	0.74	107.953	111.238	110.048	0.071	
angle	00000001_2	C2 N4 C1	Not unusual (enough hits	53	109.65	110.972	2.593	0.51	1.321	105.927	114.592	111.774	0.047	
angle	00000001_2	C3 C2 N4	Not unusual (enough hits	191	105.177	102.619	1.341	1.907	2.558	94.971	107.419	102.75	0.04	
angle	00000001_2	C2 C3 N3	Not unusual (enough hits	85	105.788	102.951	1.651	1.718	2.836	99.561	108.169	102.882	0.032	
angle	00000001_2	CL1 C4 N6	Not unusual (enough hits	239	117.447	116.229	2.378	0.512	1.218	106.087	140.591	115.898	0.033	
angle	00000001_2	C8 C4 CL1	Not unusual (enough hits	437	121.728	119.088	2.36	1.119	2.64	96.671	128.568	119.178	0.002	
angle	00000001_2	C6 C5 N6	Not unusual (enough hits	225	122.116	123.744	1.746	0.933	1.628	117.703	127.597	124.357	0.052	
angle	00000001_2	C7 C6 C5	Not unusual (enough hits	495	117.336	117.075	1.499	0.174	0.261	105.829	123.29	116.994	0	
angle	00000001_2	C9 C6 C5	Not unusual (enough hits	155	117.779	121.018	1.641	1.974	3.239	113.768	126.783	120.987	0.086	
angle	00000001_2	C8 C7 C6	Not unusual (enough hits	11395	119.245	121.039	1.437	1.249	1.794	93.35	147.791	121.028	0.001	
angle	00000001_2	C7 C8 C4	Not unusual (enough hits	289	117.629	117.43	0.964	0.207	0.199	114.685	123.178	117.353	0.001	
angle	00000001_2	C9 N3 C1	Unusual (enough hits)	15	127.896	124.917	0.706	4.22	2.979	123.364	126.201	124.859	1.695	
angle	00000001_2	C8 C4 N6	Unusual (enough hits)	167	120.824	124.711	1.675	2.32	3.887	117.068	127.876	125.155	0.001	
angle	00000001_2	C5 N6 C4	Unusual (enough hits)	179	122.85	116.435	1.303	4.924	6.415	112.785	121.37	116.186	1.48	
angle	00000001_2	C9 C6 C7	Unusual (enough hits)	10997	124.884	120.774	1.905	2.158	4.11	90.622	143.824	120.777	0.002	
angle	00000001_2	C6 C9 N3	Unusual (enough hits)	764	122.038	113.088	1.717	5.214	8.951	104.07	122.755	113.045	0.716	
angle	00000001_3	C3 N3 C1	Not unusual (enough hits	23	108.683	109.675	2.799	0.355	0.993	104.343	112.076	111.094	1.339	
angle	00000001_3	C9 N3 C3	Not unusual (enough hits	109	123.416	120.505	2.722	1.07	2.911	110.736	125.952	121.036	0.098	
angle	00000001_3	N3 C1 N2	Not unusual (enough hits	16	123.975	125.746	3.213	0.551	1.771	120.039	133.881	124.868	0.017	
angle	00000001_3	N4 C1 N2	Not unusual (enough hits	5	125.574	122.569	2.404	1.25	3.005	120.265	126.041	122.711	0.467	
angle	00000001_3	N4 C1 N3	Not unusual (enough hits	19	110.451	109.894	0.771	0.722	0.557	107.953	111.238	110.048	0.037	
angle	00000001_3	C2 N4 C1	Not unusual (enough hits	53	109.935	110.972	2.593	0.4	1.037	105.927	114.592	111.774	0.146	
angle	00000001_3	C3 C2 N4	Not unusual (enough hits	191	105.164	102.619	1.341	1.897	2.544	94.971	107.419	102.75	0.054	
angle	00000001_3	C2 C3 N3	Not unusual (enough hits	85	105.768	102.951	1.651	1.706	2.816	99.561	108.169	102.882	0.052	
angle	00000001_3	CL1 C4 N6	Not unusual (enough hits	239	117.956	116.229	2.378	0.726	1.727	106.087	140.591	115.898	0.066	
angle	00000001_3	C8 C4 CL1	Not unusual (enough hits	437	120.802	119.088	2.36	0.726	1.713	96.671	128.568	119.178	0.008	
angle	00000001_3	C6 C5 N6	Not unusual (enough hits	225	121.845	123.744	1.746	1.088	1.899	117.703	127.597	124.357	0.024	
angle	00000001_3	C7 C6 C5	Not unusual (enough hits	495	117.333	117.075	1.499	0.172	0.258	105.829	123.29	116.994	0.001	
angle	00000001_3	C9 C6 C5	Not unusual (enough hits	155	118.809	121.018	1.641	1.347	2.209	113.768	126.783	120.987	0.027	
angle	00000001_3	C9 C6 C7	Not unusual (enough hits	10997	123.855	120.774	1.905	1.617	3.081	90.622	143.824	120.777	0	
angle	00000001_3	C8 C7 C6	Not unusual (enough hits	11395	119.413	121.039	1.437	1.132	1.627	93.35	147.791	121.028	0	
angle	00000001_3	C7 C8 C4	Not unusual (enough hits	289	117.72	117.43	0.964	0.3	0.289	114.685	123.178	117.353	0.009	
angle	00000001_3	C9 N3 C1	Unusual (enough hits)	15	127.897	124.917	0.706	4.221	2.98	123.364	126.201	124.859	1.696	
angle	00000001_3	C8 C4 N6	Unusual (enough hits)	167	121.241	124.711	1.675	2.071	3.47	117.068	127.876	125.155	0.067	

angle	00000001_3	C5 N6 C4	Unusual (enough hits)	179	122.448	116.435	1.303	4.615	6.012	112.785	121.37	116.186	1.078	
angle	00000001_3	C6 C9 N3	Unusual (enough hits)	764	121.45	113.088	1.717	4.871	8.363	104.07	122.755	113.045	1.304	
angle	00000001_4	C3 N3 C1	Not unusual (enough hits	23	108.524	109.675	2.799	0.411	1.152	104.343	112.076	111.094	1.18	
angle	00000001_4	C9 N3 C3	Not unusual (enough hits	109	123.536	120.505	2.722	1.114	3.031	110.736	125.952	121.036	0.154	
angle	00000001_4	N3 C1 N2	Not unusual (enough hits	16	124.276	125.746	3.213	0.457	1.47	120.039	133.881	124.868	0.229	
angle	00000001_4	N4 C1 N2	Not unusual (enough hits	5	125.151	122.569	2.404	1.074	2.583	120.265	126.041	122.711	0.889	
angle	00000001_4	N4 C1 N3	Not unusual (enough hits	19	110.572	109.894	0.771	0.879	0.678	107.953	111.238	110.048	0.009	
angle	00000001_4	C2 N4 C1	Not unusual (enough hits	53	109.804	110.972	2.593	0.451	1.168	105.927	114.592	111.774	0.015	
angle	00000001_4	C2 C3 N3	Not unusual (enough hits	85	105.747	102.951	1.651	1.693	2.795	99.561	108.169	102.882	0.047	
angle	00000001_4	CL1 C4 N6	Not unusual (enough hits	239	119.486	116.229	2.378	1.37	3.257	106.087	140.591	115.898	0.087	
angle	00000001_4	C8 C4 CL1	Not unusual (enough hits	437	119.159	119.088	2.36	0.03	0.071	96.671	128.568	119.178	0.003	
angle	00000001_4	C6 C5 N6	Not unusual (enough hits	225	120.945	123.744	1.746	1.604	2.799	117.703	127.597	124.357	0.066	
angle	00000001_4	C7 C6 C5	Not unusual (enough hits	495	117.372	117.075	1.499	0.199	0.298	105.829	123.29	116.994	0.008	
angle	00000001_4	C9 C6 C5	Not unusual (enough hits	155	122.716	121.018	1.641	1.035	1.698	113.768	126.783	120.987	0.013	
angle	00000001_4	C9 C6 C7	Not unusual (enough hits	10997	119.911	120.774	1.905	0.453	0.863	90.622	143.824	120.777	0	
angle	00000001_4	C8 C7 C6	Not unusual (enough hits	11395	120.37	121.039	1.437	0.466	0.669	93.35	147.791	121.028	0	
angle	00000001_4	C7 C8 C4	Not unusual (enough hits	289	117.804	117.43	0.964	0.388	0.374	114.685	123.178	117.353	0.002	
angle	00000001_4	C9 N3 C1	Unusual (enough hits)	15	127.938	124.917	0.706	4.279	3.021	123.364	126.201	124.859	1.737	
angle	00000001_4	C3 C2 N4	Unusual (enough hits)	191	105.354	102.619	1.341	2.039	2.734	94.971	107.419	102.75	0.016	
angle	00000001_4	C8 C4 N6	Unusual (enough hits)	167	121.355	124.711	1.675	2.003	3.356	117.068	127.876	125.155	0.01	
angle	00000001_4	C5 N6 C4	Unusual (enough hits)	179	122.154	116.435	1.303	4.39	5.719	112.785	121.37	116.186	0.784	
angle	00000001_4	C6 C9 N3	Unusual (enough hits)	764	119.182	113.088	1.717	3.55	6.094	104.07	122.755	113.045	0.004	
angle	00000001_5	C3 N3 C1	Not unusual (enough hits	23	108.254	109.675	2.799	0.508	1.421	104.343	112.076	111.094	0.91	
angle	00000001_5	C9 N3 C3	Not unusual (enough hits	109	123.052	120.505	2.722	0.936	2.547	110.736	125.952	121.036	0.036	
angle	00000001_5	N3 C1 N2	Not unusual (enough hits	16	124.084	125.746	3.213	0.517	1.662	120.039	133.881	124.868	0.037	
angle	00000001_5	N4 C1 N2	Not unusual (enough hits	5	125.201	122.569	2.404	1.095	2.632	120.265	126.041	122.711	0.84	
angle	00000001_5	N4 C1 N3	Not unusual (enough hits	19	110.714	109.894	0.771	1.064	0.821	107.953	111.238	110.048	0.081	
angle	00000001_5	C2 N4 C1	Not unusual (enough hits	53	109.704	110.972	2.593	0.489	1.267	105.927	114.592	111.774	0.068	
angle	00000001_5	C3 C2 N4	Not unusual (enough hits	191	105.253	102.619	1.341	1.964	2.634	94.971	107.419	102.75	0.035	
angle	00000001_5	C2 C3 N3	Not unusual (enough hits	85	106.074	102.951	1.651	1.892	3.122	99.561	108.169	102.882	0.255	
angle	00000001_5	CL1 C4 N6	Not unusual (enough hits	239	119.79	116.229	2.378	1.498	3.561	106.087	140.591	115.898	0.184	
angle	00000001_5	C8 C4 CL1	Not unusual (enough hits	437	119.258	119.088	2.36	0.072	0.17	96.671	128.568	119.178	0.001	
angle	00000001_5	C6 C5 N6	Not unusual (enough hits	225	120.795	123.744	1.746	1.689	2.949	117.703	127.597	124.357	0.07	
angle	00000001_5	C7 C6 C5	Not unusual (enough hits	495	117.455	117.075	1.499	0.254	0.38	105.829	123.29	116.994	0.001	
angle	00000001_5	C9 C6 C5	Not unusual (enough hits	155	123.047	121.018	1.641	1.237	2.029	113.768	126.783	120.987	0.033	
angle	00000001_5	C9 C6 C7	Not unusual (enough hits	10997	119.497	120.774	1.905	0.671	1.277	90.622	143.824	120.777	0.001	
angle	00000001_5	C8 C7 C6	Not unusual (enough hits	11395	120.486	121.039	1.437	0.385	0.553	93.35	147.791	121.028	0	
angle	00000001_5	C7 C8 C4	Not unusual (enough hits	289	117.986	117.43	0.964	0.576	0.556	114.685	123.178	117.353	0.007	
angle	00000001_5	C9 N3 C1	Unusual (enough hits)	15	128.689	124.917	0.706	5.343	3.772	123.364	126.201	124.859	2.488	
angle	00000001_5	C8 C4 N6	Unusual (enough hits)	167	120.952	124.711	1.675	2.244	3.759	117.068	127.876	125.155	0.129	
angle	00000001_5	C5 N6 C4	Unusual (enough hits)	179	122.326	116.435	1.303	4.522	5.891	112.785	121.37	116.186	0.956	
angle	00000001_5	C6 C9 N3	Unusual (enough hits)	764	120.784	113.088	1.717	4.483	7.696	104.07	122.755	113.045	1.095	
torsion	00000001_1	C6 C9 N3 C1	Not unusual (enough hits	48	102.73								1.264	0.229
torsion	00000001_1	C6 C9 N3 C3	Not unusual (enough hits	182	−78.141								0.005	0.511
torsion	00000001_1	C5 C6 C9 N3	Not unusual (enough hits	349	165.409								0.17	0.089

torsion	00000001_1	C7 C6 C9 N3	Not unusual (enough hits	10853	−15.076								0.002	0.074
torsion	00000001_2	C6 C9 N3 C1	Not unusual (enough hits	48	107.075								0.075	0.208
torsion	00000001_2	C6 C9 N3 C3	Not unusual (enough hits	182	−73.623								0.032	0.665
torsion	00000001_2	C5 C6 C9 N3	Not unusual (enough hits	349	166.57								0.11	0.086
torsion	00000001_2	C7 C6 C9 N3	Not unusual (enough hits	10853	−13.773								0.002	0.072
torsion	00000001_3	C6 C9 N3 C1	Not unusual (enough hits	48	111.301								0.661	0.188
torsion	00000001_3	C6 C9 N3 C3	Not unusual (enough hits	182	−69.51								0.128	0.692
torsion	00000001_3	C5 C6 C9 N3	Not unusual (enough hits	349	159.533								1.446	0.08
torsion	00000001_3	C7 C6 C9 N3	Not unusual (enough hits	10853	−21.14								0.001	0.086
torsion	00000001_4	C6 C9 N3 C1	Not unusual (enough hits	48	−114.975								0.097	0.271
torsion	00000001_4	C6 C9 N3 C3	Not unusual (enough hits	182	65.555								0.024	0.588
torsion	00000001_4	C5 C6 C9 N3	Not unusual (enough hits	349	20.861								0.053	0.106
torsion	00000001_4	C7 C6 C9 N3	Not unusual (enough hits	10853	−159.262								0.021	0.095
torsion	00000001_5	C6 C9 N3 C1	Not unusual (enough hits	48	−102.043								1.951	0.229
torsion	00000001_5	C6 C9 N3 C3	Not unusual (enough hits	182	78.83								0.183	0.505
torsion	00000001_5	C5 C6 C9 N3	Not unusual (enough hits	349	11.305								0.013	0.086
torsion	00000001_5	C7 C6 C9 N3	Not unusual (enough hits	10853	−169.011								0.011	0.077
ring	00000001_1	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.706	16.329			0.771
ring	00000001_1	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.067	8.297			1
ring	00000001_2	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.703	16.289			0.771
ring	00000001_2	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.026	8.249			1
ring	00000001_3	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.615	16.318			0.771
ring	00000001_3	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.079	8.156			1
ring	00000001_4	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.661	16.321			0.771
ring	00000001_4	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.077	8.285			1
ring	00000001_5	N3 C1 N4 C2 C3	Not unusual (enough hits	35						0.639	16.299			0.771
ring	00000001_5	C4 N6 C5 C6 C7 C8	Not unusual (enough hits	320						0.009	8.378			1