Supporting Information

Hydrogen-bond dynamics, proton transfer, and water mobility in crystalline guanidinium carbonates for direct air capture

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Supplementary Note 1. Complementary Results

Table S1. Linear fit parameters obtained from the temperature dependence of the lattice parameters and unit-cell volume using the relation $y(T) = mT + k$ for the P1 and P3 phases from neutron and X-ray diffraction data. The slopes (m) describe the thermal expansion coefficients of the corresponding structural parameters, while the intercepts (k) represent the extrapolated values at T = 0 K. Uncertainties correspond to the standard errors from the linear regression fits.

Parameter	Method	P1 phase		P3 phase	
		m	*k*	*m*	*k*
a (Å)	Neutron	$(9.21\pm0.90)\times10^{-4}$	9.957±0.025	$(8.53\pm0.04)\times10^{-4}$	6.916±0.001
	X-ray	$(1.15\pm0.01)\times10^{-3}$	9.943±0.002	$(9.55\pm0.61)\times10^{-4}$	6.919±0.017
b (Å)	Neutron	$(1.14\pm0.20)\times10^{-4}$	10.05±0.01	$(4.66\pm0.87)\times10^{-5}$	8.670±0.020
	X-ray	$(3.26\pm0.12)\times10^{-4}$	10.040±0.03	$(1.97\pm0.53)\times10^{-4}$	8.676±0.015
c (Å)	Neutron	$(1.40\pm0.60)\times10^{-4}$	10.979±0.017	$(0.86\pm1.04)\times10^{-4}$	21.569±0.029
	X-ray	$(4.82\pm0.09)\times10^{-4}$	10.946±0.003	$(6.93\pm0.49)\times10^{-4}$	21.549±0.014
V (Å^3)	Neutron	$(1.430\pm0.069)\times10^{-1}$	1088.4±1.9	$(1.715\pm0.062)\times10^{-1}$	1285.5±1.8
	X-ray	$(2.246\pm0.016)\times10^{-1}$	1082.3±0.4	$(2.531\pm0.228)\times10^{-1}$	1285.1±6.4

Table S2. Comparison of experimental (neutron diffraction) and AIMD-simulated H··· Acceptor distances for the P1 phase. Atomic labels are defined in Figure 5a. Standard deviations indicate the extent of distance fluctuations during the simulation.

Type of Proton	Atom Label	Experimental (Neutron)		AIMD Simulations	
		T=300 K	T = 320 K	T= 320 K	T= 400 K
NH	O1···H6	1.643(4)	1.633(2)	1.667±0.144	1.662 ±0.181
NH_2	O2···H8B	1.649(3)	1.635(1)	1.642±0.123	1.659±0.147
NH_2	O1···H2A	1.893(5)	1.923(2)	1.897±0.158	1.926±0.191
NH_2	O1···H1B	2.002(5)	2.001(2)	2.013±0.196	2.049±0.239
H_w	N3···H3B	2.094(5)	2.114(2)	2.189±0.256	2.251±0.316
H_w	N4···H3A	1.936(5)	1.955(2)	1.897±0.162	1.935±0.205

Table S3. Comparison of experimental (neutron diffraction) and AIMD-simulated H··· Acceptor distances for the P3 phase. Atomic labels are defined in Figure 5b. Standard deviations indicate the extent of distance fluctuations during the simulation.

Type of Proton	Atom Label	Experimental (Neutron)		AIMD Simulations	
		T=320 K	T = 343 K	T= 320 K	T= 400 K
NH	O1···H6	1.740(5)	1.741(5)	1.754±0.150	1.755±0.170
NH	O2···H3	1.901(5)	1.918(4)	1.923±0.169	1.938±0.197
NH_2	O3···H8B	1.669(5)	1.671(5)	1.687±0.112	1.694±0.129
NH_2	O3···H1B	1.748(6)	1.757(5)	1.748±0.141	1.763±0.170
NH_2	O2···H1A	1.740(6)	1.744(5)	1.750±0.145	1.765±0.170
NH_2	O1···H2D	1.905(6)	1.907(6)	1.946±0.186	1.961±0.215
H_w	O3···H2	1.776(6)	1.782(5)	1.774±0.153	1.808±0.189
H_w	O2···H1	1.791(6)	1.802(6)	1.797±0.155	1.835±0.188
H_w	O1···H7	1.943(9)	1.957(7)	2.000±0.264	2.037±0.321

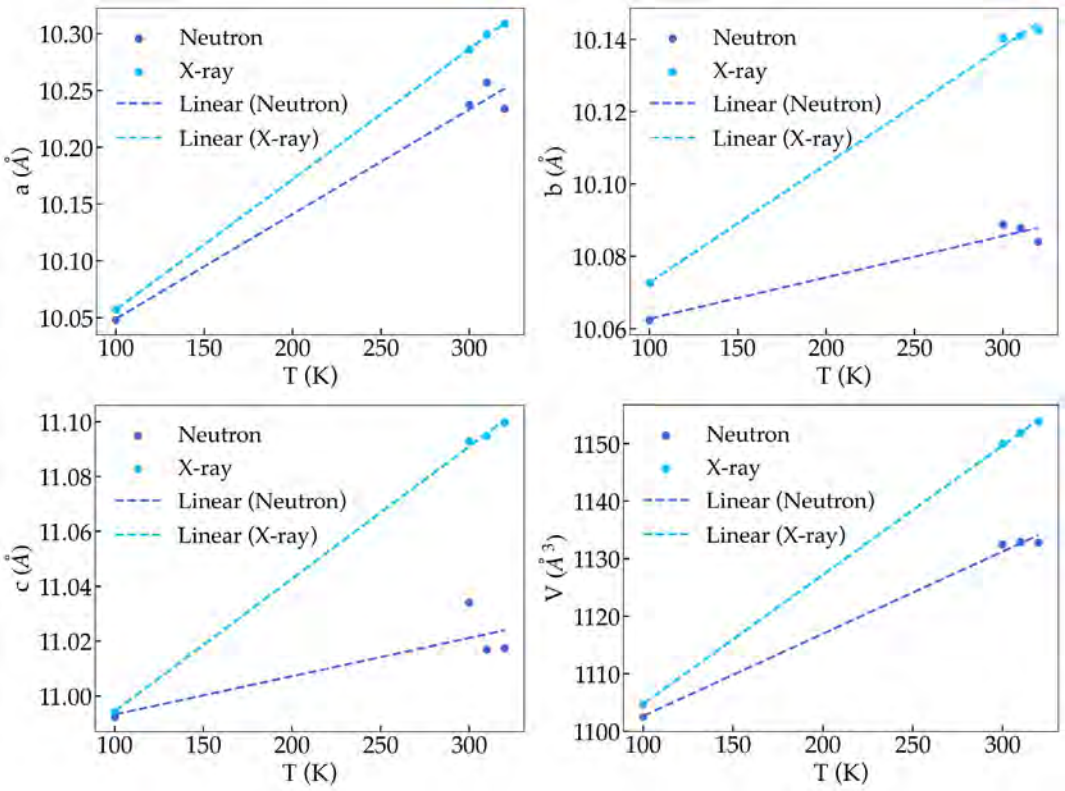


Figure S1. Temperature dependence of the P1 unit-cell parameters from variable-temperature neutron and X-ray diffraction.

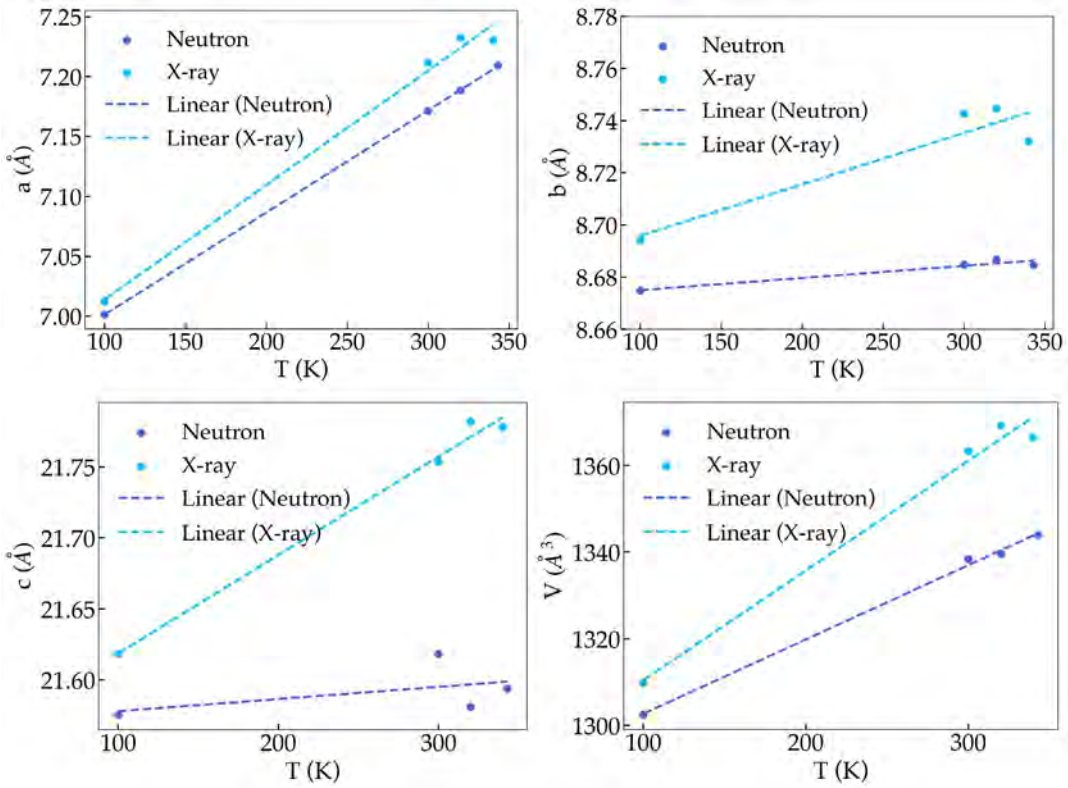


Figure S2. Temperature dependence of the P3 unit-cell parameters from variable-temperature neutron and X-ray diffraction.

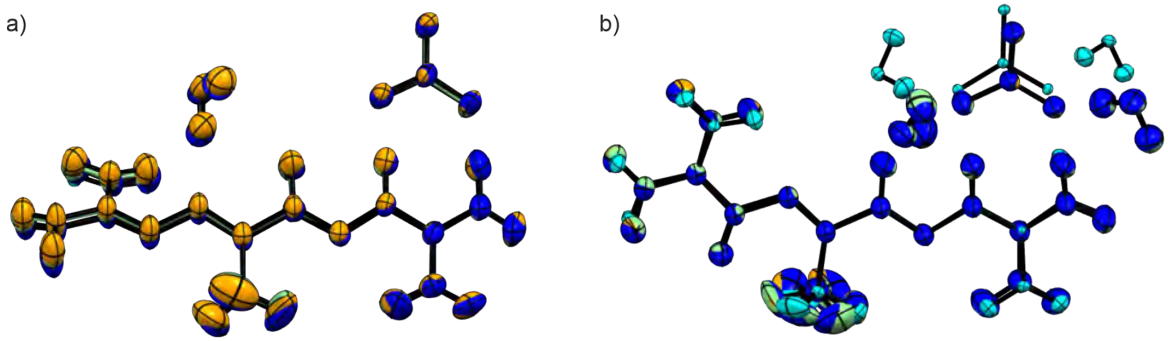


Figure S3. Overlaid neutron crystal structures of a) P1 phase and b) P3 phase from the variable-temperature study. The coloring scheme for P1 phase is cyan for 100 K, orange for 300 K, green for 310 K, and blue for 320 K. The coloring scheme for the P3 phase is cyan for 100 K, orange for 300 K, green for 320 K, and blue for 343 K.

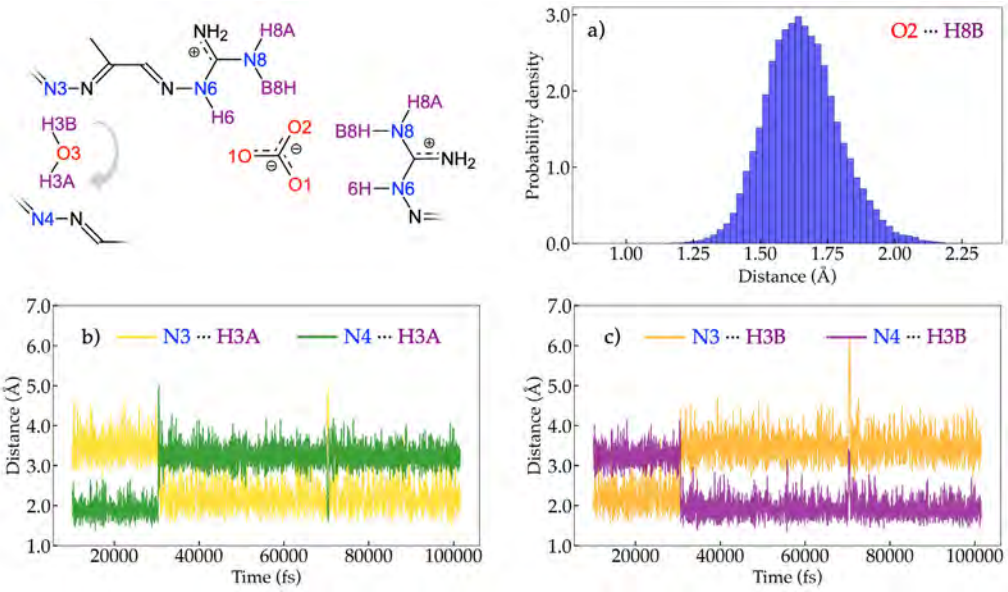


Figure S4. Complementary AIMD analysis of proton dynamics in the P1 phase. (a) Probability distribution of the O2···H8B hydrogen-bond distance in the bulk P1 structure at 400 K, indicating no proton transfer to the carbonate oxygen. (b) Time evolution of the N3···H3A and N4···H3A distances at 400 K, and of the (c) N3···H3B and N4···H3B distances at 400 K, showing hydrogen-bond switching caused by in-place rotation of the lattice-water molecule

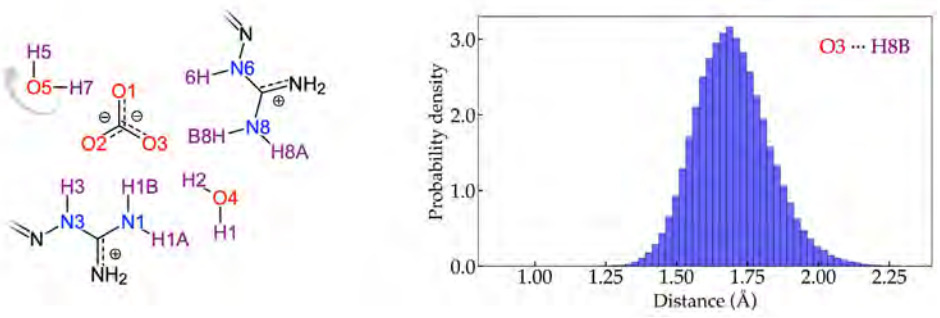


Figure S5. Complementary AIMD analysis of proton dynamics in the P3 phase. The right plot shows the probability distribution of the O3···H8B distances in the bulk P3 phase at 400 K, exhibiting no proton transfer.

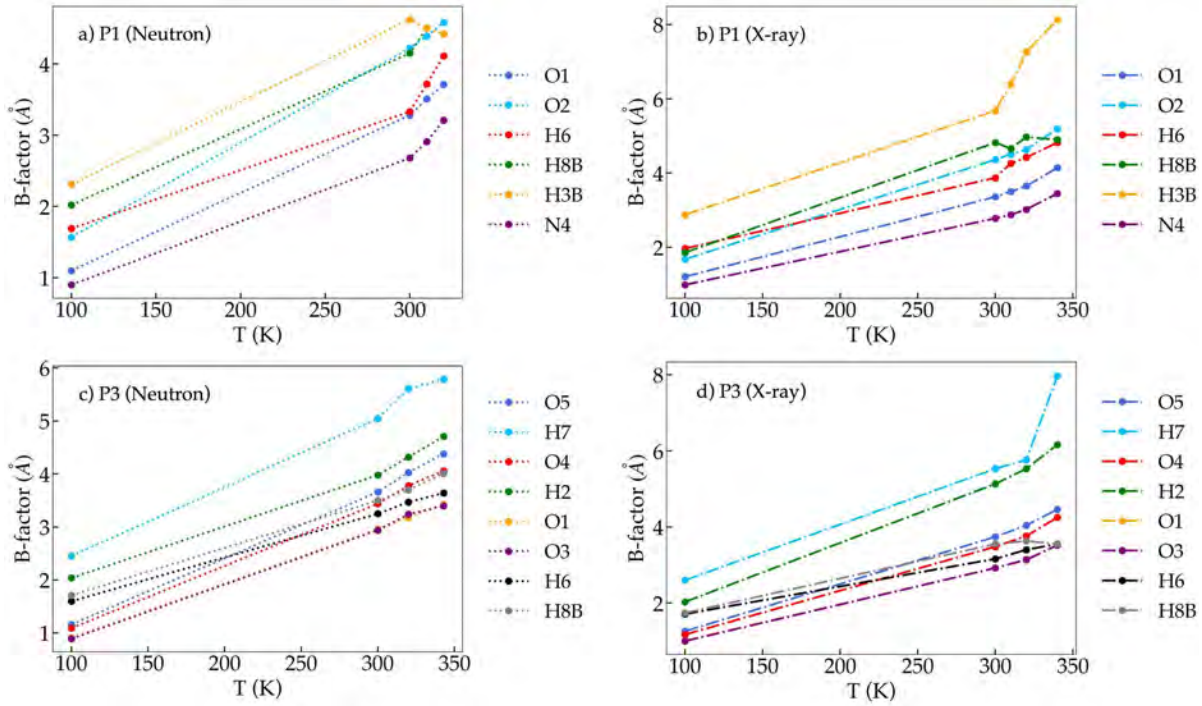


Figure S6. Temperature vs. specific Debye–Waller B-factor for P1 obtained from (a) neutron and (b) X-ray results, as well as for P3 obtained from (c) neutron and (d) X-ray results.

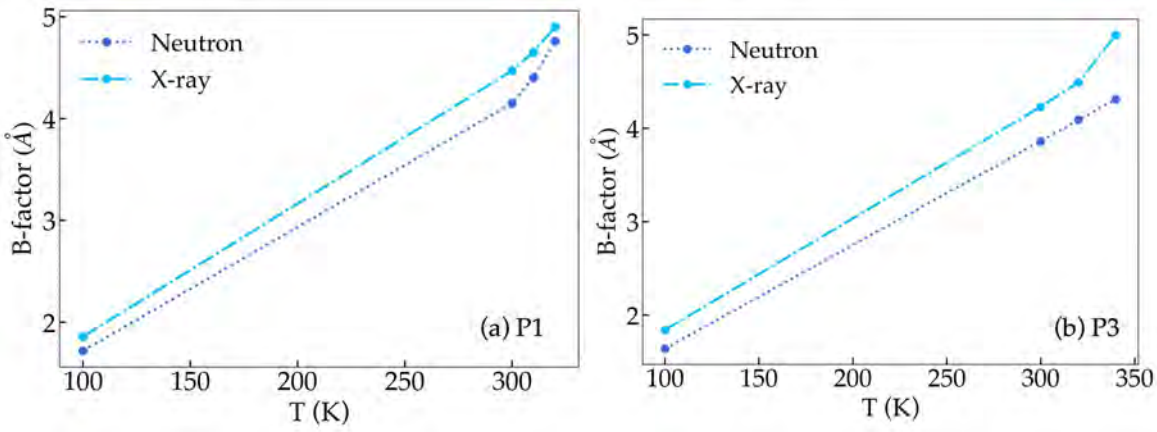


Figure S7. Temperature vs. Debye–Waller B-factor obtained from neutron and SCXRD studies for (a) P1 and (b) P3 systems.

1.1. Complementary AIMD surface analysis

1.1.1. Correlation analysis of equivalent proton transfer events at the P1 surface (100)

The correlation between equivalent proton transfer events was quantified using the Pearson correlation coefficient, defined as $\rho = \mathrm{cov}(A,B)/(\sigma_A\,\sigma_B)$, where A and B correspond to the time-dependent proton transfer coordinates associated with the two equivalent proton environments. For each trajectory frame, the proton transfer coordinates A and B were defined as the difference between the donor(N6)–H bond and the acceptor(O1)–H bond, such that positive and negative values indicate localization of the proton toward the acceptor and donor groups, respectively. The resulting time series were used to compute the covariance of A and B and their standard deviations, yielding a Pearson correlation coefficient of −0.841. The negative value of ρ therefore indicates anticorrelated proton transfer dynamics between the equivalent sites. Figure 3(c) shows the corresponding time series for the proton transfer coordinates A and B.

1.1.2. Correlation analysis of proton transfer events at the P3 surface (001)

The correlation between proton transfer events and local water coordination at the P3 solid–vacuum interface was also quantified using the Pearson correlation coefficient. The proton transfer coordinates, A and B, were defined as the difference between the donor(N6)–H6 and acceptor(O1)–H6 bonds and between the donor(N3)–H3 and acceptor(O2)–H3 bonds, respectively, such that positive and negative values indicate proton localization toward the acceptor and donor groups. The correlation between the two simultaneous proton transfer to carbonate, namely H3 and H6, yielded a Pearson correlation coefficient of −0.223. Although smaller than for the P1 phase, this reduction primarily reflects the much lower frequency of proton transfer events in P3, causing the trajectory to be dominated by uncorrelated thermal fluctuations that shift the Pearson correlation coefficient toward zero. The negative coefficient nevertheless indicates that H6 and H3 proton transfer events remain anticorrelated.

To assess the relationship between proton transfer and carbonate dehydration, the O1···H_w and O3···H_w distances, denoted as C and D, respectively, were monitored throughout the trajectory. The O···H_w distance was defined as the distance between each carbonate oxygen atom and the closest proton of a water molecule in each trajectory frame, since water molecules can exchange coordination sites throughout the trajectory at the surface. Correlation analysis further showed that H6 proton transfer is positively correlated with increasing O1···H_w and O3···H_w distances (average Pearson correlation coefficient of +0.381), whereas H3 proton transfer exhibits essentially no correlation with carbonate dehydration (average Pearson correlation coefficient of -0.002). The near-zero Pearson correlation coefficient for H3 primarily

reflects the very low frequency of H3 proton transfer events, such that the correlation is dominated by the much larger number of uncorrelated thermal fluctuations, effectively diluting any statistically resolvable relationship with carbonate dehydration. Nevertheless, the overall correlation analysis clearly shows that proton transfer at the P3 surface is associated primarily with H6 transfer, which is positively correlated with increasing O1···H_w and O3···H_w distances and therefore with the loss of directly coordinating water molecules at the carbonate site.

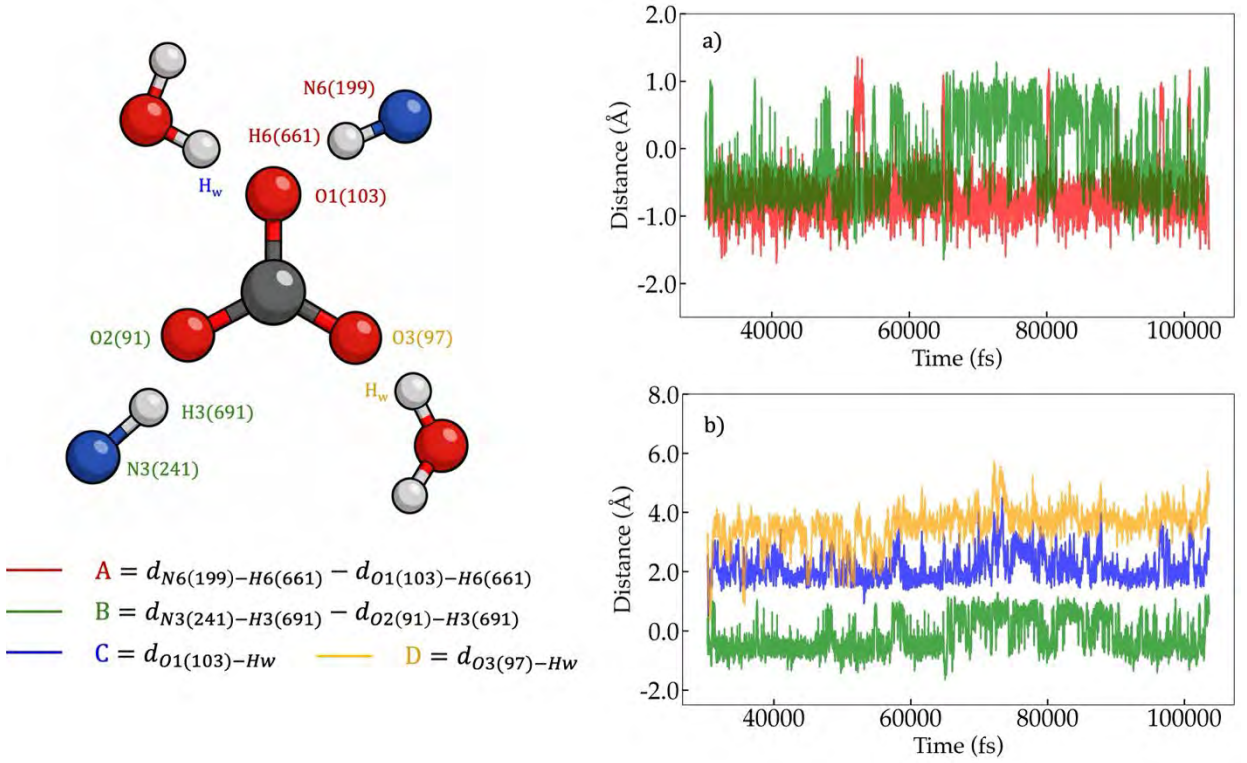


Figure S8. Time-dependent correlation analysis of proton transfer and carbonate dehydration at the P3 solid–vacuum interface at 453 K. (a) Time-dependent proton transfer coordinates A for H6 transfer and B for H3 transfer, showing anticorrelation between the two proton transfer pathways (Pearson correlation coefficient = −0.223). (b) Correlation between the H6 proton transfer coordinate (A) and the O1···H_w (C) and O3···H_w (D) distances, with an average Pearson correlation coefficient of +0.381. (c) Correlation between the H3 proton transfer coordinate (B) and the O1···H_w (C) and O3···H_w (D) distances, with an average Pearson correlation coefficient of -0.002.

2. Supplementary Note 2. Crystallographic data

Crystallographic data for the P1 and P3 phases have been deposited with the Cambridge Crystallographic Data Centre (CCDC) under deposition numbers 2591699–2591714.

For P1, the neutron diffraction structures are deposited as CCDC 2591706 (100 K), 2591705 (300 K), 2591704 (310 K), and 2591703 (320 K). The corresponding single-crystal X-ray diffraction structures are deposited as CCDC 2591712 (100 K), 2591713 (300 K), 2591714 (310 K), and 2591707 (320 K).

For P3, the neutron diffraction structures are deposited as CCDC 2591702 (100 K), 2591701 (300 K), 2591700 (320 K), and 2591699 (343 K). The corresponding single-crystal X-ray diffraction structures are deposited as CCDC 2591708 (100 K), 2591709 (300 K), 2591710 (320 K), and 2591711 (340 K).

Table S4. Crystal data and structure refinement for MGBIG carbonate hydrate, P1 (100 K), single-crystal neutron diffraction.

Chemical formula	C5.50 H15 N8 O2.50
Chemical formula weight	233.25
Crystal system, space group	monoclinic, *P* 1 2/n 1
Temperature (K)	100.0
a (Å)	10.0572(2)
b (Å)	10.07258(17)
c (Å)	10.99430(19)
α, β, γ (°)	90, 97.3011(17), 90
V (Å^3)	1104.72(3)
Z	4
Calculated density (g cm^{-3})	1.402
μ (mm^{-1})	0.1604 + 0.1077λ
Crystal size (mm^3)	1.75 × 1.4 × 0.85
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.396–78.620
Reflections measured	17360
Independent reflections	4226
Observed reflections [I > 2σ(I)]	3757
R_{int}	0.0710
Data/restraints/parameters	4226 / 0 / 282
R [$F^2 > 2\sigma(F^2)$]	0.0409
R (all data)	0.0542
wR(F^2)	0.0738
Goodness-of-fit on F^2	1.297
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm Å^{-3})	0.796, −0.784

Table S5. Crystal data and structure refinement for MGBIG carbonate hydrate, P1 (300 K), single-crystal neutron diffraction.

Parameter	**Value**
Chemical formula	C5.50 H15 N8 O2.50
Chemical formula weight	233.25
Crystal system, space group	monoclinic, P 1 2/n 1
Temperature (K)	300
a (Å)	10.2874(5)
b (Å)	10.1395(4)
c (Å)	11.0940(5)
α, β, γ (°)	90, 96.326(4), 90
V (Å^3)	1150.16(9)
Z	4
Calculated density (g cm^{-3})	1.347
μ (mm^{-1})	0.1604 + 0.1077λ
Crystal size (mm^3)	1.75 × 1.4 × 0.85
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.439–76.187
Reflections measured	12270
Independent reflections	3568
R_{int}	0.1609
Data/restraints/parameters	3568 / 0 / 282
R [$F^2 > 2\sigma(F^2)$]	0.0669
R (all data)	0.0711
wR(F^2)	0.1452
Goodness-of-fit on F^2	1.164
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm Å^{-3})	1.03, −1.08

Table S6. Crystal data and structure refinement for MGBIG carbonate hydrate, P1 (310 K), single-crystal neutron diffraction.

Parameter	**Value**
Chemical formula	C5.50 H15 N8 O2.50
Chemical formula weight	233.25
Crystal system, space group	monoclinic, P 1 2/n 1
Temperature (K)	310
a (Å)	10.2992(5)
b (Å)	10.1411(4)
c (Å)	11.0948(5)
α, β, γ (°)	90, 96.2450(5), 90
V (Å^3)	1151.92(9)
Z	4
Calculated density (g cm^{-3})	1.345
μ (mm^{-1})	0.1604 + 0.1077λ
Crystal size (mm^3)	1.75 × 1.4 × 0.85
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.547–77.089
Reflections measured	6289
Independent reflections	6289
R_{int}	0.1066
Data/restraints/parameters	6289/3/310
R [$F^2 > 2\sigma(F^2)$]	0.0575
R (all data)	0.0575
wR(F^2)	0.1602
Goodness-of-fit on F^2	1.222
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm Å^{-3})	0.83, −0.76

Table S7. Crystal data and structure refinement for MGBIG carbonate hydrate, P1 (320 K), single-crystal neutron diffraction.

Parameter	**Value**
Chemical formula	C5.50 H15 N8 O2.50
Chemical formula weight	233.25
Crystal system, space group	monoclinic, P 1 2/n 1
Temperature (K)	320
a (Å)	10.3087(5)
b (Å)	10.1426(4)
c (Å)	11.0997(6)
α, β, γ (°)	90, 96.154(4), 90
V (Å^3)	1153.86(9)
Z	4
Calculated density (g cm^{-3})	1.343
μ (mm^{-1})	0.1604 + 0.1077λ
Crystal size (mm^3)	1.75 × 1.4 × 0.85
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.391–76.151
Reflections measured	1879
Independent reflections	1879
R_{int}	0.1335
Data/restraints/parameters	1879/0/283
R [$F^2 > 2\sigma(F^2)$]	0.0905
R (all data)	0.0924
wR(F^2)	0.2304
Goodness-of-fit on F^2	1.112
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm Å^{-3})	0.94, −0.87

Table S8. Crystal data and structure refinement for MGBIG carbonate hydrate, P3 (100 K), single-crystal neutron diffraction.

Parameter	**Value**
Chemical formula	C6 H18 N8 O5
Chemical formula weight	282.28
Crystal system, space group	monoclinic, *P* 1 2_1/c 1
Temperature (K)	100
a (Å)	7.01229(3)
b (Å)	8.69421(4)
c (Å)	21.61828(10)
α, β, γ (°)	90, 96.3788(5), 90
V ($Å^3$)	1309.828(10)
Z	4
Calculated density (g cm^{-3})	1.431
μ (mm^{-1})	0.1593 + 0.1091λ
Crystal size (mm^3)	1.84 × 1.04 × 0.65
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.467–78.529
Reflections measured	22281
Independent reflections	4939
R_{int}	0.1036
Data/restraints/parameters	4939 / 0 / 327
R [$F^2 > 2\sigma(F^2)$]	0.0384
R (all data)	0.0528
wR(F^2)	0.0719
Goodness-of-fit on F^2	1.175
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm $Å^{-3}$)	1.52, −1.81

Table S9. Crystal data and structure refinement for MGBIG carbonate hydrate, P3 (300 K), single-crystal neutron diffraction.

Parameter	**Value**
Chemical formula	C6 H18 N8 O5
Chemical formula weight	282.28
Crystal system, space group	monoclinic, *P* 1 2_1/c 1
Temperature (K)	300
a (Å)	7.2114(3)
b (Å)	8.7426(4)
c (Å)	21.7535(6)
α, β, γ (°)	90, 96.246(3), 90
V ($Å^3$)	1363.34(9)
Z	4
Calculated density (g cm^{-3})	1.375
μ (mm^{-1})	0.1588 + 0.1088λ
Crystal size (mm^3)	2.35 × 1.5 × 1.02
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.333–76.529
Reflections measured	9645
Independent reflections	9654
R_{int}	0.1178
Data/restraints/parameters	9654 / 0 / 346
R [$F^2 > 2\sigma(F^2)$]	0.0582
R (all data)	0.0582
wR(F^2)	0.1523
Goodness-of-fit on F^2	1.092
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm $Å^{-3}$)	0.72, −0.91

Table S10. Crystal data and structure refinement for MGBIG carbonate hydrate, P3 (320 K), single-crystal neutron diffraction.

Parameter	**Value**
Chemical formula	C6 H18.04 N8 O5.02
Chemical formula weight	282.65
Crystal system, space group	monoclinic, P 1 21/c 1
Temperature (K)	320
a (Å)	7.2323(5)
b (Å)	8.7447(7)
c (Å)	21.7818(12)
α, β, γ (°)	90
V (Å^3)	96.266(6)1369.3(2)
Z	4
Calculated density (g cm^{-3})	1.371
μ (mm^{-1})	0.1588 + 0.1088λ
Crystal size (mm^3)	2.35 × 1.5 × 1.02
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.364–76.182
Reflections measured	7170
Independent reflections	2308
R_{int}	0.1109
Data/restraints/parameters	2308 / 0 / 348
R [$F^2 > 2\sigma(F^2)$]	0.0456
R (all data)	0.0461
wR(F^2)	0.1127
Goodness-of-fit on F^2	1.171
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm Å^{-3})	0.66, −0.71

Table S11. Crystal data and structure refinement for MGBIG carbonate hydrate, P3 (343 K), single-crystal neutron diffraction.

Parameter	**Value**
Chemical formula	C6 H18 N8 O5
Chemical formula weight	282.28
Crystal system, space group	monoclinic, P 1 21/c 1
Temperature (K)	343
a (Å)	7.2601(5)
b (Å)	8.7691(5)
c (Å)	21.8645(10)
α, β, γ (°)	90, 96.411(5), 90
V (Å^3)	1383.30(14)
Z	4
Calculated density (g cm^{-3})	1.355
μ (mm^{-1})	0.1588 + 0.1088λ
Crystal size (mm^3)	2.35 × 1.5 × 1.02
Radiation type	neutrons
Wavelength (Å)	0.4 – 3.5
θ range for data collection (°)	7.435–76.233
Reflections measured	8555
Independent reflections	2353
R_{int}	0.1096
Data/restraints/parameters	2353 / 9 / 363
R [$F^2 > 2\sigma(F^2)$]	0.0426
R (all data)	0.0437
wR(F^2)	0.1012
Goodness-of-fit on F^2	1.176
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (fm Å^{-3})	0.62, −0.70

1.1. Temperature-dependent bond distances, angles, and hydrogen-bond geometries

The complete sets of bond distances and bond angles extracted from the neutron CIF files for all temperatures are summarized in Tables S12–S15. Tables S12 and S13 list distinct bond lengths for P1 and P3, respectively, while Tables S14 and S15 list the corresponding bond angles. These tables provide the numerical basis for the trends discussed in the main text, including the stability of the guanidinium and carbonate fragments and the modest temperature dependence of the intramolecular geometry.

To highlight the hydrogen bonding that governs proton migration and water behavior, we collect the H···O and H···N contacts and associated D–H···A angles (D = N or O, A = O or N) in separate tables for each polymorph. Table S13 lists the key N–H···O and O–H···N hydrogen bonds in P1 as a function of temperature, and Table S14 provides the analogous data for P3. These hydrogen-bond geometries are derived directly from the neutron structural models (CIFs) and correspond to the contacts used in the main text to interpret proton migration pathways and water dynamics.

Together, Tables S12–S17 provide a complete crystallographic description of the temperature-dependent local bonding environment, separating intramolecular geometry (S12–S15) from intermolecular hydrogen bonding (S16–S17).

Table S12. Selected bond lengths (Å) for P1 at all temperatures (neutron single-crystal data).

Bond	100 K	300 K	310 K	320 K
C3-C2	1.4965(11)	1.498(2)	1.497(5)	1.496(11)
C3-C4	1.4573(10)	1.4637(19)	1.467(4)	1.459(10)
N1-C1	1.3530(9)	1.3584(17)	1.355(4)	1.355(8)
N2-C1	1.3436(9)	1.3477(18)	1.349(4)	1.352(7)
N3-C1	1.3365(9)	1.3379(18)	1.330(4)	1.338(9)
N3-N4	1.3861(7)	1.3906(15)	1.393(3)	1.379(7)
N4-C3	1.3004(9)	1.3030(18)	1.298(4)	1.307(8)
N5-C4	1.2868(9)	1.2879(17)	1.282(4)	1.284(8)
N6-C5	1.3487(9)	1.3476(17)	1.346(4)	1.356(8)
N6-N5	1.3657(7)	1.3718(14)	1.376(3)	1.364(7)
N7-C5	1.3283(10)	1.329(2)	1.328(4)	1.325(10)
N8-C5	1.3246(9)	1.3291(19)	1.329(4)	1.328(10)
O1-C6	1.2932(10)	1.293(2)	1.289(5)	1.292(10)
O2-C6	1.2766(16)	1.277(3)	1.271(8)	1.290(16)

Table S13. Selected bond angles (°) for P1 at all temperatures (neutron single-crystal data).

Angle	100 K	300 K	310 K	320 K
C1-N3-N4	111.54(5)	111.61(11)	111.8(2)	112.1(4)
C3-N4-N3	116.07(6)	116.27(11)	116.5(2)	116.8(5)
C4-C3-C2	120.77(6)	120.40(13)	120.1(3)	121.2(6)

C4-N5-N6	116.80(6)	117.07(11)	117.1(2)	117.4(5)
C5-N6-N5	115.83(6)	115.71(11)	115.6(2)	115.6(5)
N2-C1-N1	117.37(6)	117.20(13)	117.1(3)	117.2(6)
N3-C1-N1	117.82(6)	117.87(13)	118.1(3)	118.5(5)
N3-C1-N2	124.79(6)	124.92(12)	124.8(3)	124.3(6)
N4-C3-C2	124.51(7)	124.83(13)	125.0(3)	123.8(6)
N4-C3-C4	114.72(7)	114.76(13)	114.9(3)	115.0(6)
N5-C4-C3	119.52(7)	119.42(13)	119.7(3)	119.7(6)
N7-C5-N6	120.11(7)	120.24(14)	120.5(3)	120.4(7)
N7-C5-N8	121.39(6)	121.20(13)	121.0(3)	121.0(6)
N8-C5-N6	118.49(7)	118.56(13)	118.5(3)	118.5(7)
N8-C5-N7	121.39(6)	121.20(13)	121.0(3)	121.0(6)
O11-C6-O1	119.68(11)	119.3(2)	119.6(5)	119.2(10)
O1-C6-O11	119.68(11)	119.3(2)	119.6(5)	119.2(10)
O2-C6-O1	120.16(6)	120.34(11)	120.2(3)	120.4(5)
O2-C6-O11	120.16(5)	120.34(11)	120.2(3)	120.4(5)

Table S14. Selected bond lengths (Å) for P3 at all temperatures (neutron single-crystal data).

Bond	100 K	300 K	320 K	343 K
C1-N1	1.3175(9)	1.319(4)	1.318(2)	1.325(2)
C1-N2	1.3294(10)	1.333(4)	1.337(2)	1.342(2)
C1-N3	1.3593(9)	1.363(4)	1.364(3)	1.363(2)
C2-C3	1.4995(11)	1.503(4)	1.511(3)	1.509(3)
C3-C4	1.4573(11)	1.468(4)	1.462(3)	1.469(2)
C3-N4	1.2950(9)	1.303(4)	1.299(3)	1.304(2)
C4-N5	1.2868(9)	1.288(4)	1.286(3)	1.295(2)
C5-N6	1.3513(9)	1.357(3)	1.356(3)	1.358(2)
C5-N7	1.3323(9)	1.333(4)	1.335(3)	1.340(2)
C5-N8	1.3204(9)	1.328(3)	1.325(2)	1.329(2)
N3-N4	1.3645(8)	1.372(3)	1.373(2)	1.3790(18)
N5-N6	1.3685(8)	1.374(3)	1.3779(19)	1.3800(17)
O3-C6	1.2847(11)	1.288(4)	1.289(3)	1.293(3)
O2-C6	1.2895(12)	1.284(4)	1.290(3)	1.297(3)
O1-C6	1.2862(11)	1.287(4)	1.285(3)	1.289(3)

Table S15. Selected bond angles (°) for P3 at all temperatures (neutron single-crystal data).

Angle	100 K	300 K	320 K	343 K

C1-N3-N4	116.49(6)	116.5(2)	116.79(14)	116.57(13)
C3-N4-N3	118.98(6)	119.1(2)	119.51(15)	119.27(14)
C4-C3-C2	121.56(7)	121.2(3)	121.16(18)	121.19(17)
C4-N5-N6	113.98(6)	114.2(2)	114.47(15)	114.38(13)
C5-N6-N5	119.20(6)	118.9(2)	119.06(14)	118.96(13)
N1-C1-N2	120.86(7)	120.8(3)	120.73(18)	120.83(16)
N1-C1-N3	118.89(7)	119.0(3)	119.20(17)	118.91(16)
N2-C1-N3	120.25(7)	120.2(2)	120.07(17)	120.25(15)
N4-C3-C2	126.51(7)	127.0(2)	126.67(17)	126.94(16)
N4-C3-C4	111.93(7)	111.8(3)	112.17(17)	111.86(16)
N5-C4-C3	121.99(7)	121.9(3)	122.03(19)	121.88(17)
N7-C5-N6	120.88(7)	121.0(2)	120.92(16)	120.80(15)
N8-C5-N6	116.76(7)	116.7(2)	116.80(17)	116.92(15)
N8-C5-N7	122.34(7)	122.3(3)	122.26(18)	122.25(16)
O3-C6-O2	121.25(8)	119.1(3)	118.7(2)	121.2(2)
O3-C6-O1	120.09(8)	119.9(3)	120.0(2)	120.0(2)
O2-C6-O3	121.25(8)	119.1(3)	118.7(2)	121.2(2)
O2-C6-O1	118.66(8)	121.1(3)	121.3(2)	118.84(18)
O1-C6-O3	120.09(8)	119.9(3)	120.0(2)	120.0(2)
O1-C6-O2	118.66(8)	121.1(3)	121.3(2)	118.84(18)

Table S16. Neutron-derived hydrogen-bond geometry for the P1 phase of MGBIG carbonate at 100, 300, 310, and 320 K. D is the donor atom (N or O), A is the acceptor atom (O or N). Distances are given in A and angles in degrees. These data are extracted from the variable-temperature neutron CIF files and correspond to the contacts used in the main text to discuss proton migration along N6–H6···O1 and N8–H8B···O2, and the water-mediated O3–H3A/B···N4 hydrogen bond.

T (K)	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (deg)
100	N6–H6···O1	1.073(2)	1.637(2)	2.708(1)	175.9(2)
100	N8–H8B···O2	1.048(1)	1.626(1)	2.673(1)	175.5(1)
100	N2–H2A···O1	1.022(2)	1.862(2)	2.884(1)	178.2(2)
100	N1–H1B···O1	1.022(2)	1.959(2)	2.979(1)	175.0(2)
100	O3–H3B···N3	0.974(2)	2.032(2)	3.000(1)	172.2(2)
100	O3–H3A···N4	0.978(2)	1.899(2)	2.874(1)	173.9(2)
100	O3–H3B···N4	0.974(2)	2.683(2)	3.517(1)	143.9(2)
300	N6–H6···O1	1.081(4)	1.643(4)	2.722(2)	175.8(3)
300	N8–H8B···O2	1.044(3)	1.649(3)	2.690(2)	174.7(3)
300	N2–H2A···O1	1.029(4)	1.893(5)	2.922(3)	178.5(4)
300	N1–H1B···O1	1.016(4)	2.002(5)	3.015(3)	174.2(4)
300	O3–H3B···N3	0.986(6)	2.094(5)	3.073(3)	172.2(4)

300	O3–H3A···N4	0.976(5)	1.936(5)	2.909(3)	174.9(4)
300	O3–H3B···N4	0.986(6)	2.735(5)	3.583(3)	144.5(4)
310	N6–H6···O1	1.083(7)	1.637(8)	2.719(5)	176.2(6)
310	N8–H8B···O2	1.046(6)	1.654(6)	2.696(3)	174.2(6)
310	N1–H1B···O1	1.026(1)	2.002(1)	3.025(6)	174.4(8)
310	O3–H3B···N3	0.968(1)	2.837(1)	3.704(7)	149.5(8)
310	O3–H3A···N4	0.983(1)	2.743(1)	3.587(7)	144.3(9)
310	O3–H3B···N4	0.968(1)	1.941(1)	2.906(7)	174.8(9)
320	N6–H6···O1	1.096(2)	1.633(2)	2.727(1)	175.7(1)
320	N8–H8B···O2	1.060(1)	1.635(1)	2.691(7)	173.4(1)
320	N2–H2A···O1	1.014(2)	1.923(2)	2.937(1)	178.5(2)
320	N1–H1B···O1	1.003(2)	2.001(2)	3.002(1)	175.9(2)
320	O3–H3B···N3	0.957(3)	2.114(2)	3.059(2)	169.1(2)
320	O3–H3A···N4	0.987(2)	1.955(2)	2.939(2)	175.0(2)
320	O3–H3B···N4	0.957(3)	2.780(2)	3.584(2)	142.1(2)

Table S17. Neutron-derived hydrogen-bond geometry for the P3 phase of MGBIG carbonate at 100, 300, 320, and 343 K. D is the donor atom (N or O), A is the acceptor atom (O). Distances are given in A and angles in degrees. The N–H···O contacts connect guanidinium cations and carbonate anions, while the O–H···O contacts describe water–carbonate and water–water hydrogen bonds, including the O5–H7···O1 interaction whose geometry evolves with temperature in parallel with the H7 site occupancy.

T (K)	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (deg)
100	N6–H6···O1	1.052(2)	2.572(2)	3.338(1)	129.2(1)
100	N3–H3···O2	1.034(2)	1.890(2)	2.891(1)	161.9(2)
100	N8–H8B···O3	1.042(2)	2.980(2)	3.732(1)	129.7(1)
100	N1–H1B···O3	1.032(2)	3.509(2)	4.444(1)	151.6(1)
100	N1–H1A···O2	1.032(2)	1.721(2)	2.726(1)	163.5(2)
100	N2–H2D1···O1	1.028(2)	3.883(2)	4.833(1)	154.8(2)
100	O4–H2···O3	0.978(2)	3.625(2)	4.556(1)	160.1(1)
100	O4–H1···O2	0.982(2)	1.745(2)	2.724(1)	174.5(2)
100	O5–H7···O1	0.967(3)	3.597(3)	4.407(1)	143.0(2)
100	O5–H5···O4	0.968(2)	1.844(3)	2.748(2)	154.2(2)
300	N6–H6···O1	1.055(7)	1.746(7)	2.793(4)	171.4(6)
300	N3–H3···O2	1.045(7)	1.904(7)	2.916(4)	162.1(5)
300	N8–H8B···O3	1.044(7)	1.667(8)	2.708(4)	174.3(6)
300	N1–H1B···O3	1.037(7)	1.750(8)	2.782(4)	173.0(6)
300	N1–H1A···O2	1.027(7)	1.750(7)	2.748(4)	162.9(6)
300	N2–H2D1···O1	1.039(7)	1.890(8)	2.924(4)	173.1(6)
300	O4–H2···O3	0.980(7)	1.771(7)	2.746(5)	173.1(8)
300	O4–H1···O2	0.984(8)	1.786(8)	2.767(6)	173.8(7)
300	O5–H7···O1	0.957(1)	1.951(1)	2.884(6)	164.1(8)

300	O5–H5···O4	0.970(1)	1.887(1)	2.783(6)	152.5(8)
320	N6–H6···O1	1.063(5)	1.740(5)	2.795(3)	171.4(4)
320	N3–H3···O2	1.051(5)	1.901(5)	2.919(3)	162.0(4)
320	N8–H8B···O3	1.049(5)	1.669(5)	2.715(3)	174.4(4)
320	N1–H1B···O3	1.042(5)	1.748(6)	2.785(3)	172.8(5)
320	N1–H1A···O2	1.037(5)	1.740(6)	2.749(3)	163.5(5)
320	N2–H2D1···O1	1.020(5)	1.905(6)	2.922(3)	174.3(4)
320	O4–H2···O3	0.979(6)	1.776(6)	2.751(4)	173.1(6)
320	O4–H1···O2	0.983(7)	1.791(6)	2.771(4)	174.0(5)
320	O5–H7···O1	0.972(1)	1.943(9)	2.889(5)	163.7(6)
320	O5–H5···O4	0.955(7)	1.896(7)	2.779(5)	152.7(6)
343	N6–H6···O1	1.069(4)	1.741(5)	2.802(3)	171.1(4)
343	N3–H3···O2	1.041(4)	1.918(4)	2.927(2)	162.1(4)
343	N8–H8B···O3	1.051(4)	1.671(5)	2.719(3)	174.9(4)
343	N1–H1B···O3	1.046(5)	1.757(5)	2.797(3)	172.7(4)
343	N1–H1A···O2	1.040(5)	1.744(5)	2.757(3)	163.4(4)
343	N2–H2D1···O1	1.026(5)	1.907(6)	2.929(3)	173.4(4)
343	O4–H2···O3	0.978(5)	1.782(5)	2.756(4)	173.7(5)
343	O4–H1···O2	0.983(6)	1.802(6)	2.782(4)	174.5(5)
343	O5–H7···O1	0.963(9)	1.957(8)	2.898(4)	164.9(6)
343	O5–H5···O4	0.963(7)	1.915(6)	2.805(4)	152.4(5)

Supplementary Note 3. AIMD complementary results

3.1. Water mobility analysis

3.1.3. Water mobility at P1 surface (100)

Figure S9. Compilation of all 16 equivalent N3···H3B and N4···H3A distances at the (100) surface termination of P1 at 453 K, showing low water mobility at the surface.

3.1.4. Water mobility at P3 surface (001)

Figure S10. Compilation of all 16 equivalent O1···H5/H7 and O3···H1/H2 distances at the (001) surface termination of P3 at 453 K, showing high water mobility at the surface.

3.2. Individual hydrogen-bond distances in P1 and P3 AIMD simulations

3.2.1. P1 at 320 K - Bond distance analysis

Table S18. Individual time-averaged hydrogen-involving atomic distances for all equivalent proton environments in the P1 bulk AIMD trajectory at 320 K.

Bond type	Average distance (Å)	Standard dev. σ (Å)	Number of points
N3_143 - H3B_487	2.1848	0.2541	94257
N3_144 - H3B_488	2.1914	0.2509	94257
N3_145 - H3B_485	2.1891	0.2611	94257
N3_146 - H3B_486	2.1989	0.2627	94257
N3_19 - H3B_363	2.1901	0.2616	94257
N3_20 - H3B_364	2.1943	0.2533	94257
N3_21 - H3B_361	2.1753	0.2423	94257
N3_22 - H3B_362	2.1834	0.2586	94257
N3_267 - H3B_115	2.1942	0.2615	94257
N3_268 - H3B_116	2.1798	0.2444	94257
N3_269 - H3B_113	2.1875	0.2573	94257
N3_270 - H3B_114	2.1879	0.2489	94257
N3_391 - H3B_239	2.1922	0.2542	94257
N3_392 - H3B_240	2.1872	0.2615	94257
N3_393 - H3B_237	2.1887	0.2536	94257
N3_394 - H3B_238	2.1895	0.2557	94257
N3_515 - H3B_859	2.1868	0.2478	94257
N3_516 - H3B_860	2.1902	0.2544	94257
N3_517 - H3B_857	2.1931	0.2595	94257
N3_518 - H3B_858	2.1859	0.2480	94257
N3_639 - H3B_983	2.1860	0.2529	94257
N3_640 - H3B_984	2.1877	0.2579	94257
N3_641 - H3B_981	2.1911	0.2583	94257
N3_642 - H3B_982	2.1816	0.2444	94257
N3_763 - H3B_611	2.1861	0.2606	94257
N3_764 - H3B_612	2.1935	0.2504	94257
N3_765 - H3B_609	2.1831	0.2493	94257
N3_766 - H3B_610	2.1931	0.2662	94257
N3_887 - H3B_735	2.2014	0.2696	94257
N3_888 - H3B_736	2.1964	0.2666	94257
N3_889 - H3B_733	2.1899	0.2551	94257
N3_890 - H3B_734	2.1884	0.2510	94257
N4_147 - H3A_229	1.8997	0.1673	94257
N4_148 - H3A_230	1.9007	0.1671	94257
N4_149 - H3A_231	1.8908	0.1562	94257
N4_150 - H3A_232	1.8979	0.1608	94257
N4_23 - H3A_105	1.8979	0.1596	94257
N4_24 - H3A_106	1.8964	0.1620	94257
N4_25 - H3A_107	1.8959	0.1651	94257
N4_26 - H3A_108	1.8900	0.1559	94257
N4_271 - H3A_353	1.8951	0.1667	94257
N4_272 - H3A_354	1.9001	0.1651	94257
N4_273 - H3A_355	1.8915	0.1550	94257
N4_274 - H3A_356	1.9007	0.1647	94257
N4_395 - H3A_477	1.8920	0.1558	94257
N4_396 - H3A_478	1.8951	0.1593	94257
N4_397 - H3A_479	1.8983	0.1623	94257

N4_398 - H3A_480	1.9006	0.1693	94257
N4_519 - H3A_601	1.8933	0.1587	94257
N4_520 - H3A_602	1.8945	0.1616	94257
N4_521 - H3A_603	1.8944	0.1606	94257
N4_522 - H3A_604	1.8917	0.1563	94257
N4_643 - H3A_725	1.8978	0.1637	94257
N4_644 - H3A_726	1.8920	0.1550	94257
N4_645 - H3A_727	1.9035	0.1703	94257
N4_646 - H3A_728	1.8976	0.1634	94257
N4_767 - H3A_849	1.8980	0.1597	94257
N4_768 - H3A_850	1.8953	0.1651	94257
N4_769 - H3A_851	1.8979	0.1628	94257
N4_770 - H3A_852	1.8934	0.1584	94257
N4_891 - H3A_973	1.9020	0.1641	94257
N4_892 - H3A_974	1.8936	0.1559	94257
N4_893 - H3A_975	1.9062	0.1741	94257
N4_894 - H3A_976	1.8978	0.1662	94257
O1_1 - H1B_94	2.0140	0.1966	94257
O1_125 - H1B_218	2.0194	0.2041	94257
O1_126 - H1B_217	2.0116	0.1900	94257
O1_127 - H1B_220	2.0117	0.1957	94257
O1_128 - H1B_219	2.0110	0.1942	94257
O1_2 - H1B_93	2.0131	0.1957	94257
O1_249 - H1B_342	2.0153	0.1952	94257
O1_250 - H1B_341	2.0128	0.1980	94257
O1_251 - H1B_344	2.0026	0.1809	94257
O1_252 - H1B_343	2.0136	0.1993	94257
O1_3 - H1B_96	2.0114	0.1951	94257
O1_373 - H1B_466	2.0175	0.2069	94257
O1_374 - H1B_465	2.0100	0.1895	94257
O1_375 - H1B_468	2.0134	0.2017	94257
O1_376 - H1B_467	2.0128	0.1966	94257
O1_4 - H1B_95	2.0109	0.1942	94257
O1_497 - H1B_590	2.0149	0.1976	94257
O1_498 - H1B_589	2.0179	0.2014	94257
O1_499 - H1B_592	2.0186	0.2078	94257
O1_500 - H1B_591	2.0128	0.1900	94257
O1_621 - H1B_714	2.0207	0.2068	94257
O1_622 - H1B_713	2.0069	0.1854	94257
O1_623 - H1B_716	2.0052	0.1895	94257
O1_624 - H1B_715	2.0145	0.1980	94257
O1_745 - H1B_838	2.0110	0.1913	94257
O1_746 - H1B_837	2.0143	0.1976	94257
O1_747 - H1B_840	2.0089	0.1921	94257
O1_748 - H1B_839	2.0107	0.1920	94257
O1_869 - H1B_962	2.0094	0.1953	94257
O1_870 - H1B_961	2.0197	0.2070	94257
O1_871 - H1B_964	2.0095	0.1904	94257
O1_872 - H1B_963	2.0118	0.1915	94257
O1_1 - H2A_72	1.8973	0.1589	94257
O1_125 - H2A_196	1.8957	0.1565	94257
O1_126 - H2A_195	1.8998	0.1634	94257
O1_127 - H2A_194	1.9047	0.1680	94257

O1_128 - H2A_193	1.8962	0.1554	94257
O1_2 - H2A_71	1.8934	0.1583	94257
O1_249 - H2A_320	1.8949	0.1561	94257
O1_250 - H2A_319	1.8951	0.1558	94257
O1_251 - H2A_318	1.8993	0.1628	94257
O1_252 - H2A_317	1.8992	0.1630	94257
O1_3 - H2A_70	1.8969	0.1577	94257
O1_373 - H2A_444	1.8969	0.1558	94257
O1_374 - H2A_443	1.8983	0.1552	94257
O1_375 - H2A_442	1.8989	0.1575	94257
O1_376 - H2A_441	1.8970	0.1607	94257
O1_4 - H2A_69	1.8992	0.1623	94257
O1_497 - H2A_568	1.8986	0.1610	94257
O1_498 - H2A_567	1.9010	0.1611	94257
O1_499 - H2A_566	1.8966	0.1602	94257
O1_500 - H2A_565	1.8947	0.1554	94257
O1_621 - H2A_692	1.8961	0.1614	94257
O1_622 - H2A_691	1.8949	0.1528	94257
O1_623 - H2A_690	1.8976	0.1579	94257
O1_624 - H2A_689	1.8922	0.1547	94257
O1_745 - H2A_816	1.8953	0.1538	94257
O1_746 - H2A_815	1.8924	0.1514	94257
O1_747 - H2A_814	1.8977	0.1554	94257
O1_748 - H2A_813	1.8968	0.1589	94257
O1_869 - H2A_940	1.8920	0.1535	94257
O1_870 - H2A_939	1.8942	0.1546	94257
O1_871 - H2A_938	1.8920	0.1535	94257
O1_872 - H2A_937	1.8973	0.1561	94257
O1_1 - H6_103	1.6691	0.1373	94257
O1_125 - H6_227	1.6705	0.1403	94257
O1_126 - H6_228	1.6634	0.1453	94257
O1_127 - H6_225	1.6645	0.1409	94257
O1_128 - H6_226	1.6693	0.1414	94257
O1_2 - H6_104	1.6654	0.1458	94257
O1_249 - H6_351	1.6652	0.1430	94257
O1_250 - H6_352	1.6711	0.1388	94257
O1_251 - H6_349	1.6704	0.1463	94257
O1_252 - H6_350	1.6602	0.1452	94257
O1_3 - H6_101	1.6687	0.1346	94257
O1_373 - H6_475	1.6659	0.1499	94257
O1_374 - H6_476	1.6712	0.1386	94257
O1_375 - H6_473	1.6659	0.1435	94257
O1_376 - H6_474	1.6613	0.1486	94257
O1_4 - H6_102	1.6687	0.1428	94257
O1_497 - H6_599	1.6653	0.1543	94257
O1_498 - H6_600	1.6657	0.1490	94257
O1_499 - H6_597	1.6704	0.1456	94257
O1_500 - H6_598	1.6680	0.1432	94257
O1_621 - H6_723	1.6639	0.1525	94257
O1_622 - H6_724	1.6627	0.1370	94257
O1_623 - H6_721	1.6728	0.1455	94257
O1_624 - H6_722	1.6684	0.1413	94257
O1_745 - H6_847	1.6636	0.1492	94257

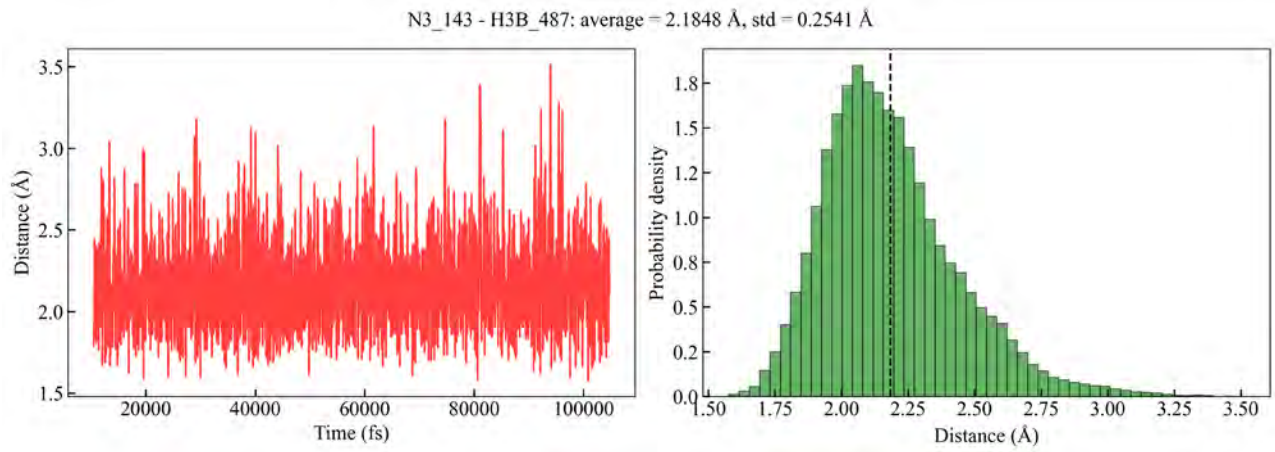
O1_746 - H6_848	1.6709	0.1445	94257
O1_747 - H6_845	1.6687	0.1420	94257
O1_748 - H6_846	1.6686	0.1444	94257
O1_869 - H6_971	1.6658	0.1422	94257
O1_870 - H6_972	1.6664	0.1453	94257
O1_871 - H6_969	1.6738	0.1428	94257
O1_872 - H6_970	1.6699	0.1440	94257
O2_10 - H8B_86	1.6419	0.1227	94257
O2_10 - H8B_88	1.6452	0.1221	94257
O2_133 - H8B_209	1.6402	0.1223	94257
O2_133 - H8B_211	1.6406	0.1243	94257
O2_134 - H8B_210	1.6424	0.1232	94257
O2_134 - H8B_212	1.6442	0.1237	94257
O2_257 - H8B_333	1.6446	0.1244	94257
O2_257 - H8B_335	1.6437	0.1238	94257
O2_258 - H8B_334	1.6440	0.1232	94257
O2_258 - H8B_336	1.6408	0.1233	94257
O2_381 - H8B_457	1.6422	0.1215	94257
O2_381 - H8B_459	1.6428	0.1274	94257
O2_382 - H8B_458	1.6448	0.1256	94257
O2_382 - H8B_460	1.6443	0.1271	94257
O2_505 - H8B_581	1.6412	0.1216	94257
O2_505 - H8B_583	1.6464	0.1273	94257
O2_506 - H8B_582	1.6437	0.1266	94257
O2_506 - H8B_584	1.6394	0.1200	94257
O2_629 - H8B_705	1.6411	0.1204	94257
O2_629 - H8B_707	1.6421	0.1202	94257
O2_630 - H8B_706	1.6433	0.1210	94257
O2_630 - H8B_708	1.6383	0.1174	94257
O2_753 - H8B_829	1.6410	0.1228	94257
O2_753 - H8B_831	1.6441	0.1268	94257
O2_754 - H8B_830	1.6404	0.1226	94257
O2_754 - H8B_832	1.6415	0.1209	94257
O2_877 - H8B_953	1.6443	0.1272	94257
O2_877 - H8B_955	1.6431	0.1234	94257
O2_878 - H8B_954	1.6402	0.1212	94257
O2_878 - H8B_956	1.6425	0.1238	94257
O2_9 - H8B_85	1.6397	0.1201	94257
O2_9 - H8B_87	1.6445	0.1253	94257

Bond Distance Plots

N3 - H3B

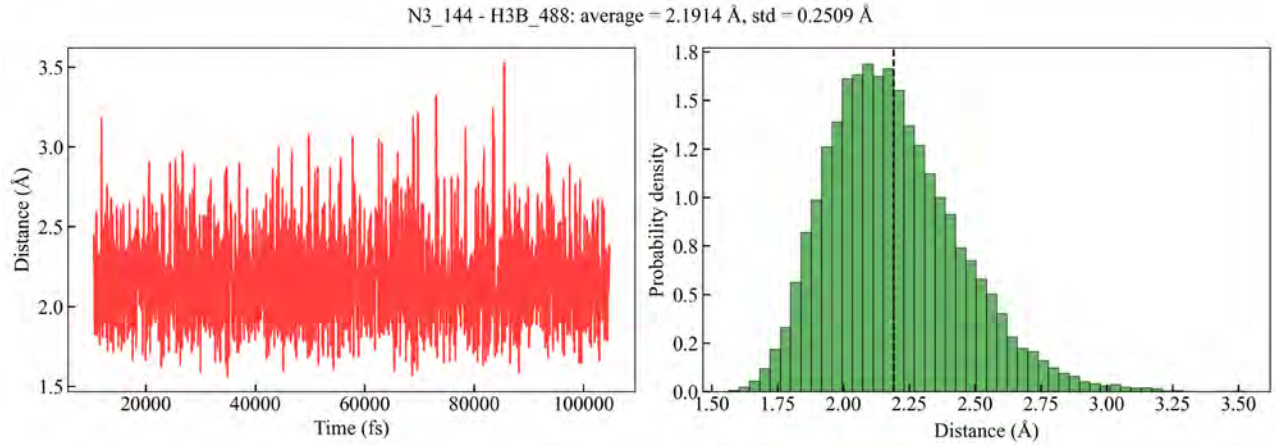
N3_143 - H3B_487

Average distance = 2.1848 Å; standard deviation = 0.2541 Å; number of points = 94257



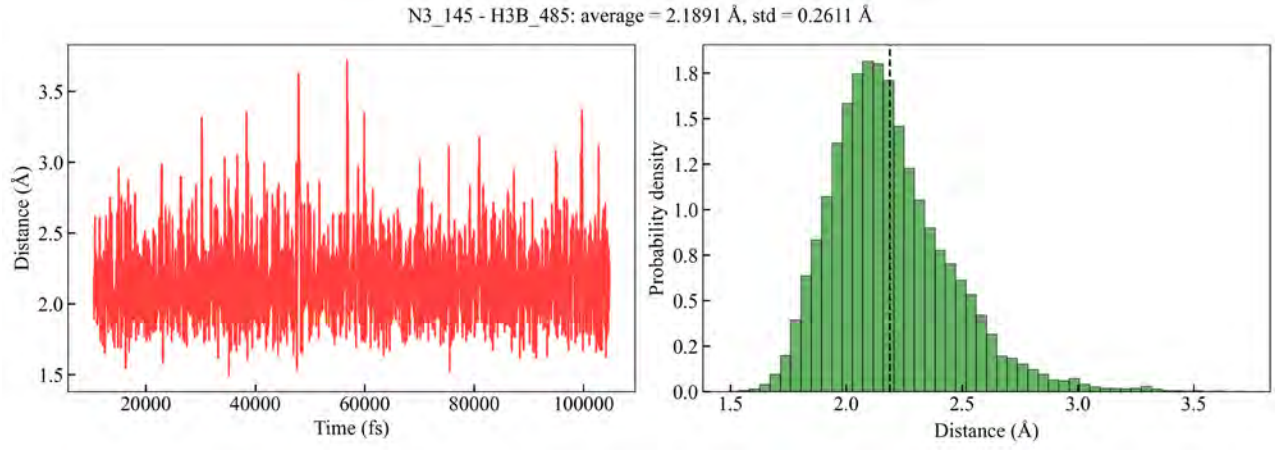
N3_144 - H3B_488

Average distance = 2.1914 Å; standard deviation = 0.2509 Å; number of points = 94257



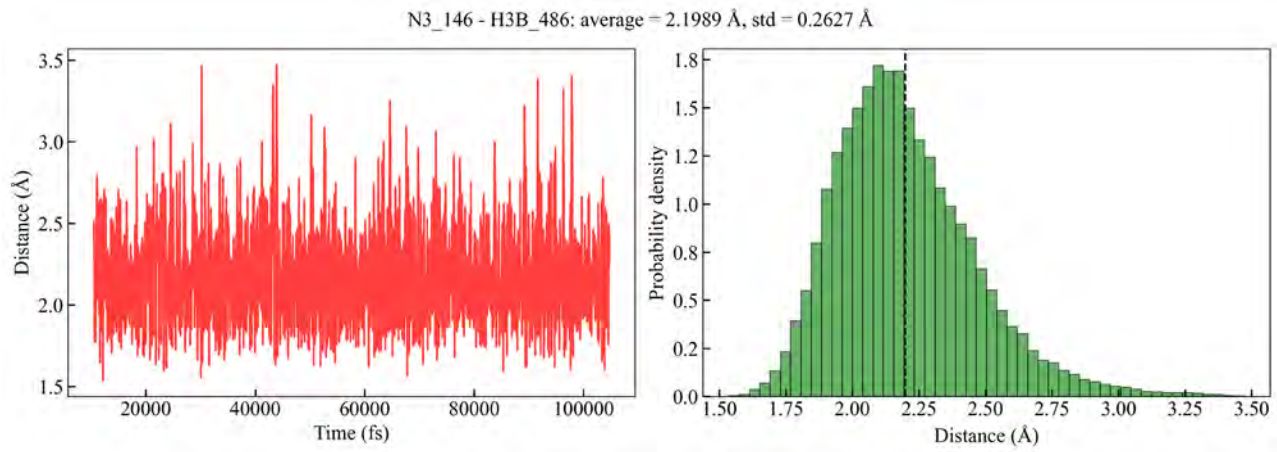
N3_145 - H3B_485

Average distance = 2.1891 Å; standard deviation = 0.2611 Å; number of points = 94257



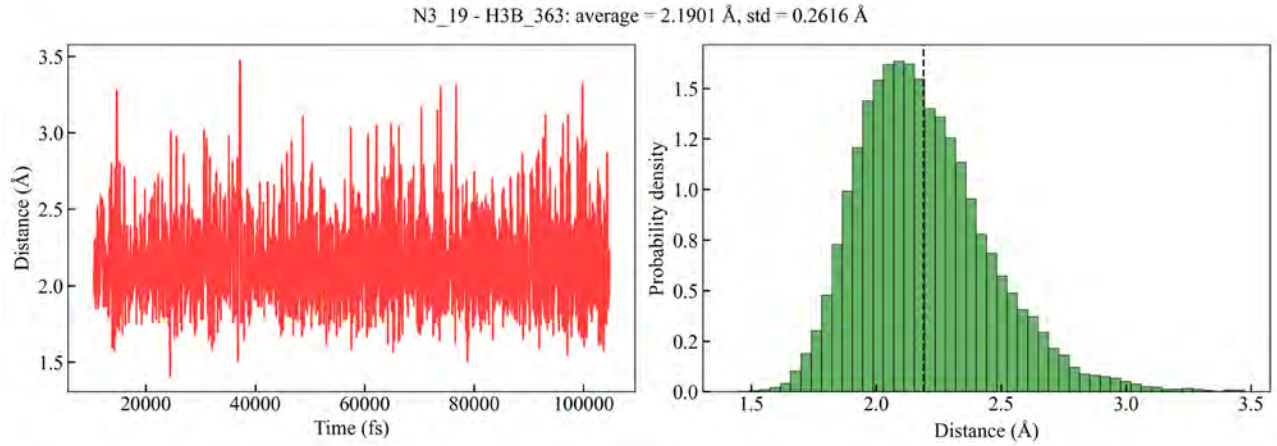
N3_146 - H3B_486

Average distance = 2.1989 Å; standard deviation = 0.2627 Å; number of points = 94257



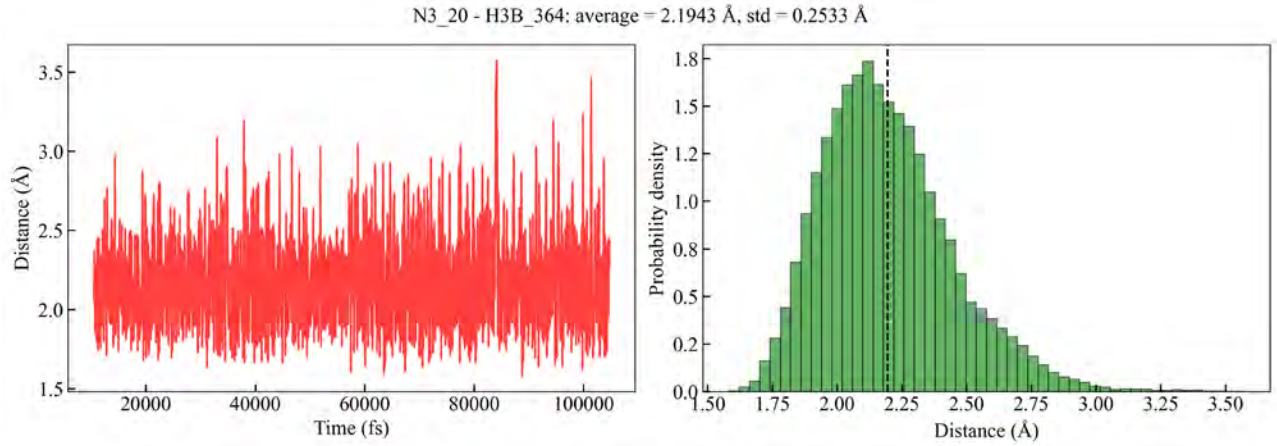
N3_19 - H3B_363

Average distance = 2.1901 Å; standard deviation = 0.2616 Å; number of points = 94257



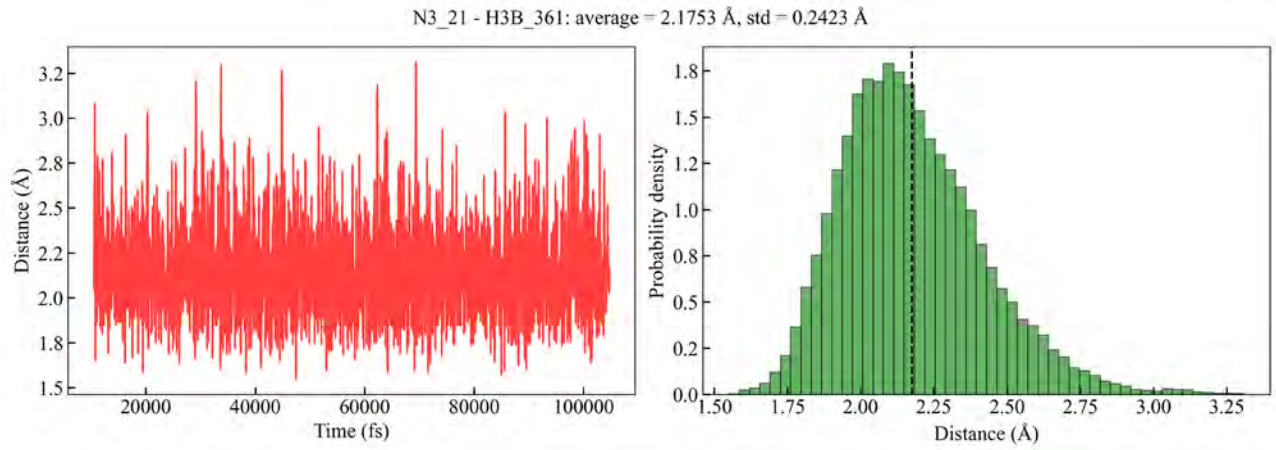
N3_20 - H3B_364

Average distance = 2.1943 Å; standard deviation = 0.2533 Å; number of points = 94257



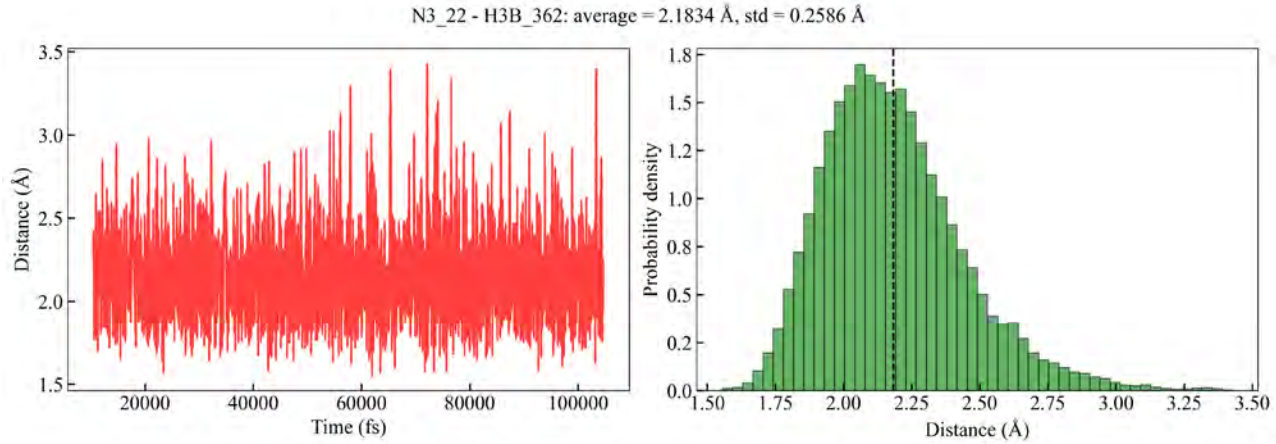
N3_21 - H3B_361

Average distance = 2.1753 Å; standard deviation = 0.2423 Å; number of points = 94257



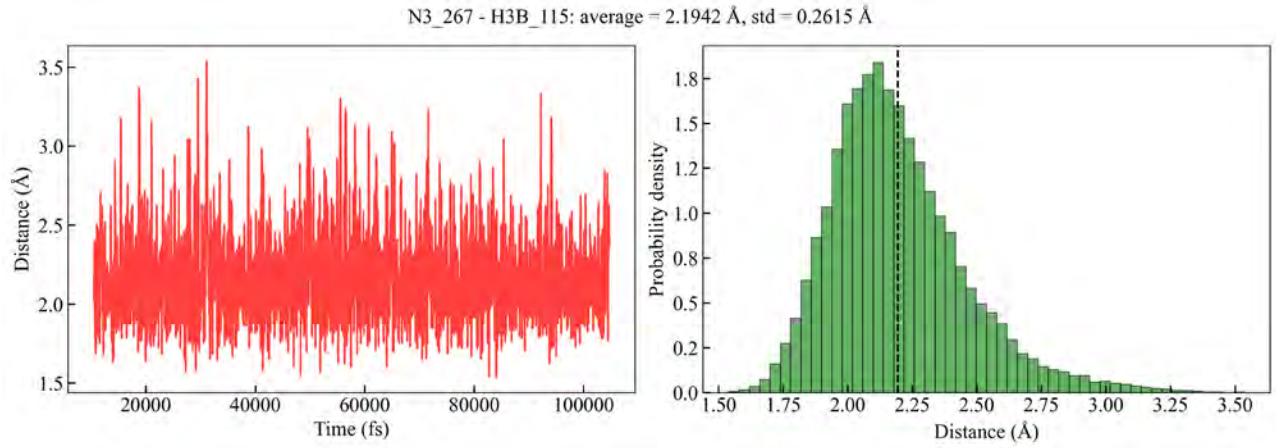
N3_22 - H3B_362

Average distance = 2.1834 Å; standard deviation = 0.2586 Å; number of points = 94257



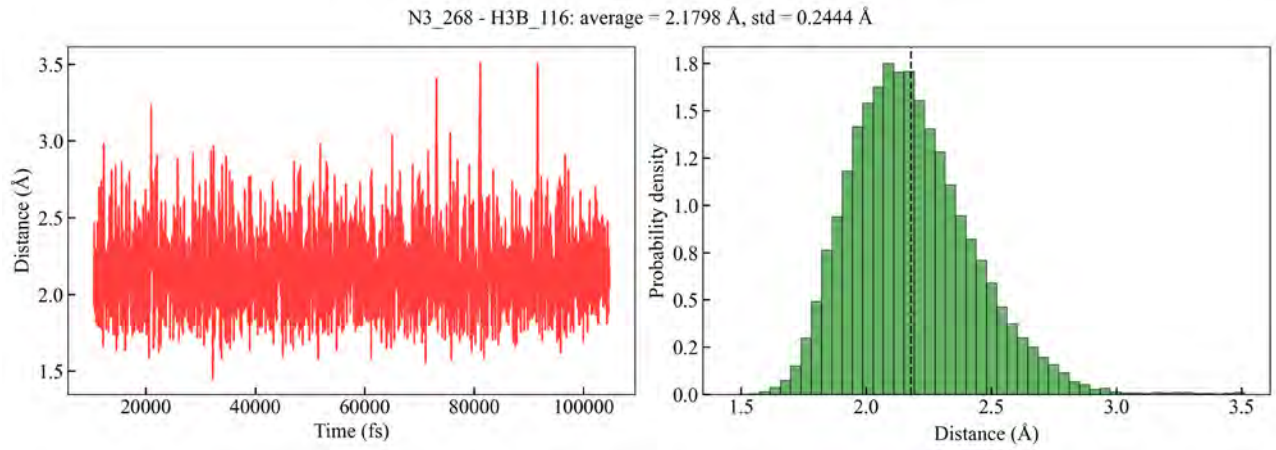
N3_267 - H3B_115

Average distance = 2.1942 Å; standard deviation = 0.2615 Å; number of points = 94257



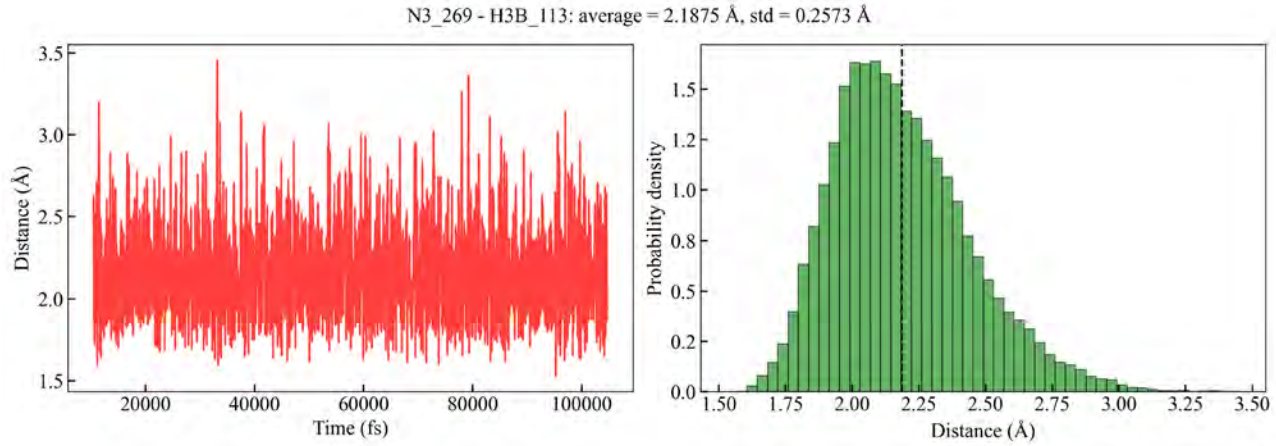
N3_268 - H3B_116

Average distance = 2.1798 Å; standard deviation = 0.2444 Å; number of points = 94257



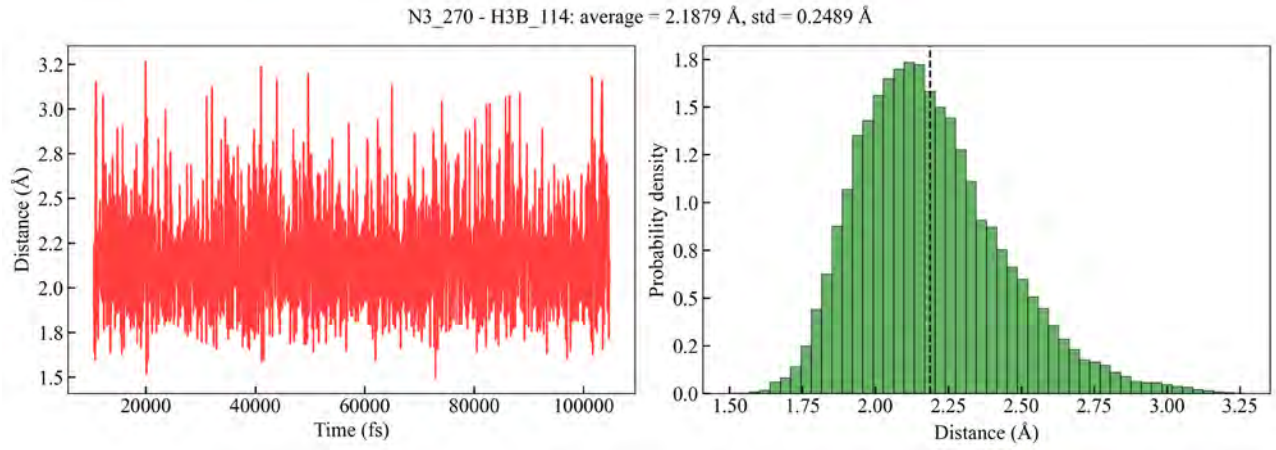
N3_269 - H3B_113

Average distance = 2.1875 Å; standard deviation = 0.2573 Å; number of points = 94257



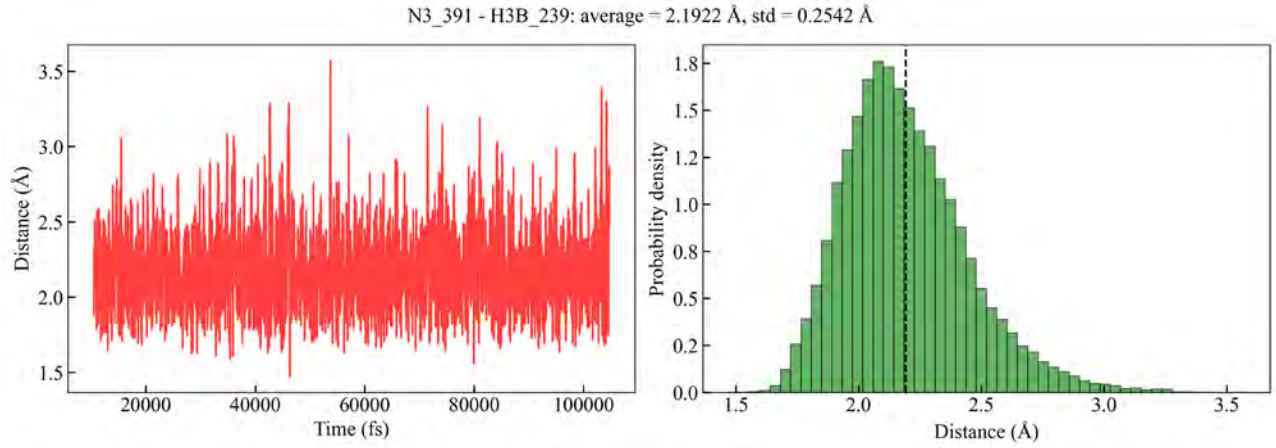
N3_270 - H3B_114

Average distance = 2.1879 Å; standard deviation = 0.2489 Å; number of points = 94257



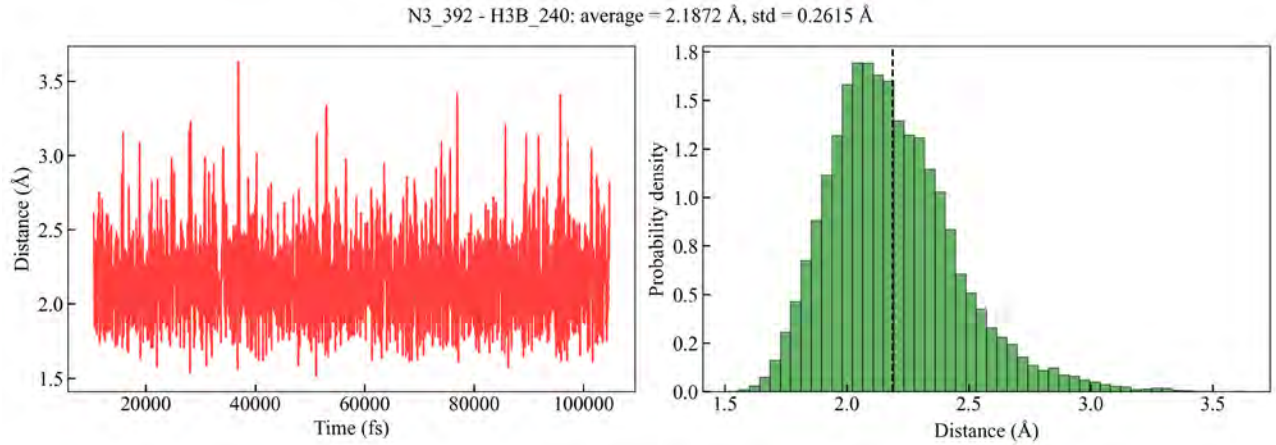
N3_391 - H3B_239

Average distance = 2.1922 Å; standard deviation = 0.2542 Å; number of points = 94257



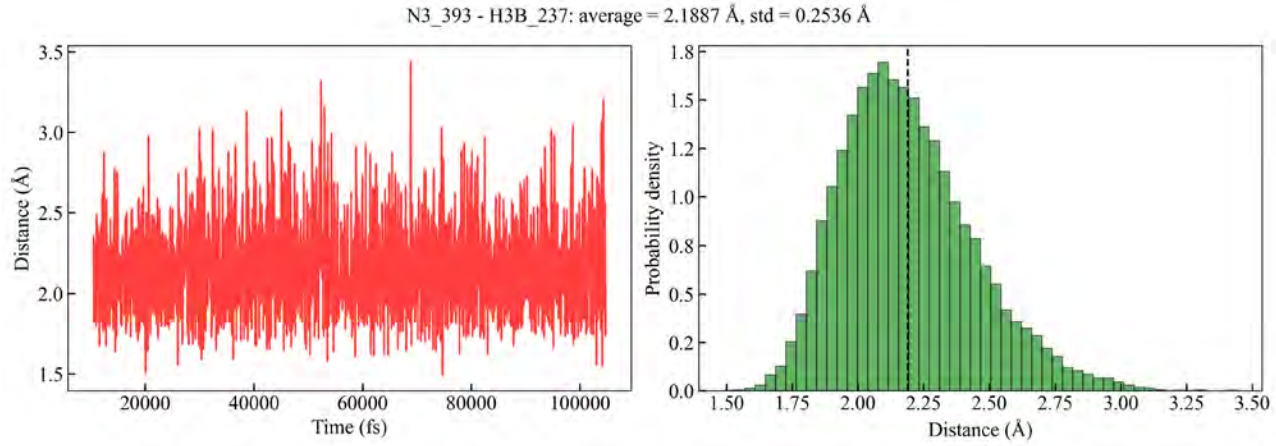
N3_392 - H3B_240

Average distance = 2.1872 Å; standard deviation = 0.2615 Å; number of points = 94257



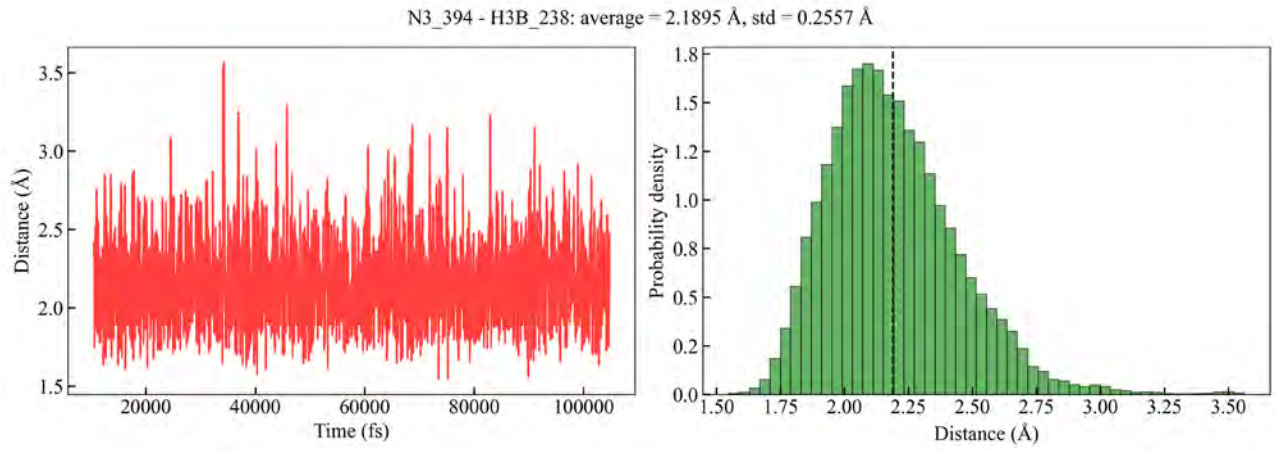
N3_393 - H3B_237

Average distance = 2.1887 Å; standard deviation = 0.2536 Å; number of points = 94257



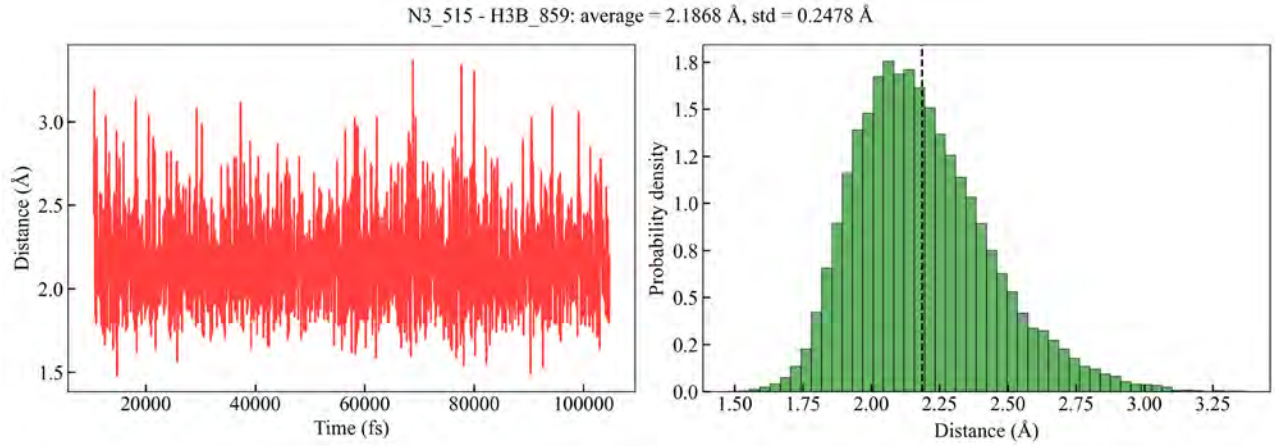
N3_394 - H3B_238

Average distance = 2.1895 Å; standard deviation = 0.2557 Å; number of points = 94257



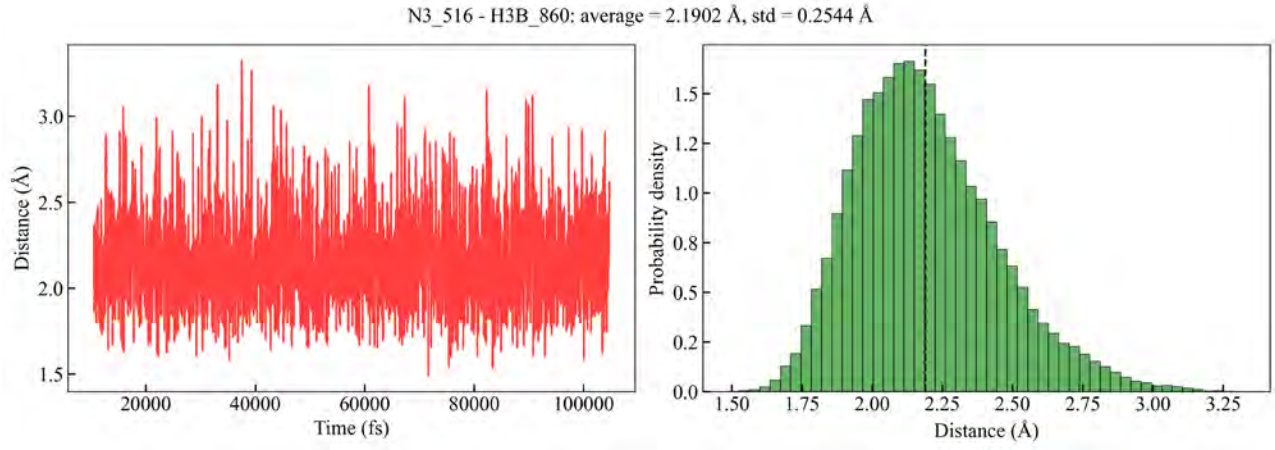
N3_515 - H3B_859

Average distance = 2.1868 Å; standard deviation = 0.2478 Å; number of points = 94257



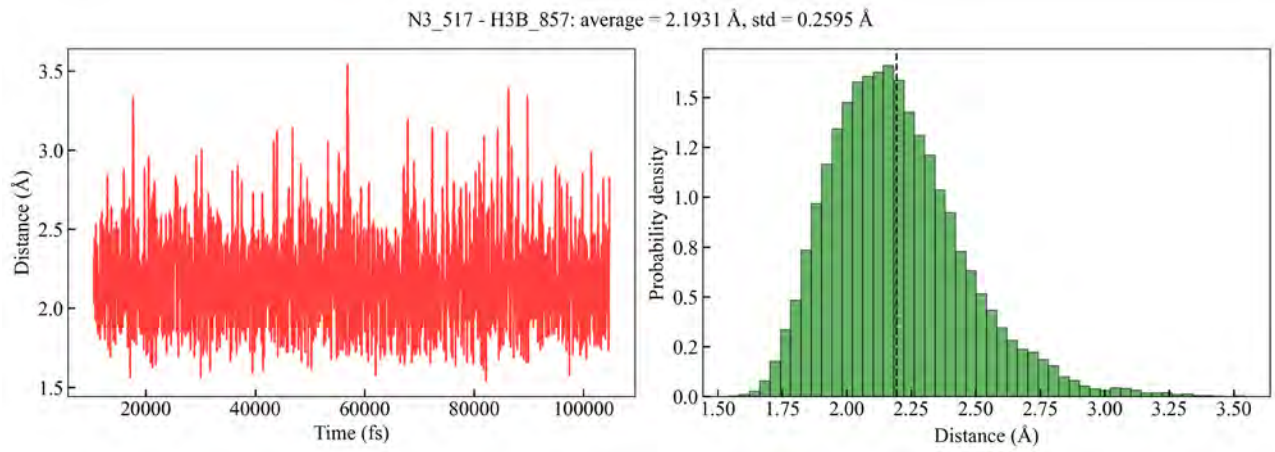
N3_516 - H3B_860

Average distance = 2.1902 Å; standard deviation = 0.2544 Å; number of points = 94257



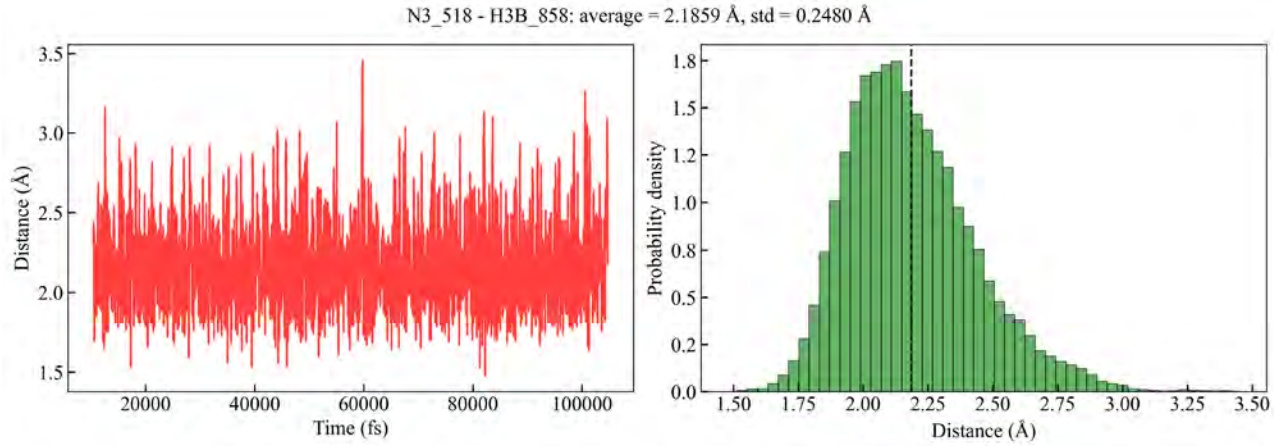
N3_517 - H3B_857

Average distance = 2.1931 Å; standard deviation = 0.2595 Å; number of points = 94257



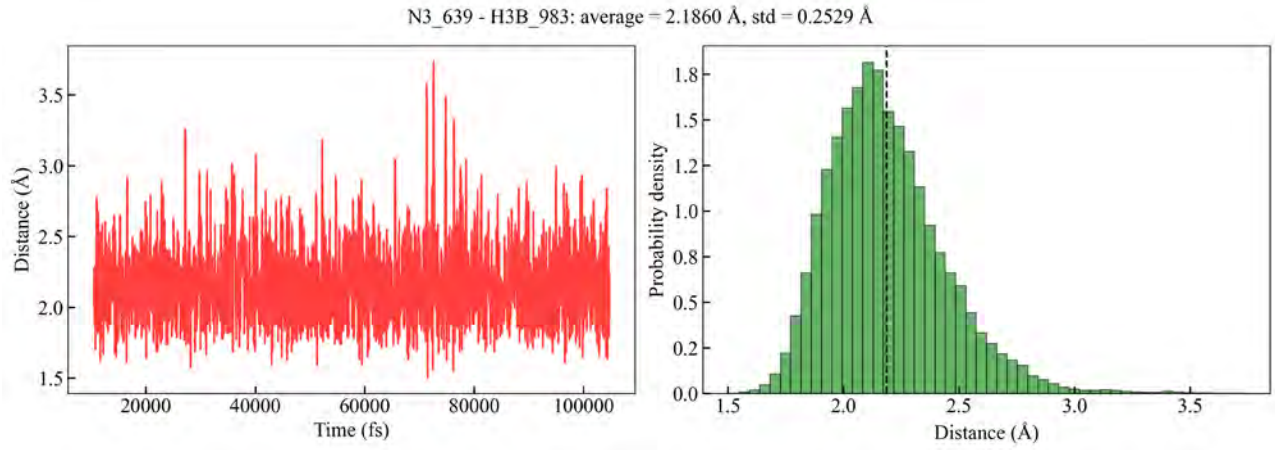
N3_518 - H3B_858

Average distance = 2.1859 Å; standard deviation = 0.2480 Å; number of points = 94257



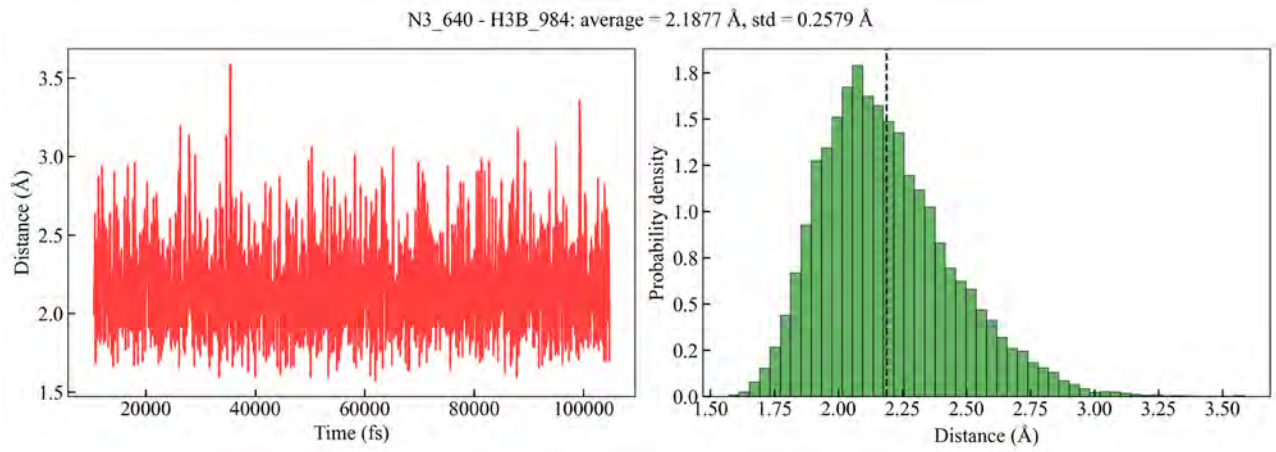
N3_639 - H3B_983

Average distance = 2.1860 Å; standard deviation = 0.2529 Å; number of points = 94257



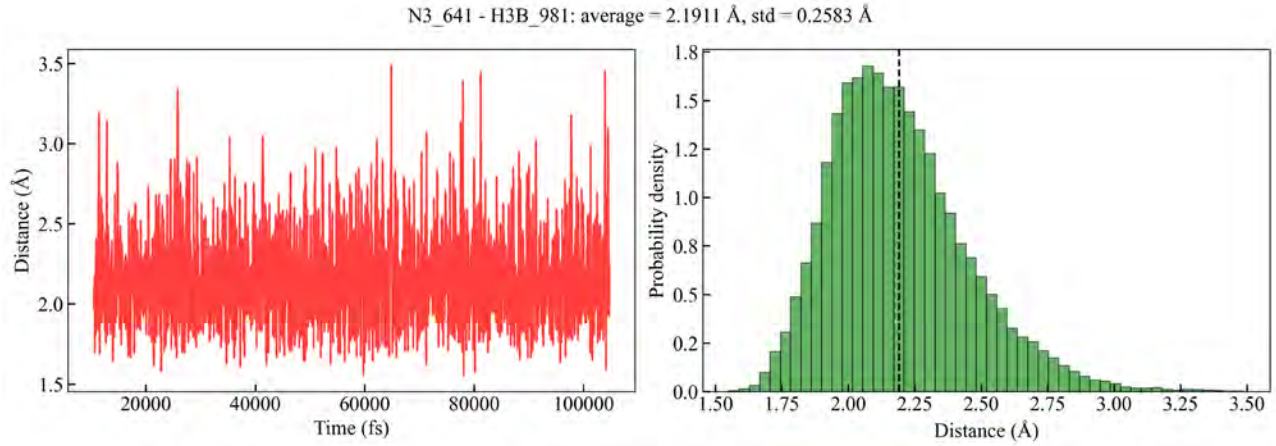
N3_640 - H3B_984

Average distance = 2.1877 Å; standard deviation = 0.2579 Å; number of points = 94257



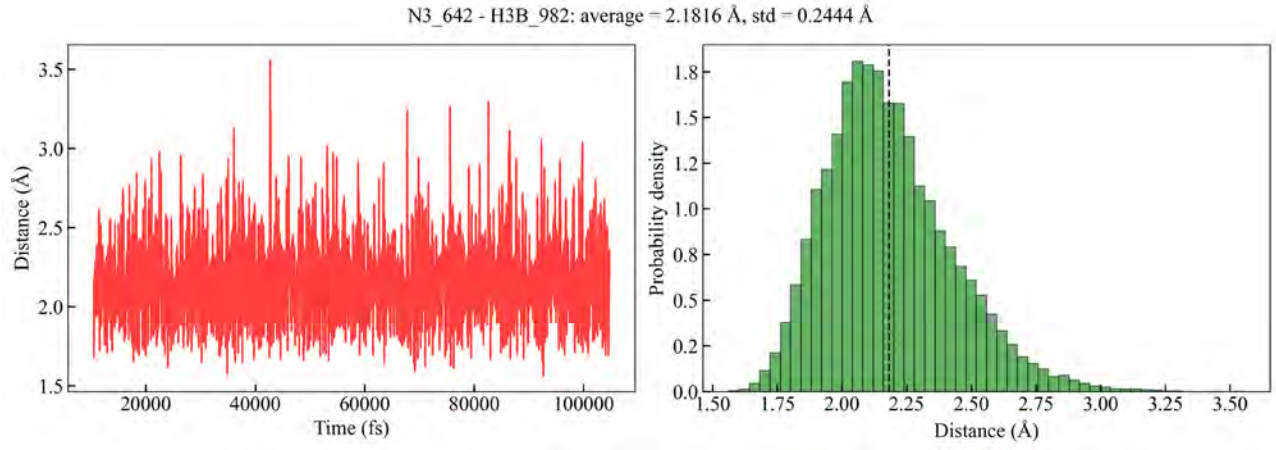
N3_641 - H3B_981

Average distance = 2.1911 Å; standard deviation = 0.2583 Å; number of points = 94257



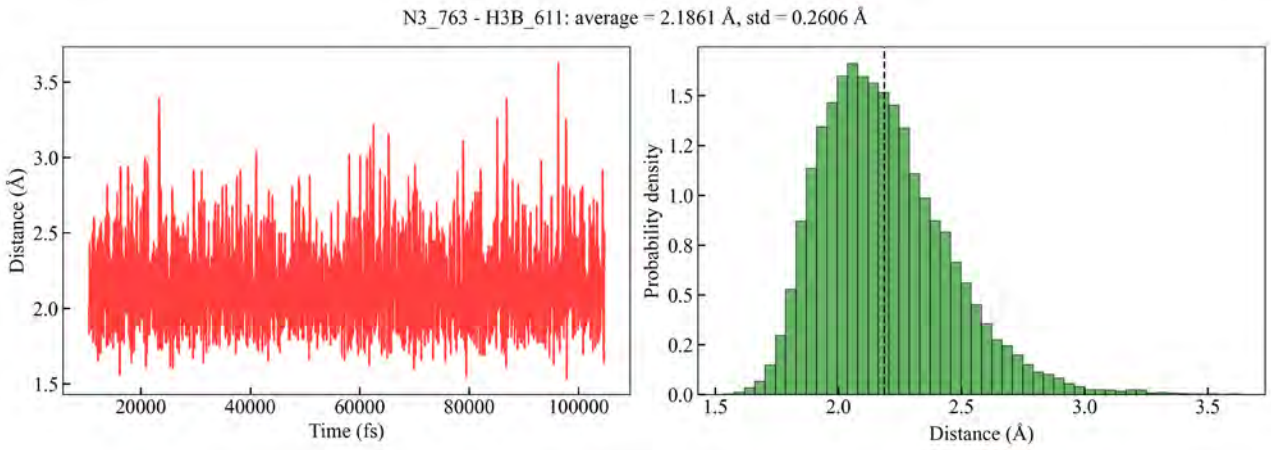
N3_642 - H3B_982

Average distance = 2.1816 Å; standard deviation = 0.2444 Å; number of points = 94257



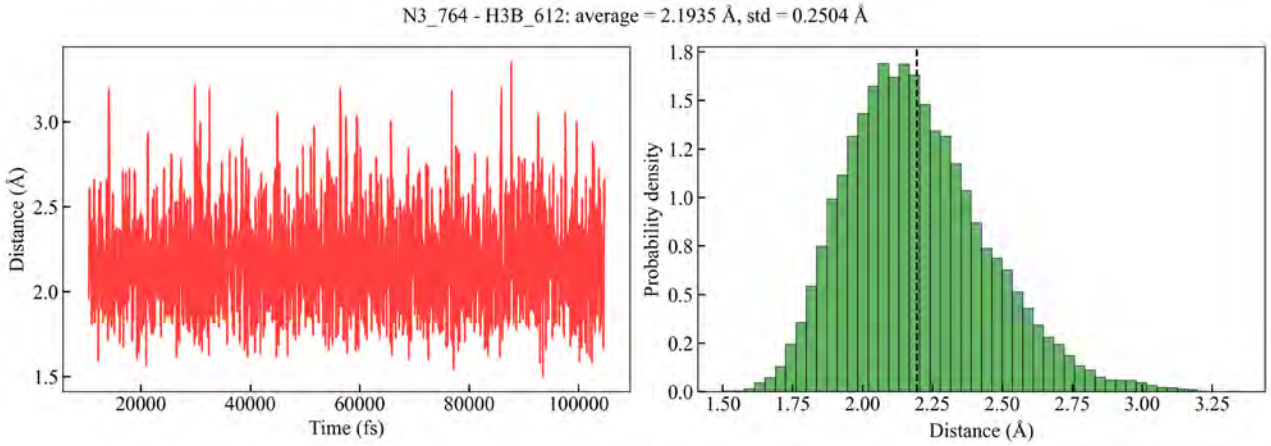
N3_763 - H3B_611

Average distance = 2.1861 Å; standard deviation = 0.2606 Å; number of points = 94257



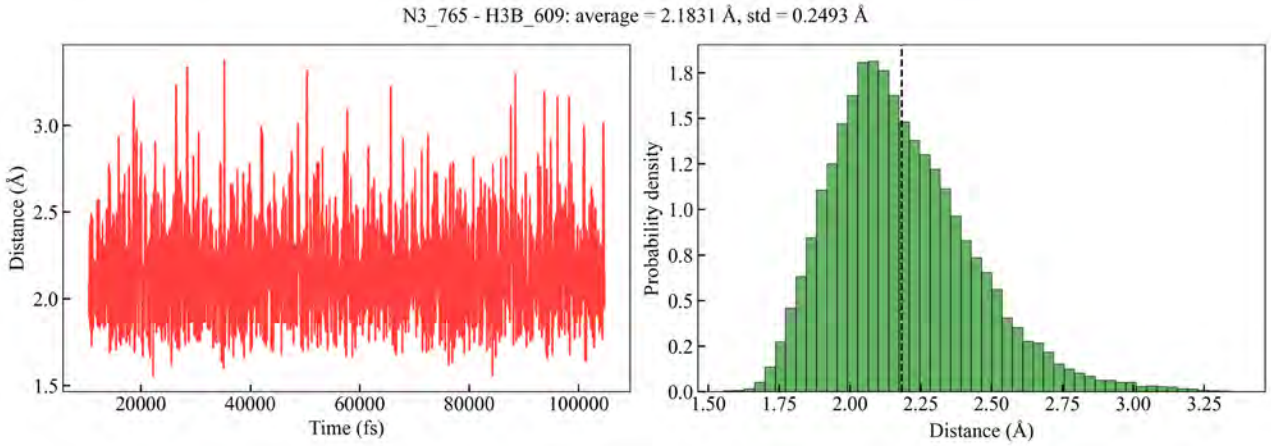
N3_764 - H3B_612

Average distance = 2.1935 Å; standard deviation = 0.2504 Å; number of points = 94257



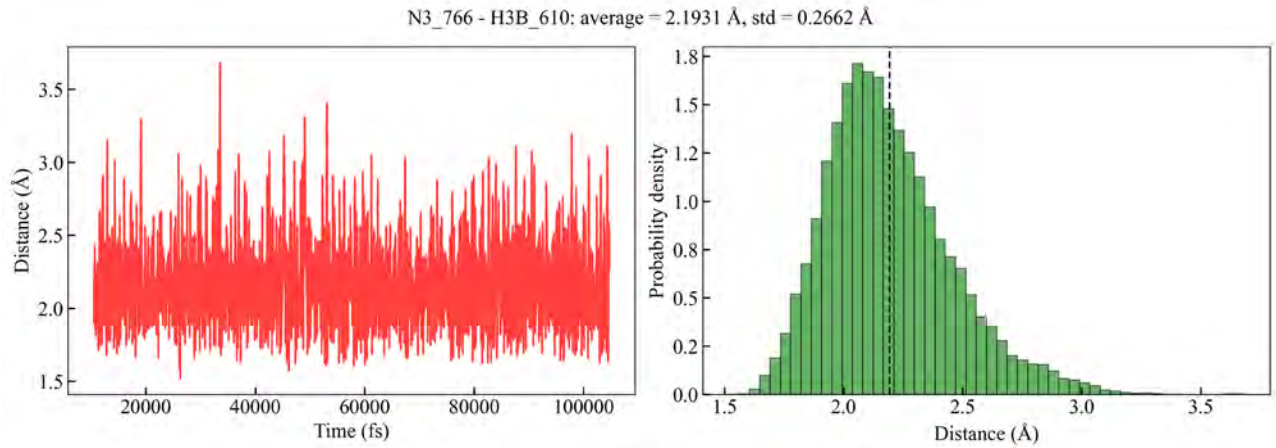
N3_765 - H3B_609

Average distance = 2.1831 Å; standard deviation = 0.2493 Å; number of points = 94257



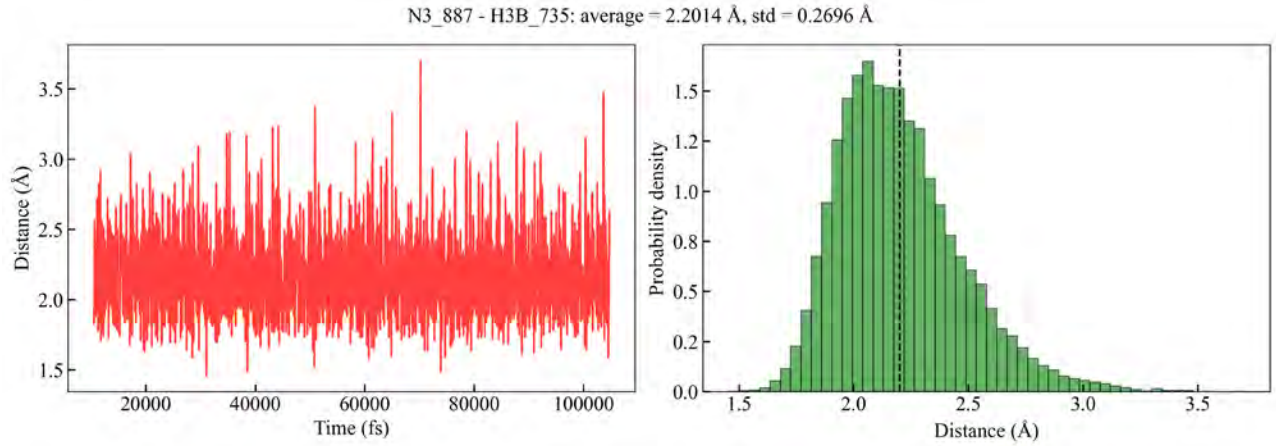
N3_766 - H3B_610

Average distance = 2.1931 Å; standard deviation = 0.2662 Å; number of points = 94257



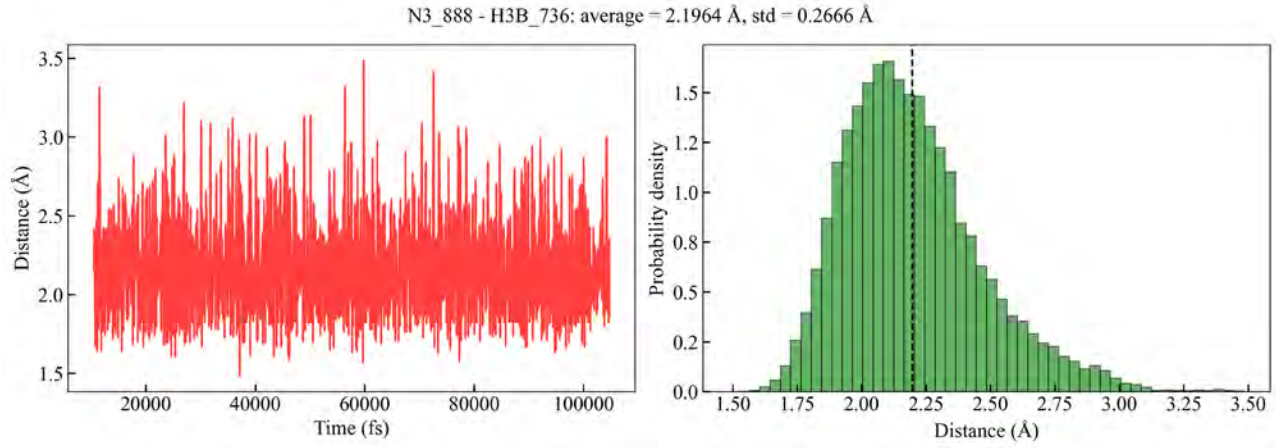
N3_887 - H3B_735

Average distance = 2.2014 Å; standard deviation = 0.2696 Å; number of points = 94257



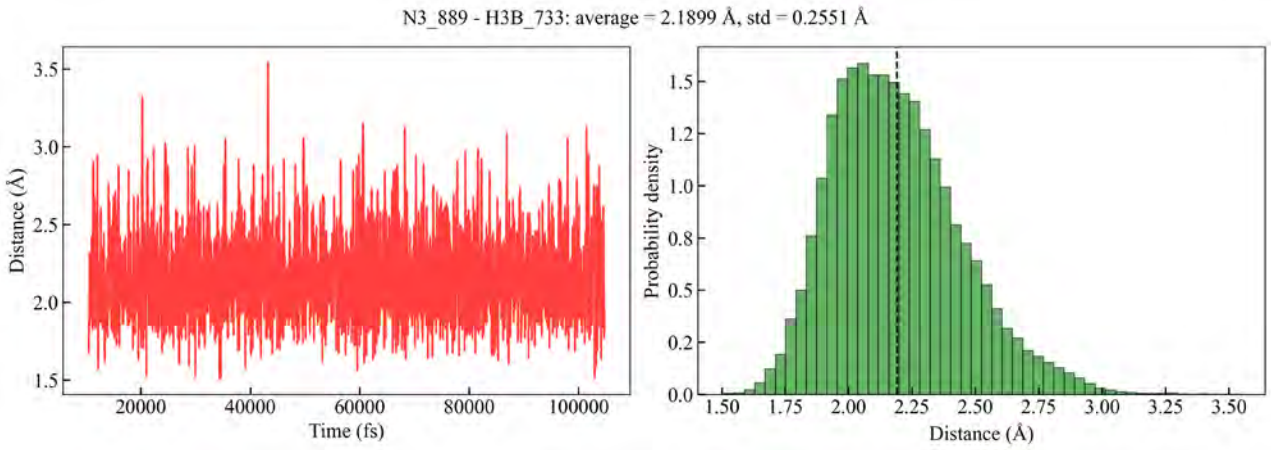
N3_888 - H3B_736

Average distance = 2.1964 Å; standard deviation = 0.2666 Å; number of points = 94257



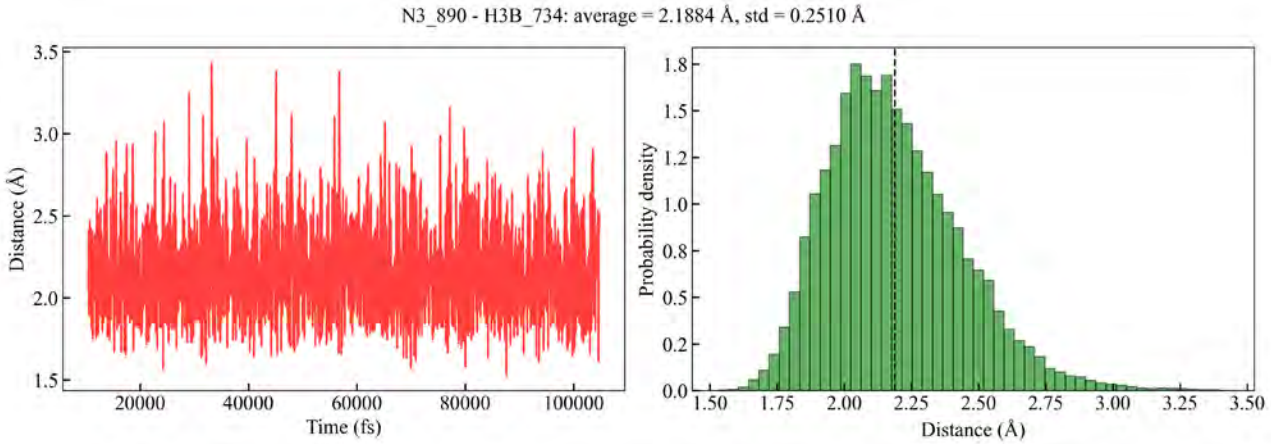
N3_889 - H3B_733

Average distance = 2.1899 Å; standard deviation = 0.2551 Å; number of points = 94257



N3_890 - H3B_734

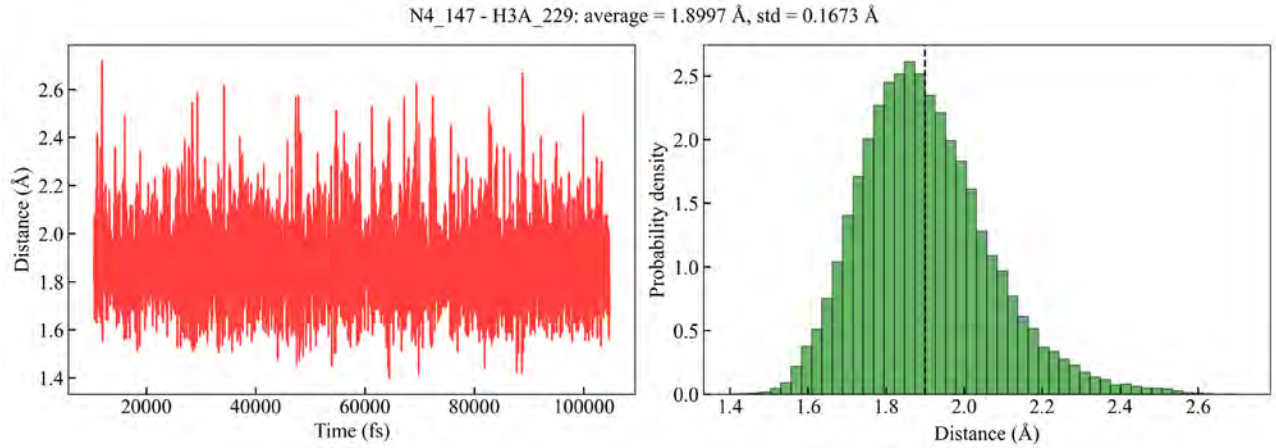
Average distance = 2.1884 Å; standard deviation = 0.2510 Å; number of points = 94257



N4 - H3A

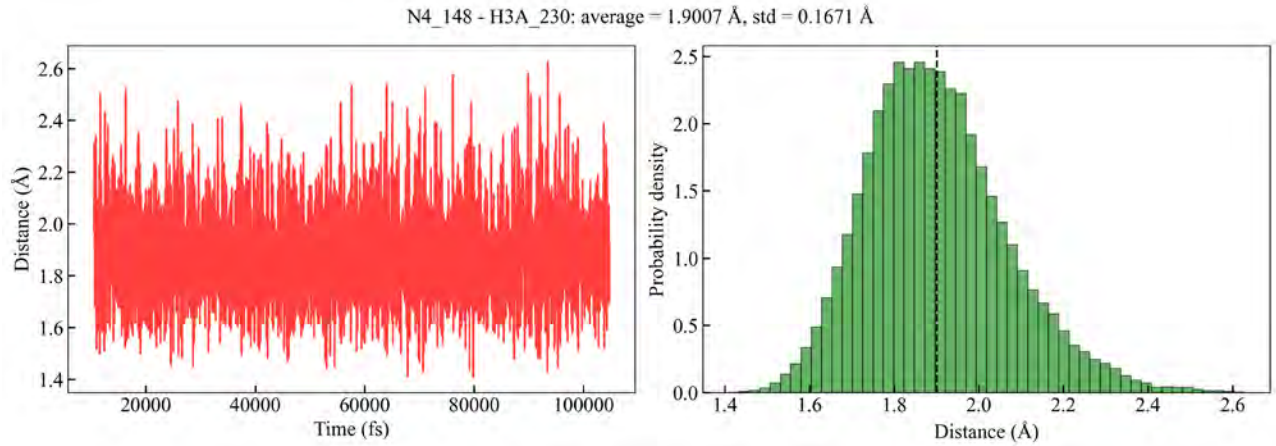
N4_147 - H3A_229

Average distance = 1.8997 Å; standard deviation = 0.1673 Å; number of points = 94257



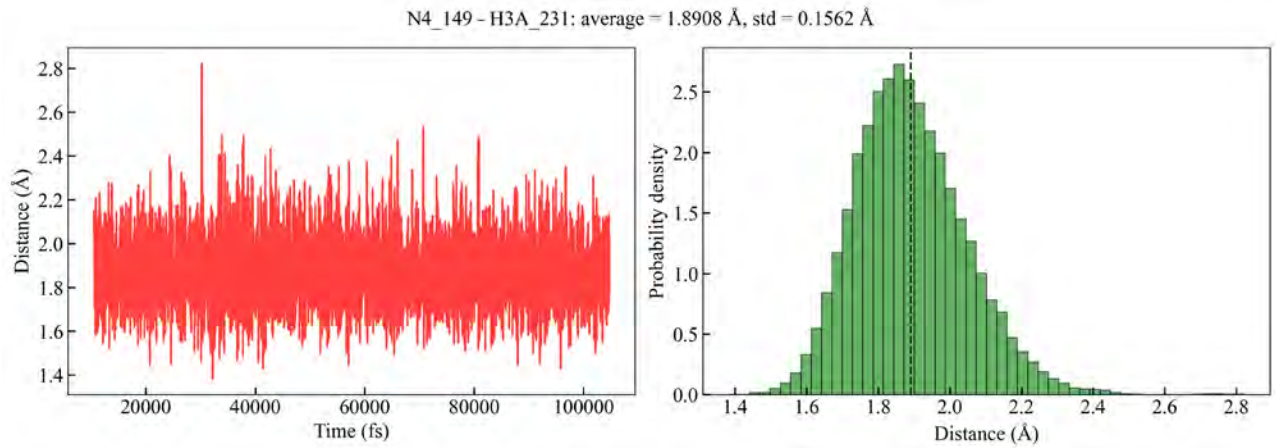
N4_148 - H3A_230

Average distance = 1.9007 Å; standard deviation = 0.1671 Å; number of points = 94257



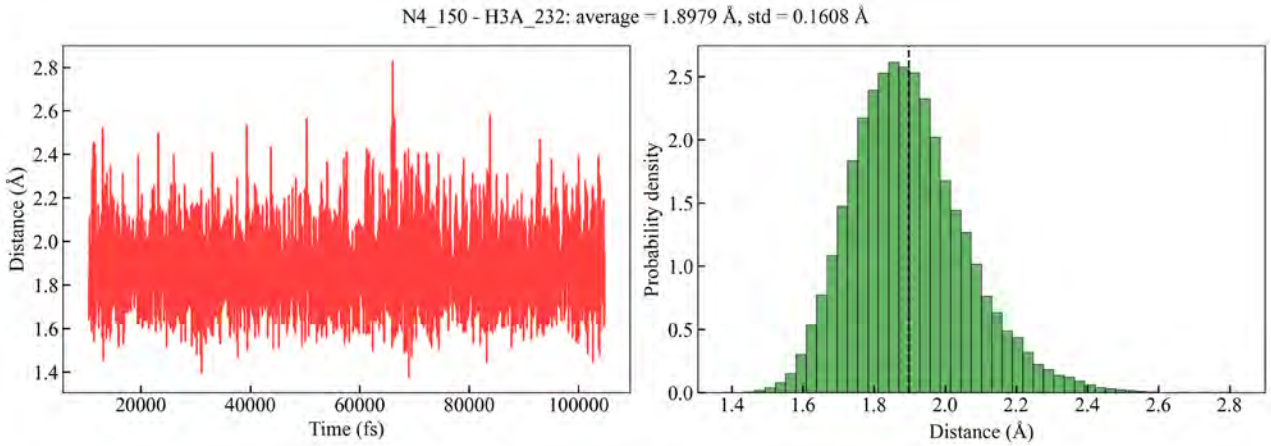
N4_149 - H3A_231

Average distance = 1.8908 Å; standard deviation = 0.1562 Å; number of points = 94257



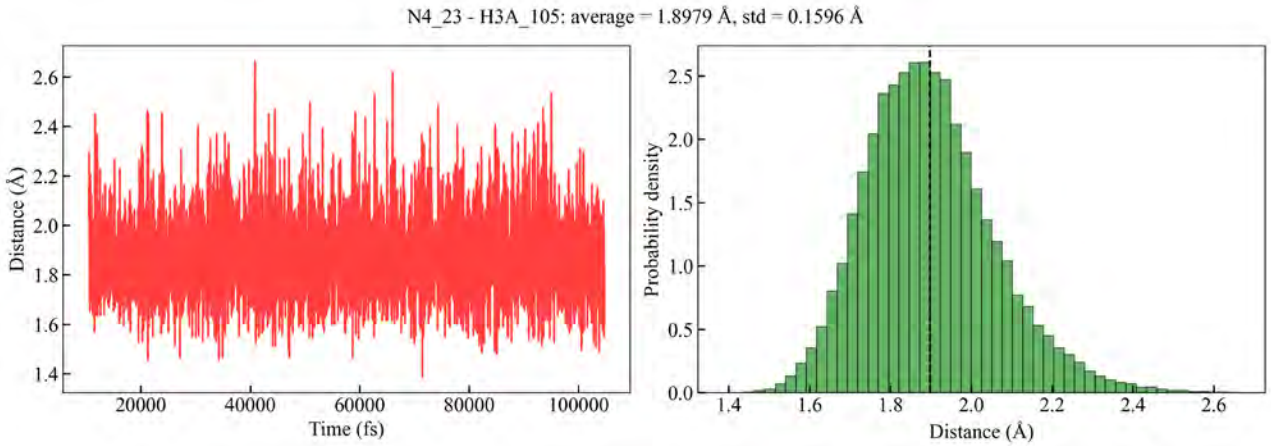
N4_150 - H3A_232

Average distance = 1.8979 Å; standard deviation = 0.1608 Å; number of points = 94257



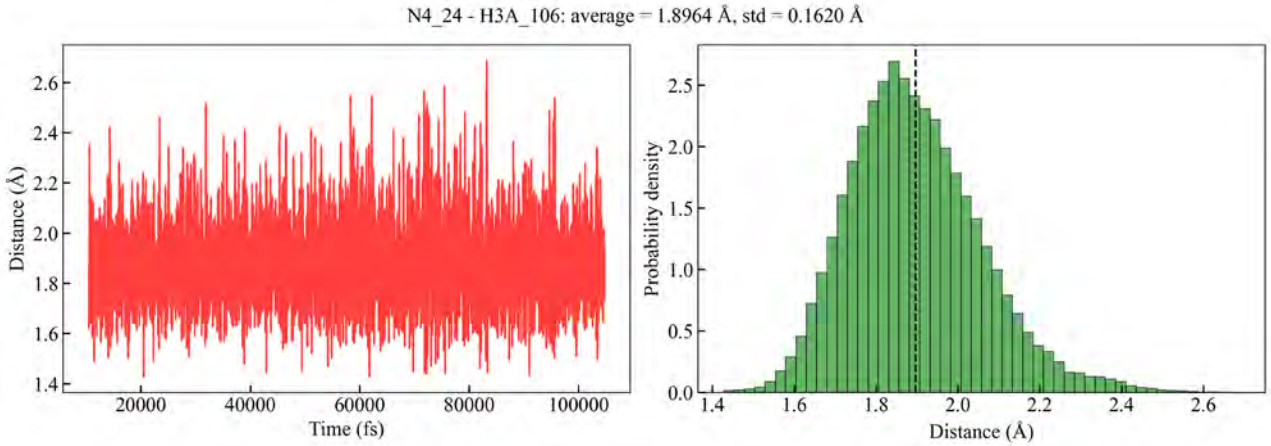
N4_23 - H3A_105

Average distance = 1.8979 Å; standard deviation = 0.1596 Å; number of points = 94257



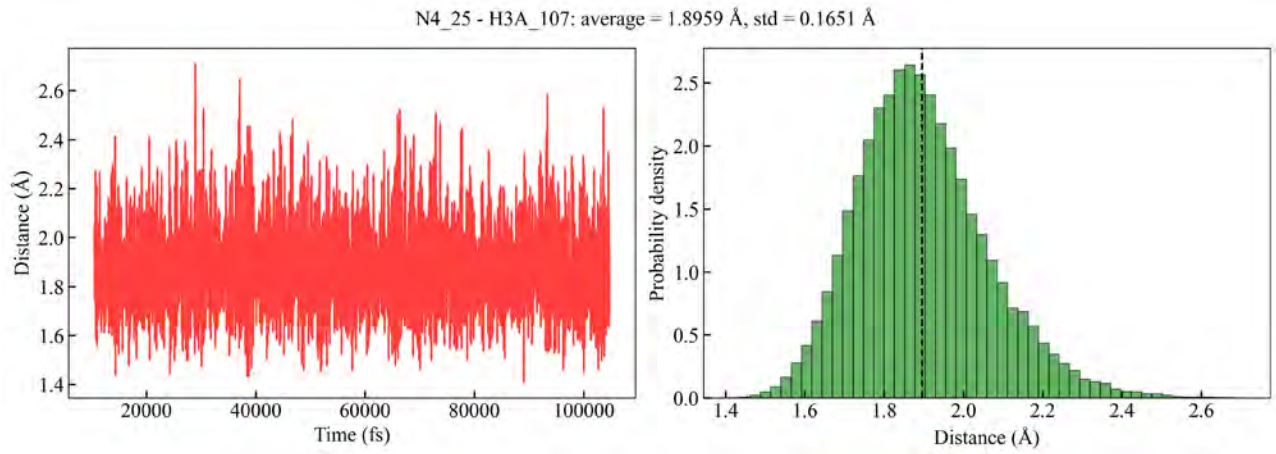
N4_24 - H3A_106

Average distance = 1.8964 Å; standard deviation = 0.1620 Å; number of points = 94257



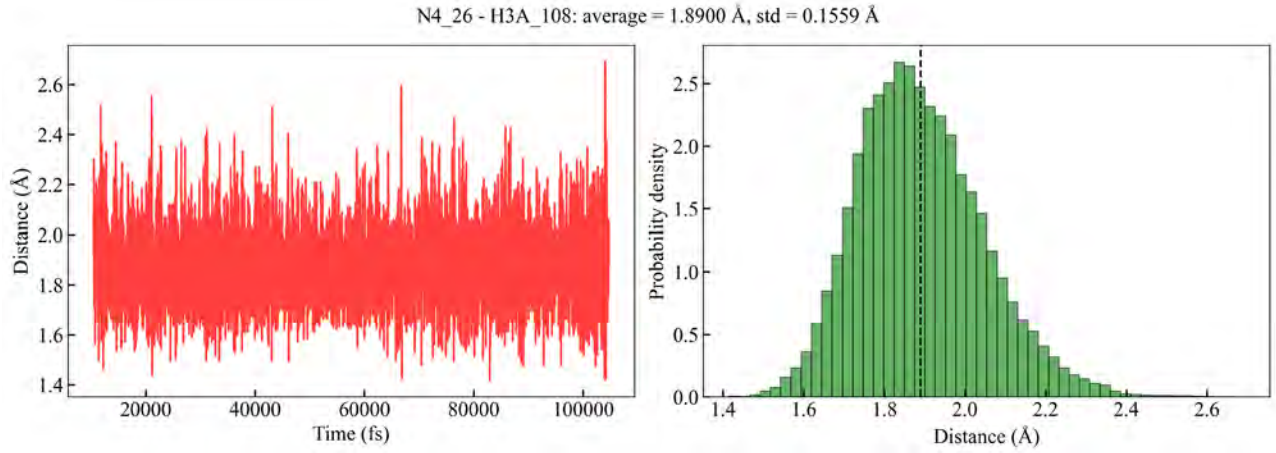
N4_25 - H3A_107

Average distance = 1.8959 Å; standard deviation = 0.1651 Å; number of points = 94257



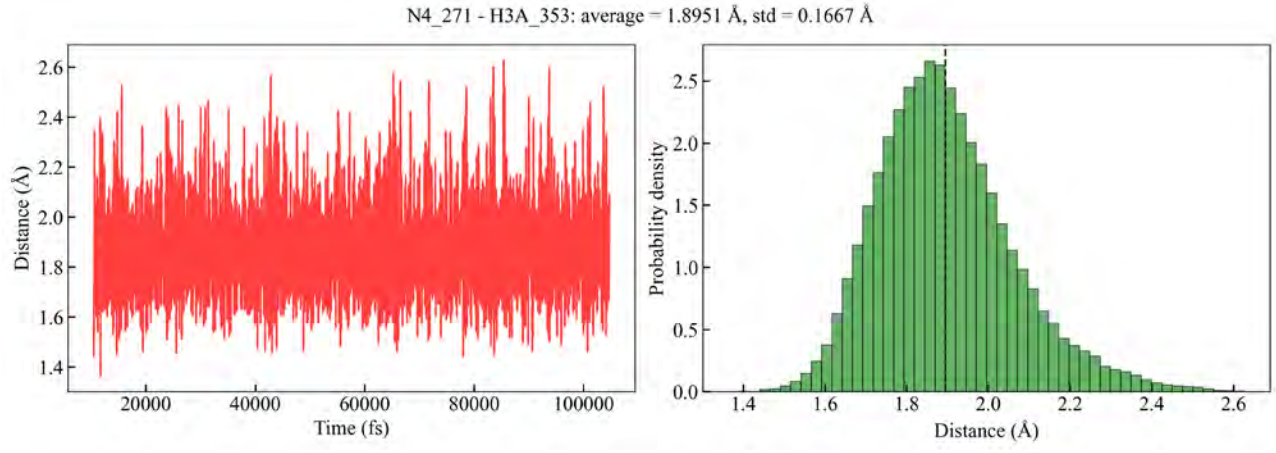
N4_26 - H3A_108

Average distance = 1.8900 Å; standard deviation = 0.1559 Å; number of points = 94257



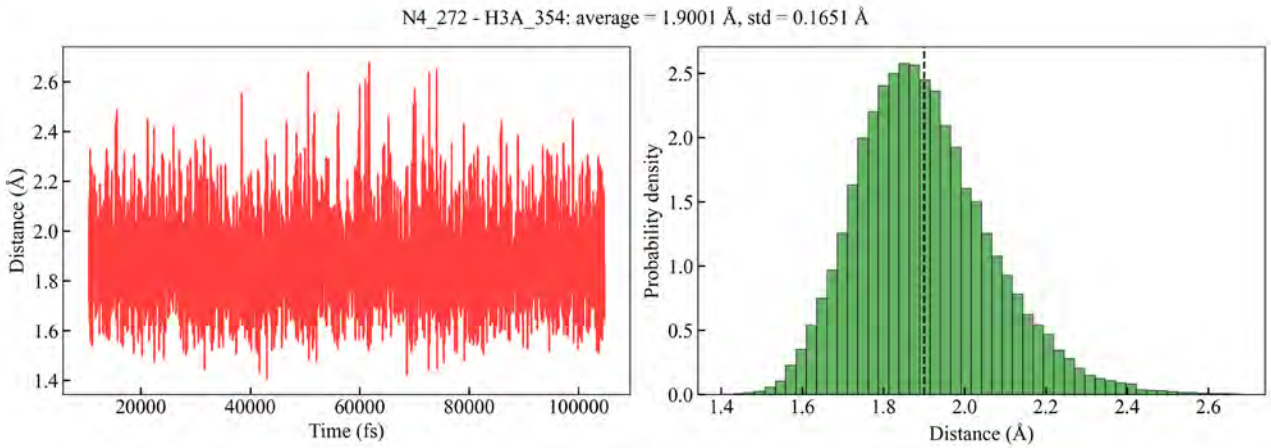
N4_271 - H3A_353

Average distance = 1.8951 Å; standard deviation = 0.1667 Å; number of points = 94257



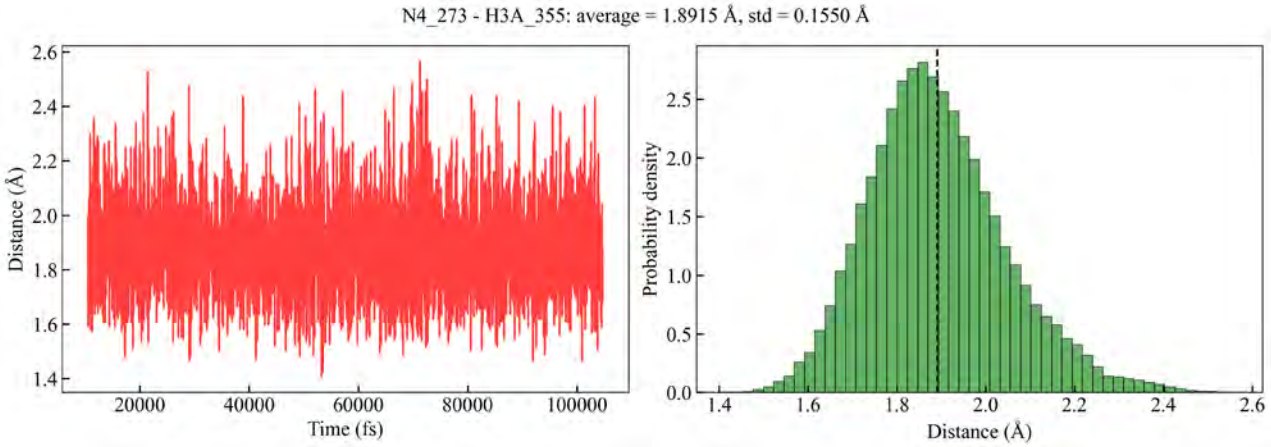
N4_272 - H3A_354

Average distance = 1.9001 Å; standard deviation = 0.1651 Å; number of points = 94257



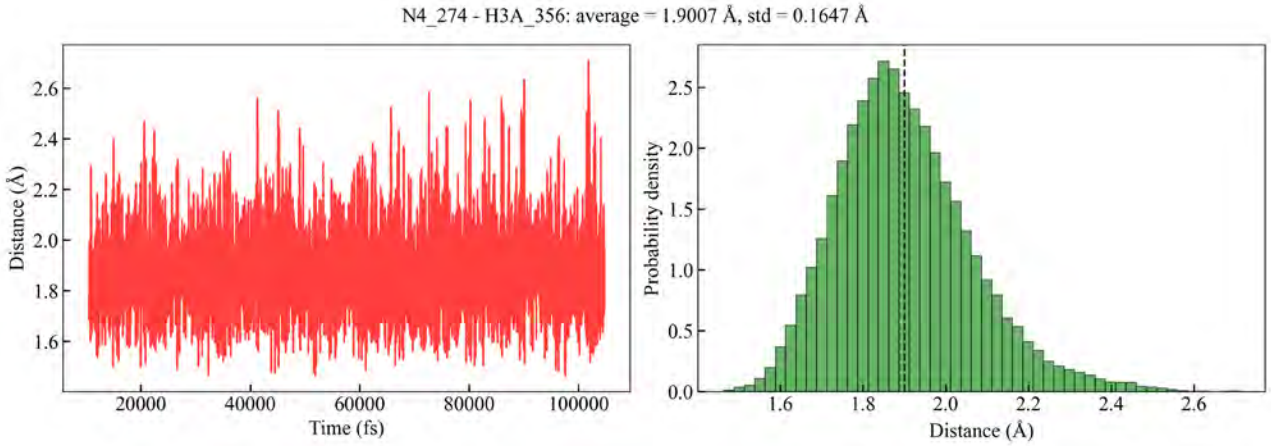
N4_273 - H3A_355

Average distance = 1.8915 Å; standard deviation = 0.1550 Å; number of points = 94257



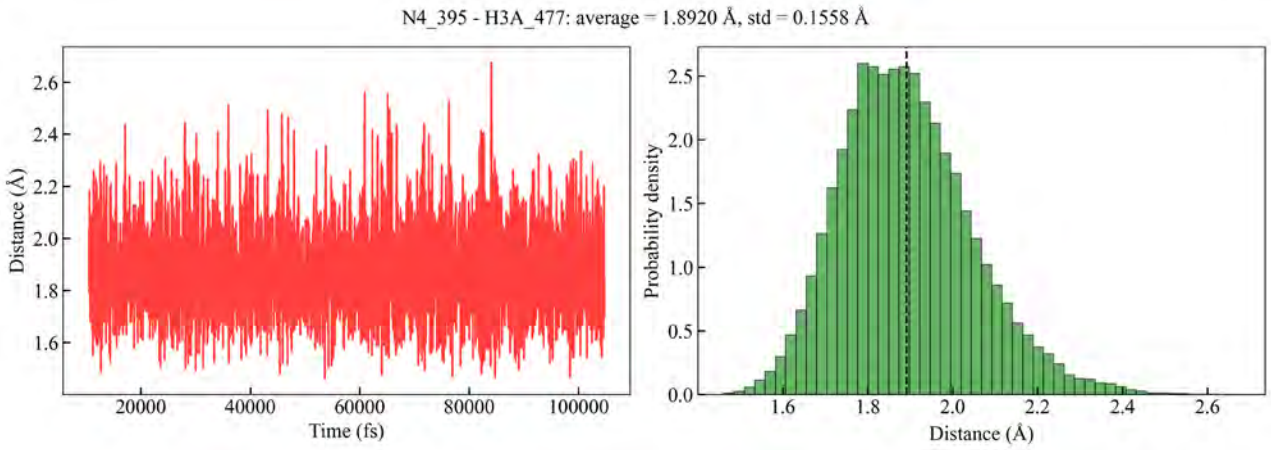
N4_274 - H3A_356

Average distance = 1.9007 Å; standard deviation = 0.1647 Å; number of points = 94257



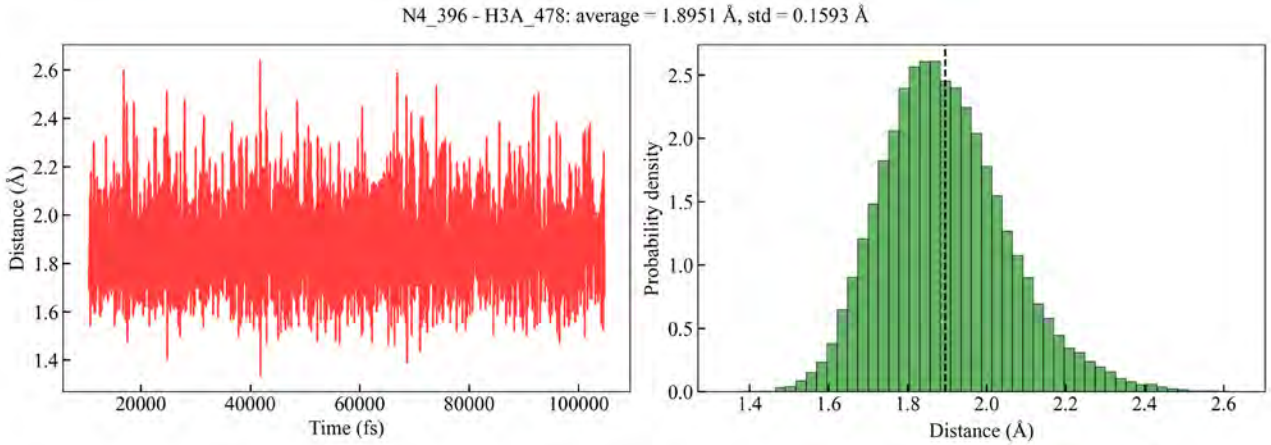
N4_395 - H3A_477

Average distance = 1.8920 Å; standard deviation = 0.1558 Å; number of points = 94257



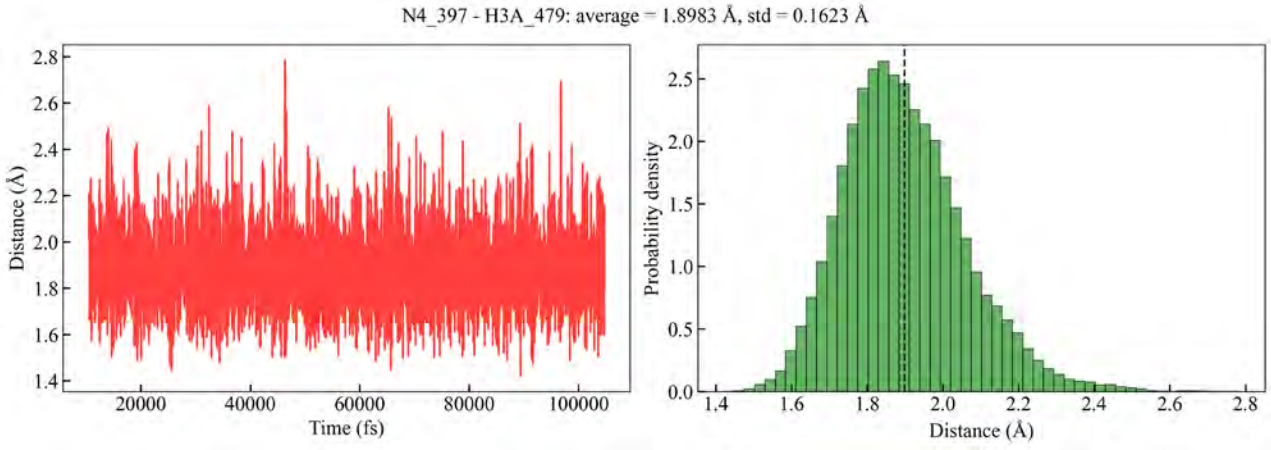
N4_396 - H3A_478

Average distance = 1.8951 Å; standard deviation = 0.1593 Å; number of points = 94257



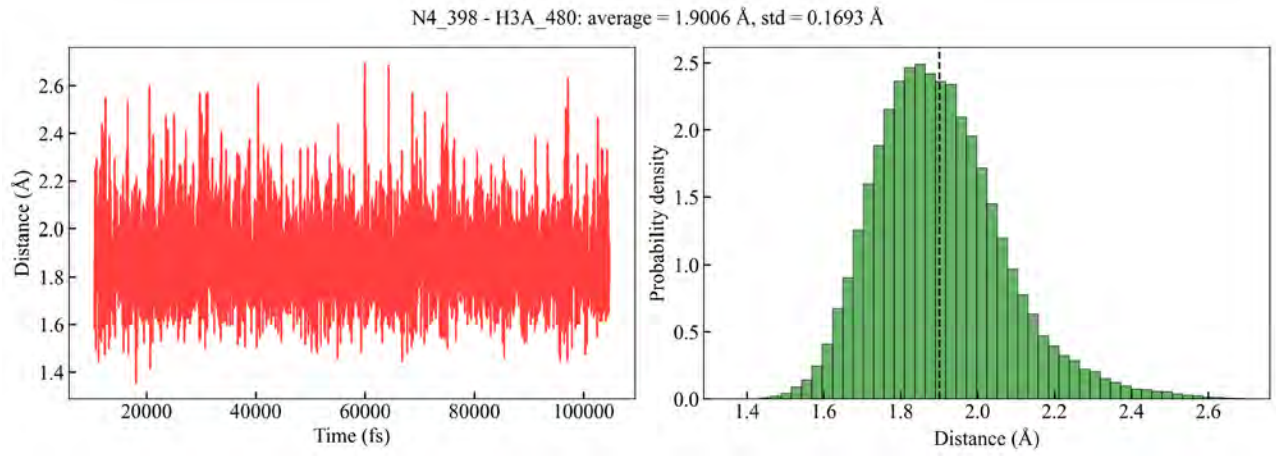
N4_397 - H3A_479

Average distance = 1.8983 Å; standard deviation = 0.1623 Å; number of points = 94257



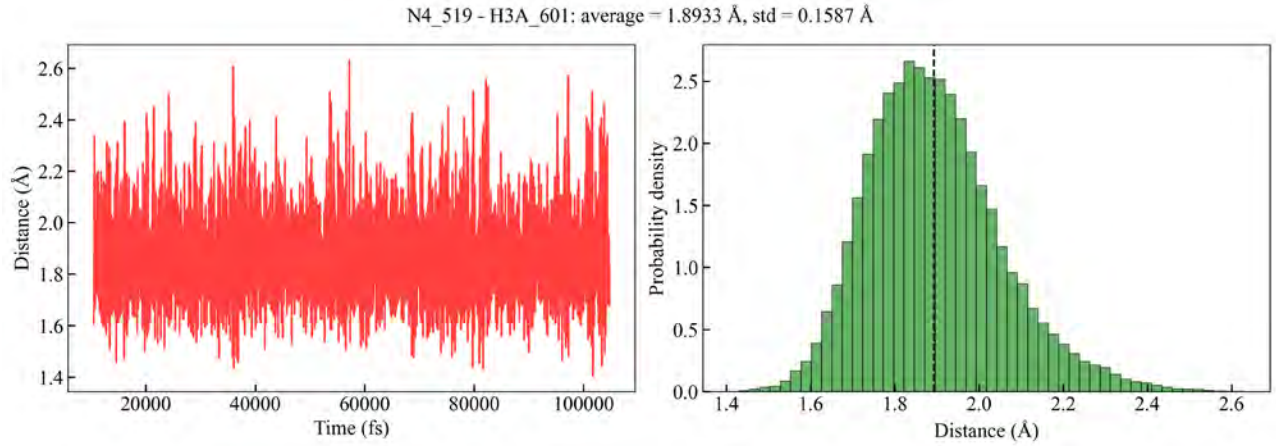
N4_398 - H3A_480

Average distance = 1.9006 Å; standard deviation = 0.1693 Å; number of points = 94257



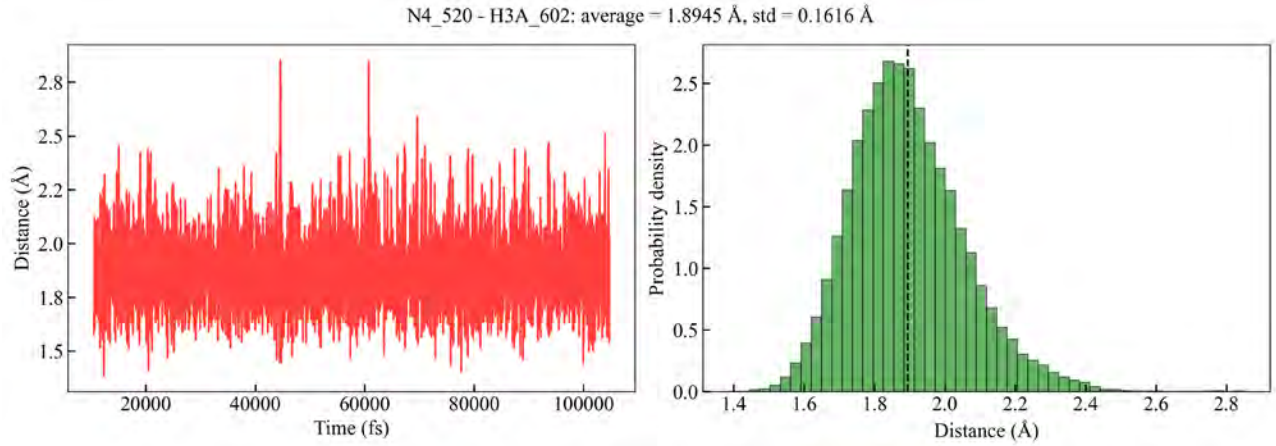
N4_519 - H3A_601

Average distance = 1.8933 Å; standard deviation = 0.1587 Å; number of points = 94257



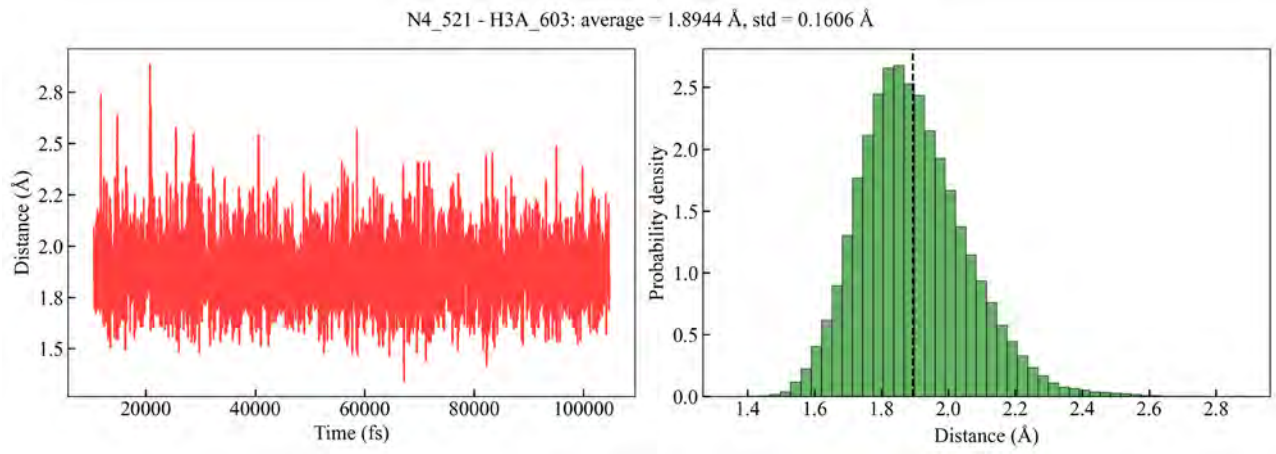
N4_520 - H3A_602

Average distance = 1.8945 Å; standard deviation = 0.1616 Å; number of points = 94257



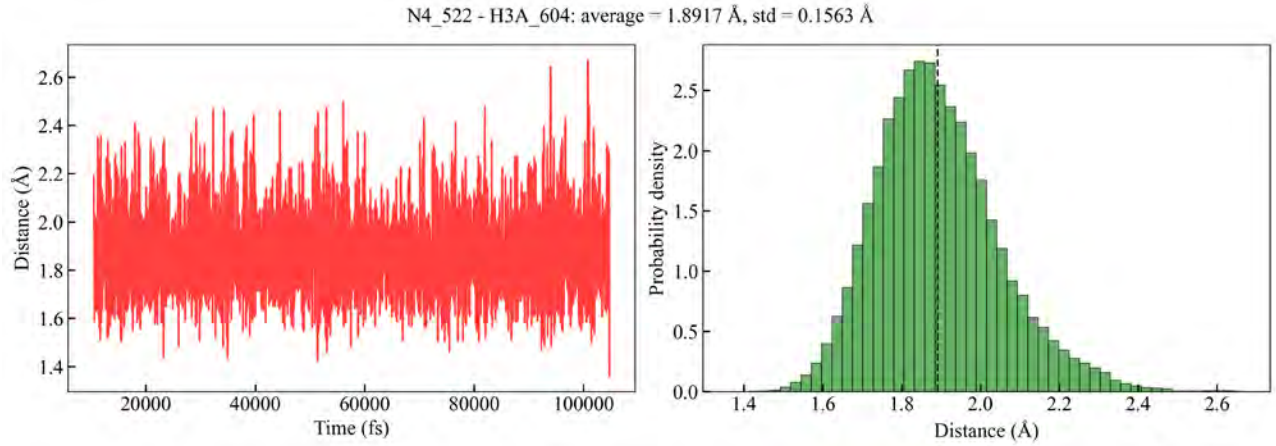
N4_521 - H3A_603

Average distance = 1.8944 Å; standard deviation = 0.1606 Å; number of points = 94257



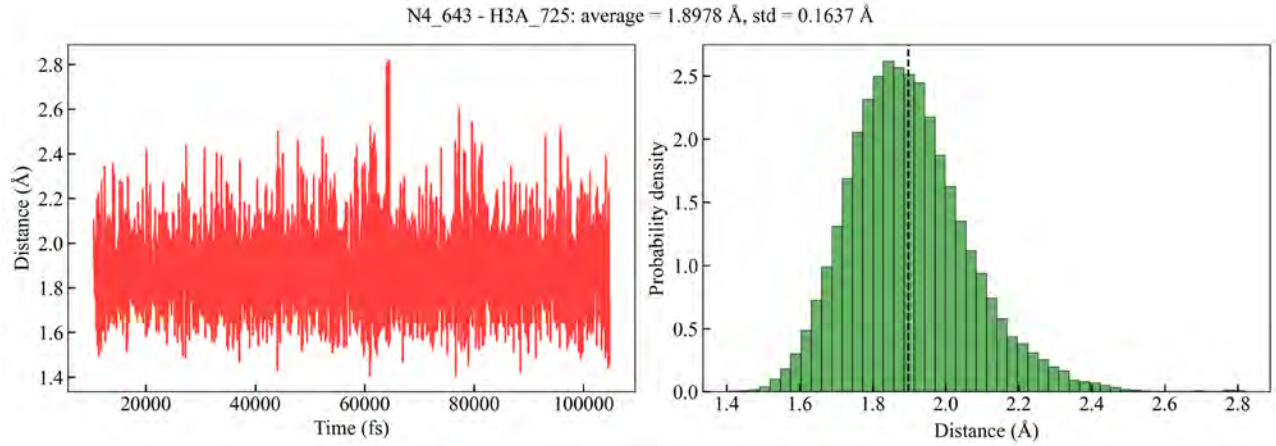
N4_522 - H3A_604

Average distance = 1.8917 Å; standard deviation = 0.1563 Å; number of points = 94257



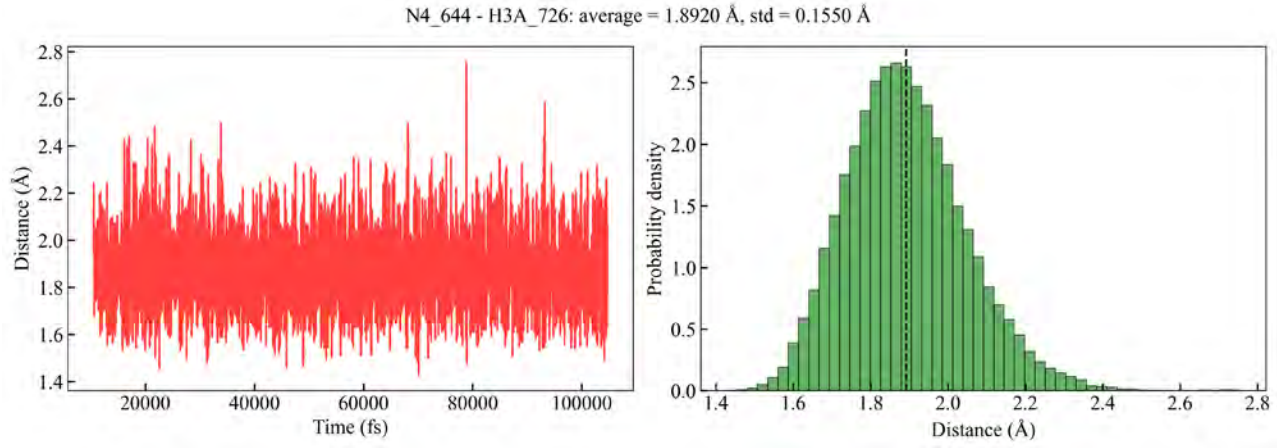
N4_643 - H3A_725

Average distance = 1.8978 Å; standard deviation = 0.1637 Å; number of points = 94257



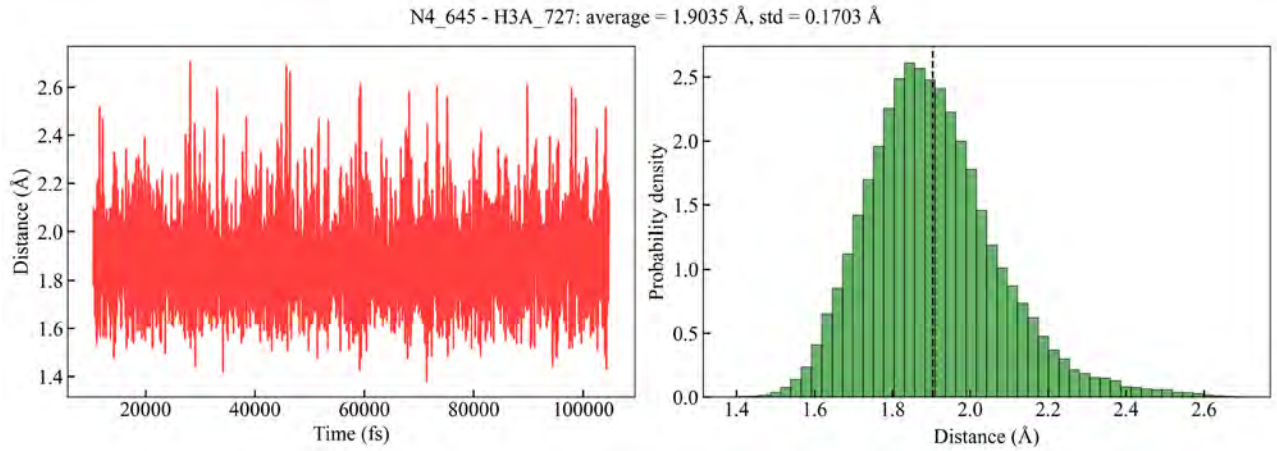
N4_644 - H3A_726

Average distance = 1.8920 Å; standard deviation = 0.1550 Å; number of points = 94257



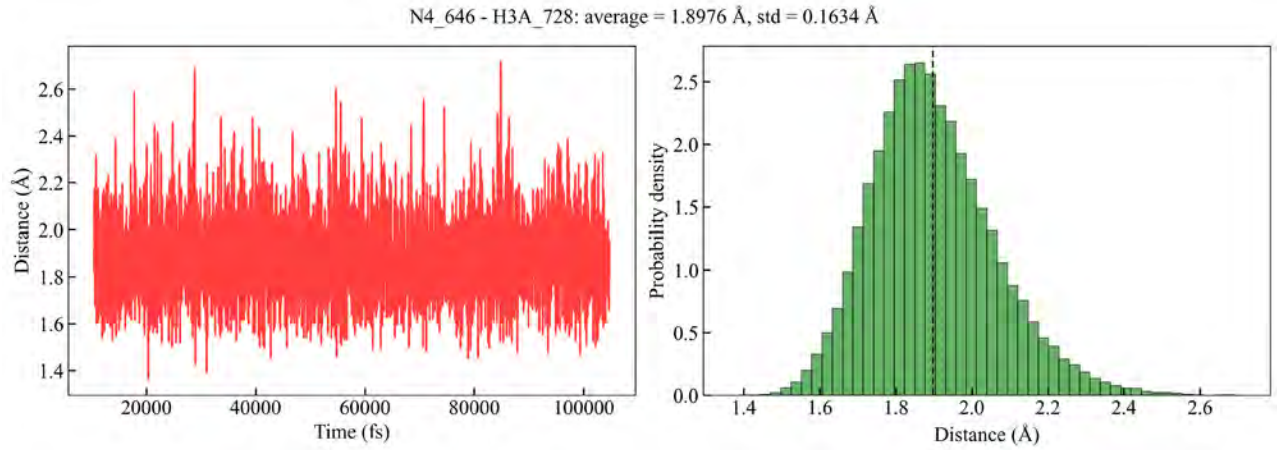
N4_645 - H3A_727

Average distance = 1.9035 Å; standard deviation = 0.1703 Å; number of points = 94257



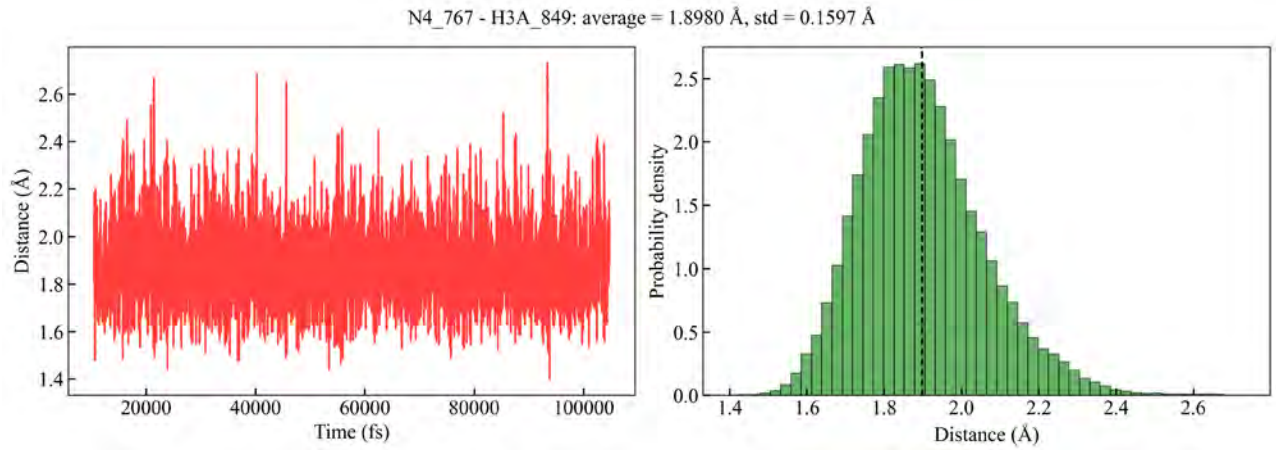
N4_646 - H3A_728

Average distance = 1.8976 Å; standard deviation = 0.1634 Å; number of points = 94257



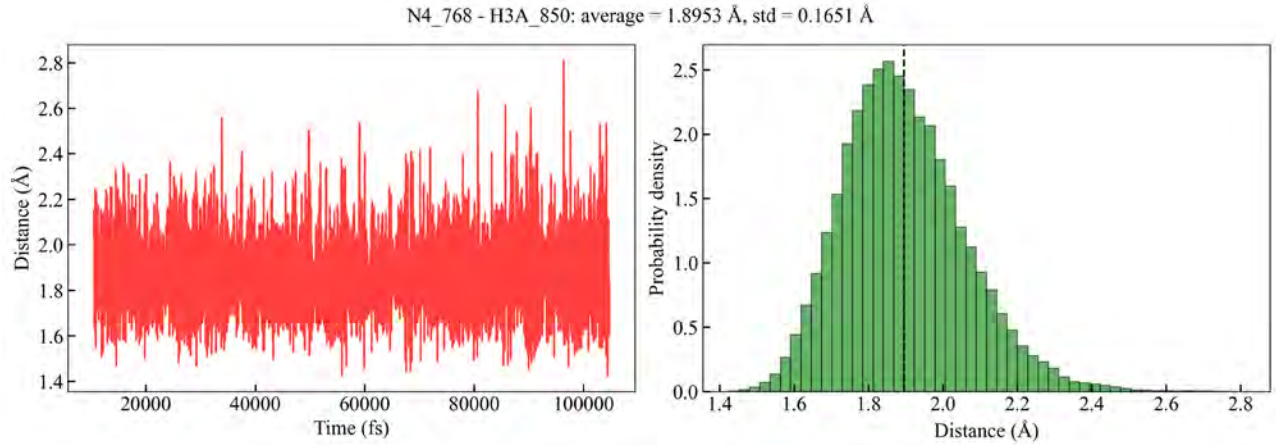
N4_767 - H3A_849

Average distance = 1.8980 Å; standard deviation = 0.1597 Å; number of points = 94257



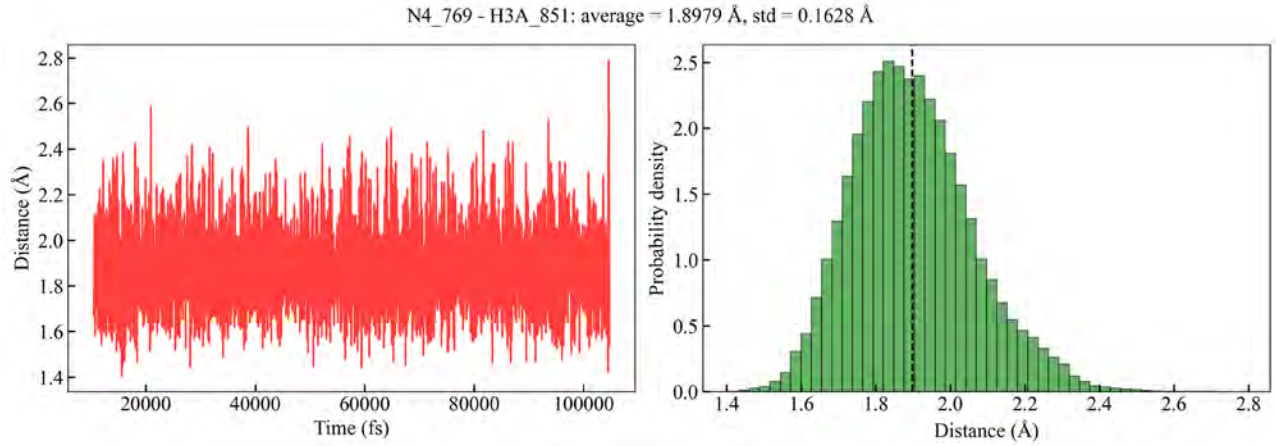
N4_768 - H3A_850

Average distance = 1.8953 Å; standard deviation = 0.1651 Å; number of points = 94257



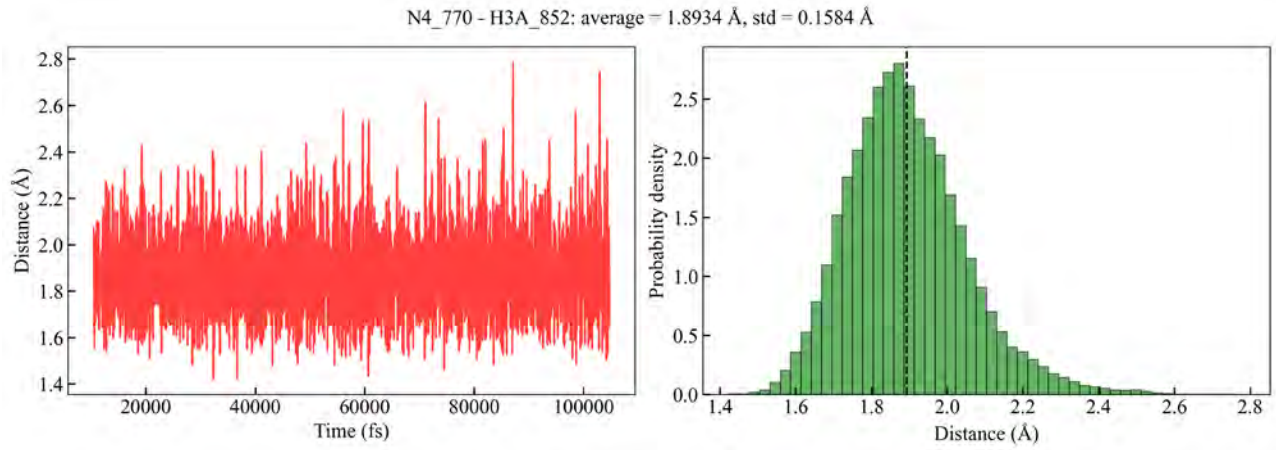
N4_769 - H3A_851

Average distance = 1.8979 Å; standard deviation = 0.1628 Å; number of points = 94257



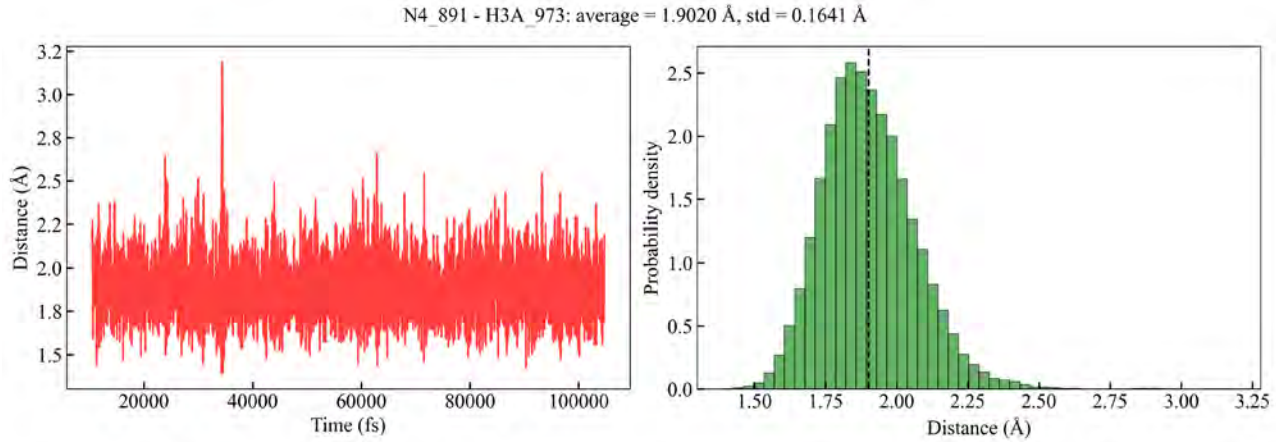
N4_770 - H3A_852

Average distance = 1.8934 Å; standard deviation = 0.1584 Å; number of points = 94257



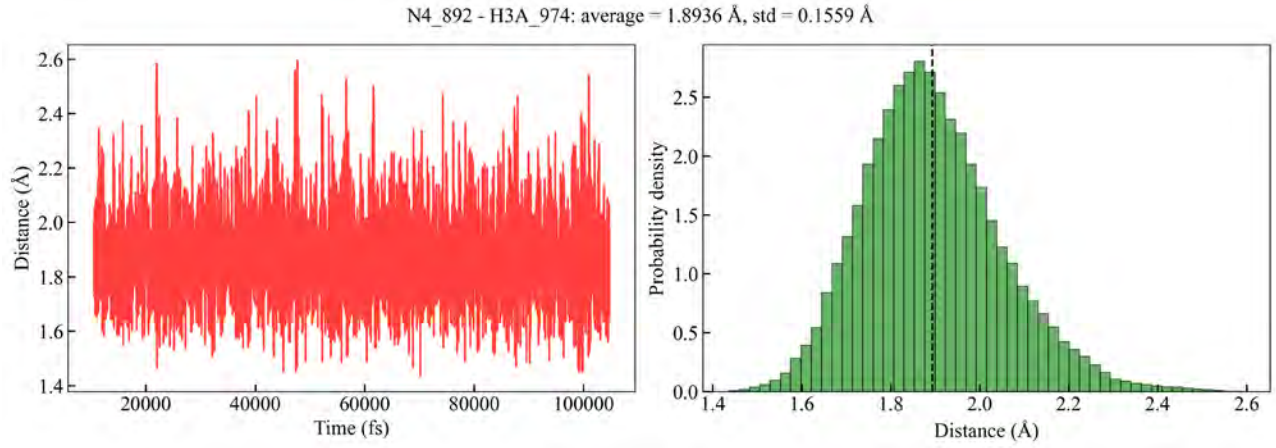
N4_891 - H3A_973

Average distance = 1.9020 Å; standard deviation = 0.1641 Å; number of points = 94257



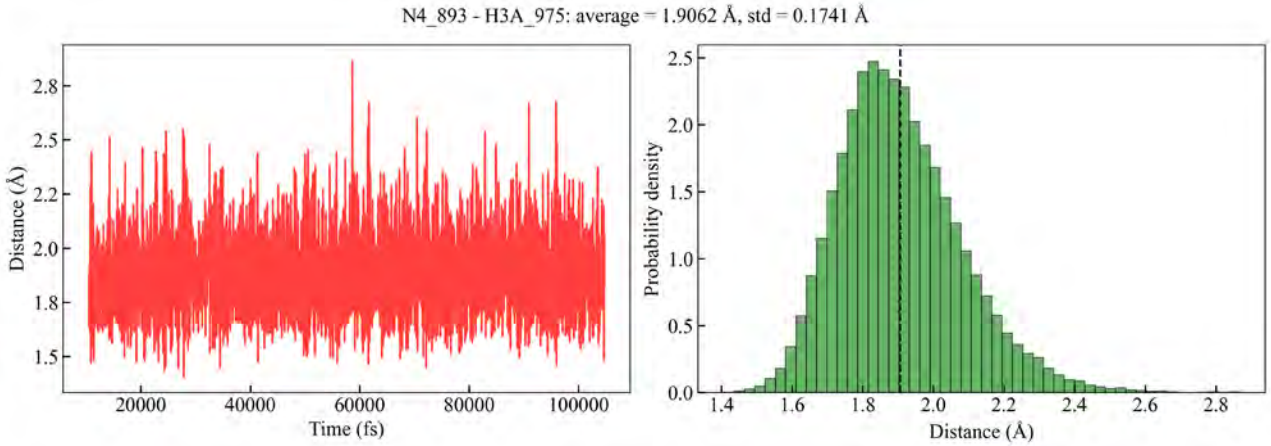
N4_892 - H3A_974

Average distance = 1.8936 Å; standard deviation = 0.1559 Å; number of points = 94257



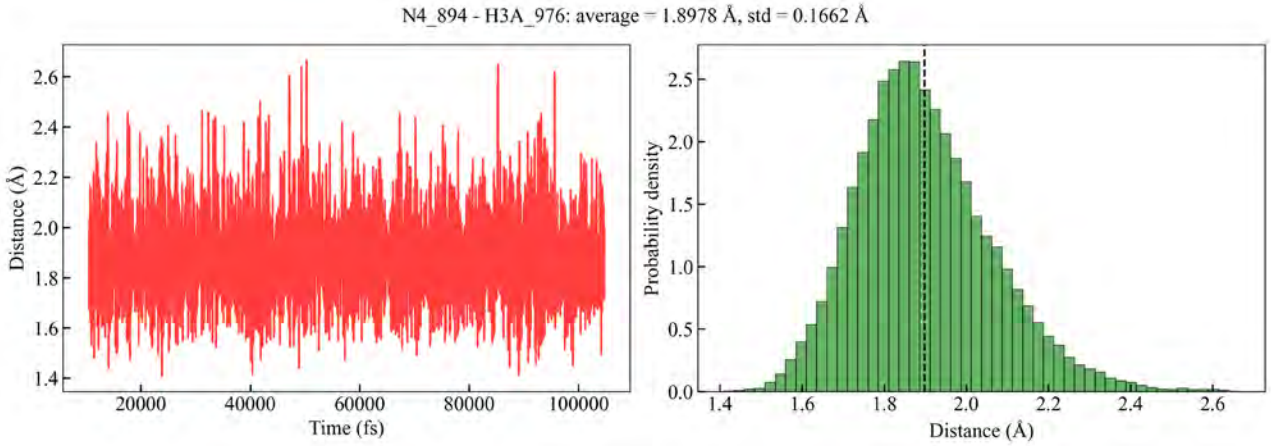
N4_893 - H3A_975

Average distance = 1.9062 Å; standard deviation = 0.1741 Å; number of points = 94257



N4_894 - H3A_976

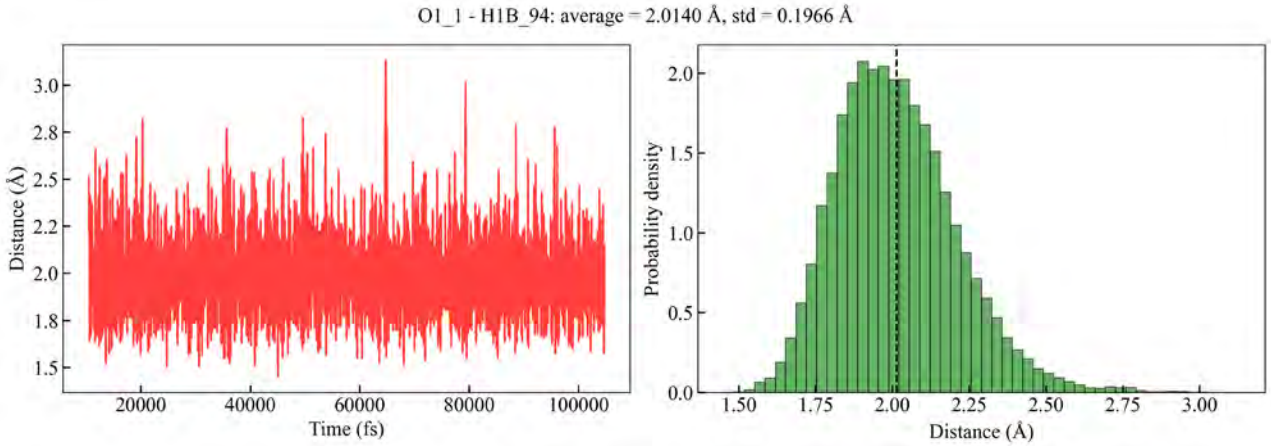
Average distance = 1.8978 Å; standard deviation = 0.1662 Å; number of points = 94257



O1 - H1B

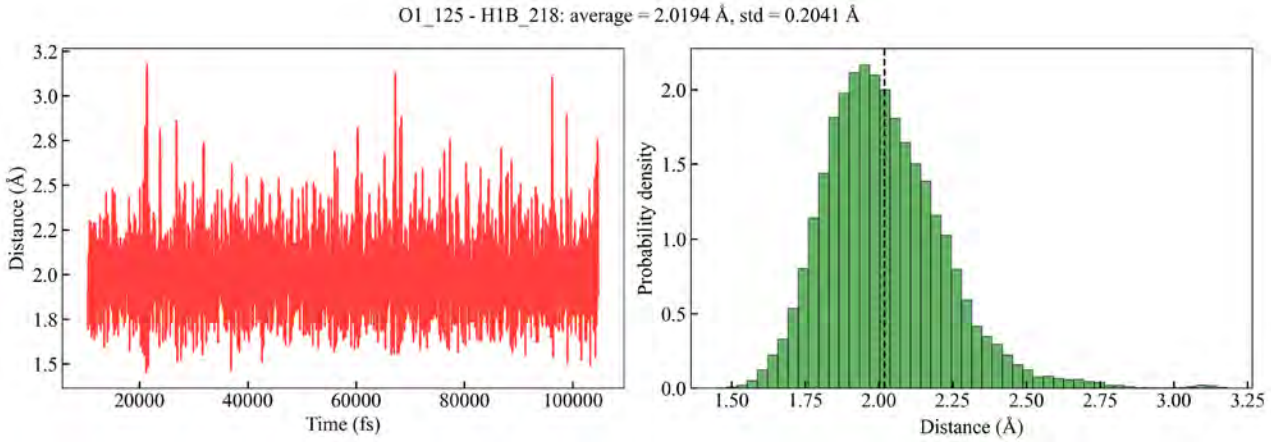
O1_1 - H1B_94

Average distance = 2.0140 Å; standard deviation = 0.1966 Å; number of points = 94257



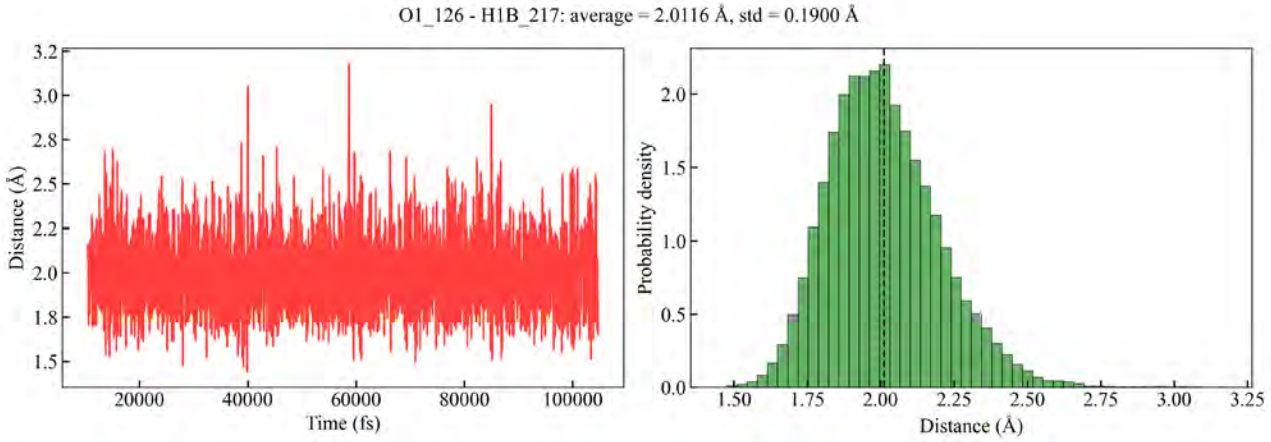
O1_125 - H1B_218

Average distance = 2.0194 Å; standard deviation = 0.2041 Å; number of points = 94257



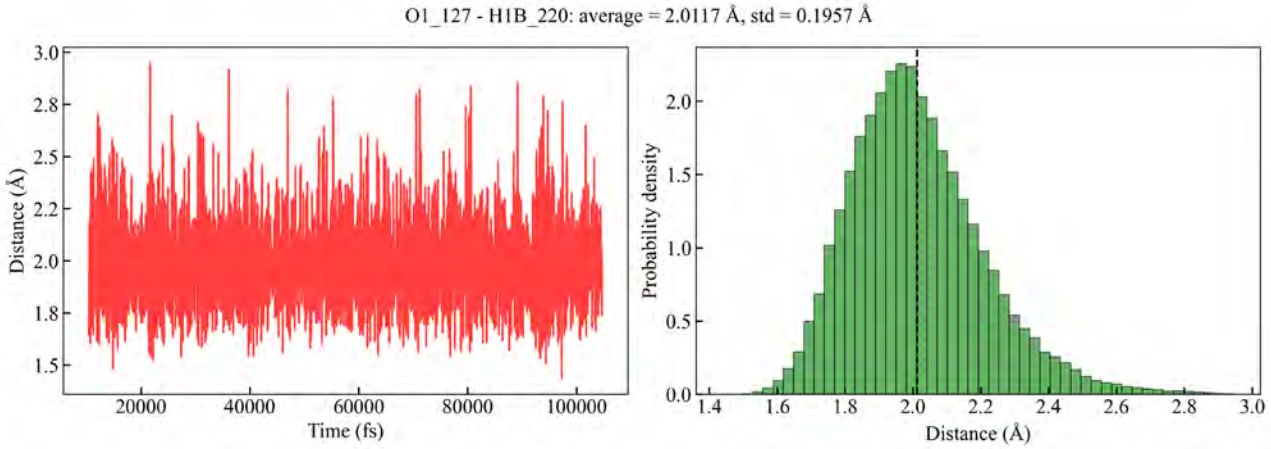
O1_126 - H1B_217

Average distance = 2.0116 Å; standard deviation = 0.1900 Å; number of points = 94257



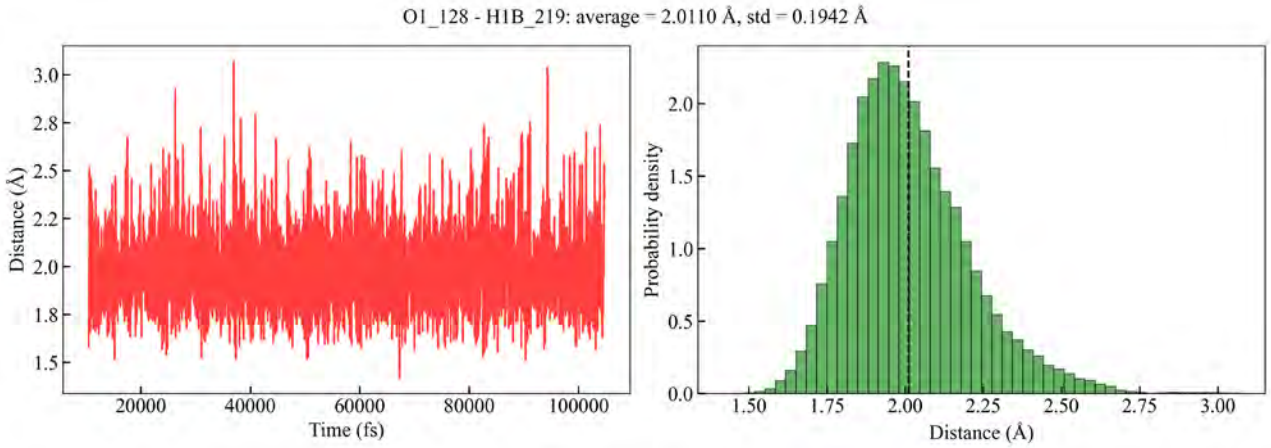
O1_127 - H1B_220

Average distance = 2.0117 Å; standard deviation = 0.1957 Å; number of points = 94257



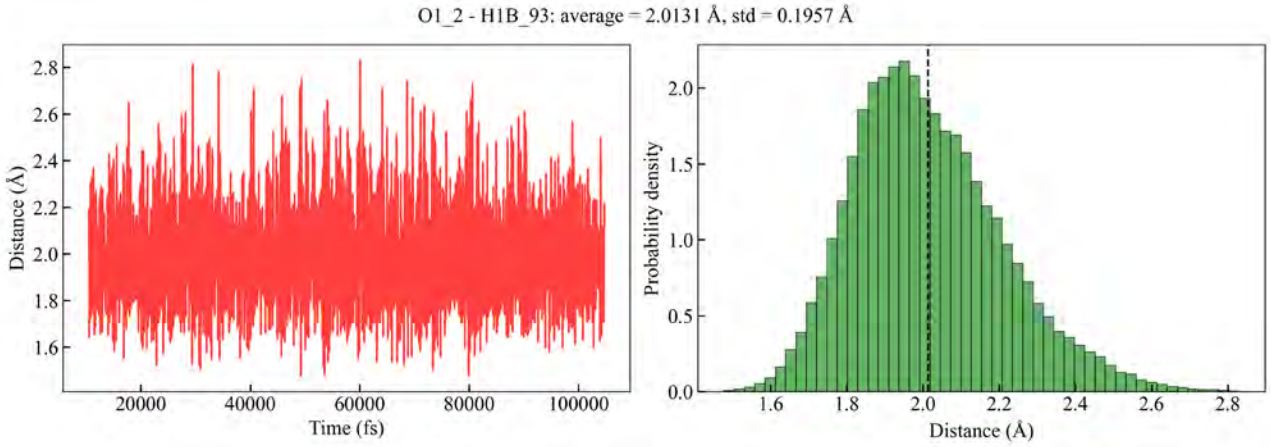
O1_128 - H1B_219

Average distance = 2.0110 Å; standard deviation = 0.1942 Å; number of points = 94257



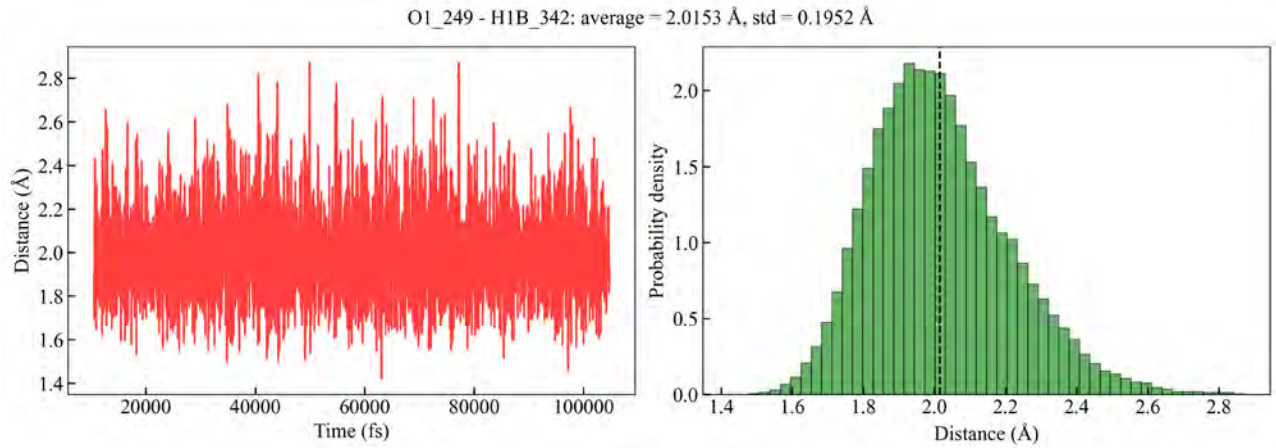
O1_2 - H1B_93

Average distance = 2.0131 Å; standard deviation = 0.1957 Å; number of points = 94257



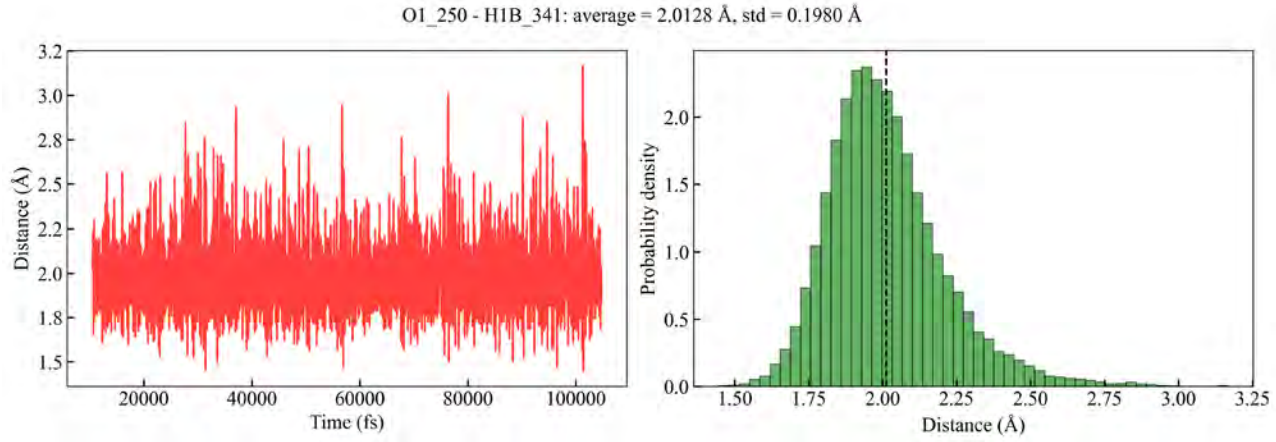
O1_249 - H1B_342

Average distance = 2.0153 Å; standard deviation = 0.1952 Å; number of points = 94257



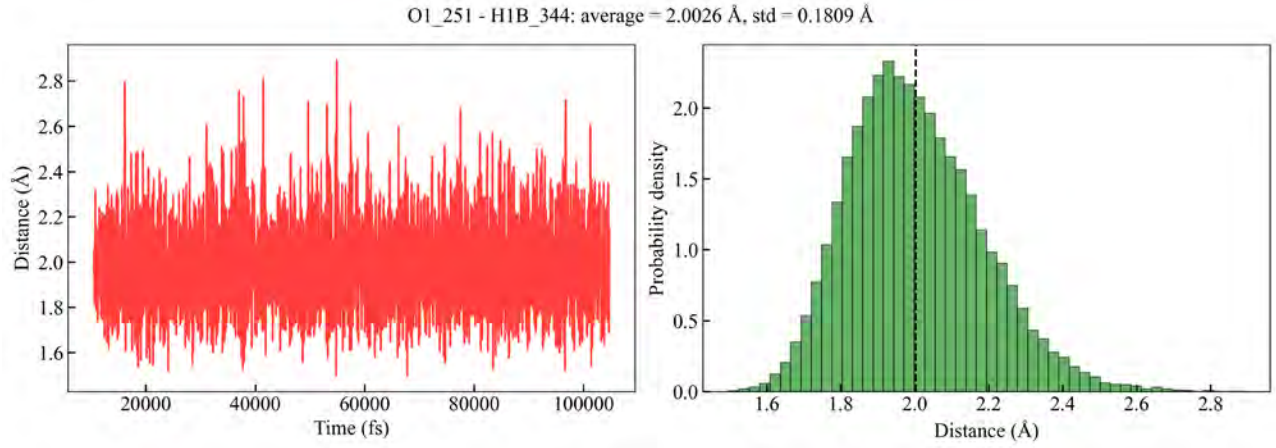
O1_250 - H1B_341

Average distance = 2.0128 Å; standard deviation = 0.1980 Å; number of points = 94257



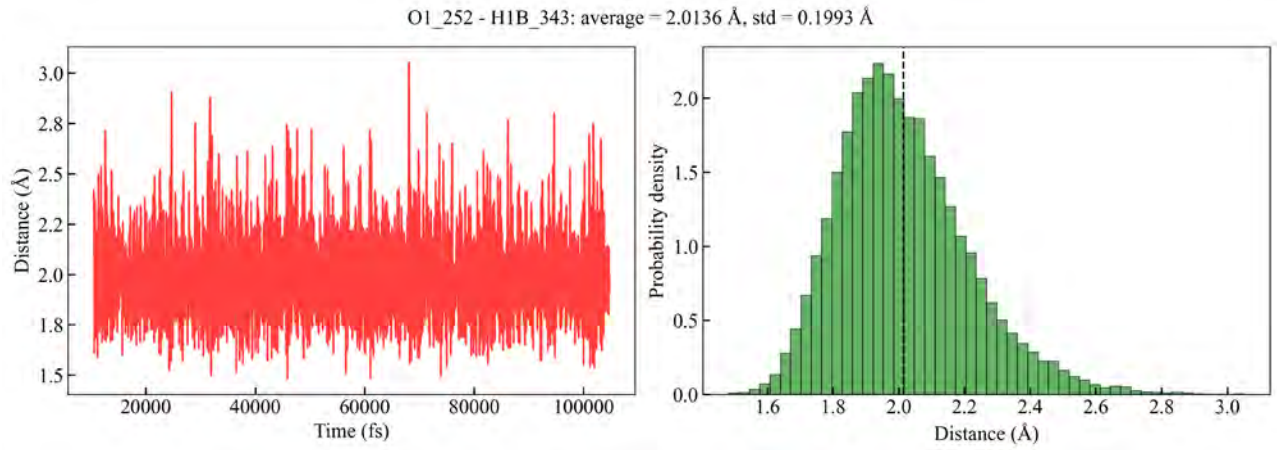
O1_251 - H1B_344

Average distance = 2.0026 Å; standard deviation = 0.1809 Å; number of points = 94257



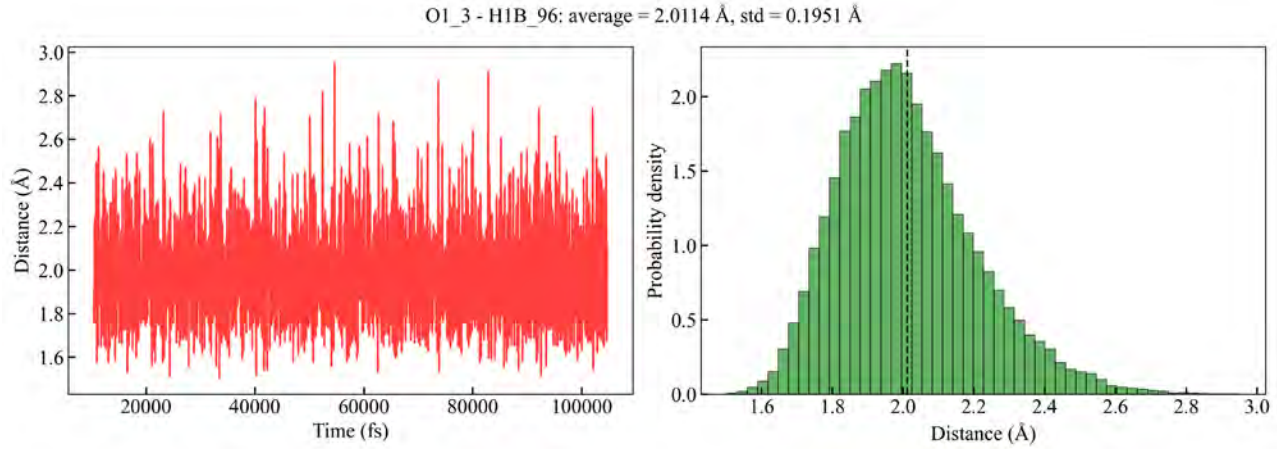
O1_252 - H1B_343

Average distance = 2.0136 Å; standard deviation = 0.1993 Å; number of points = 94257



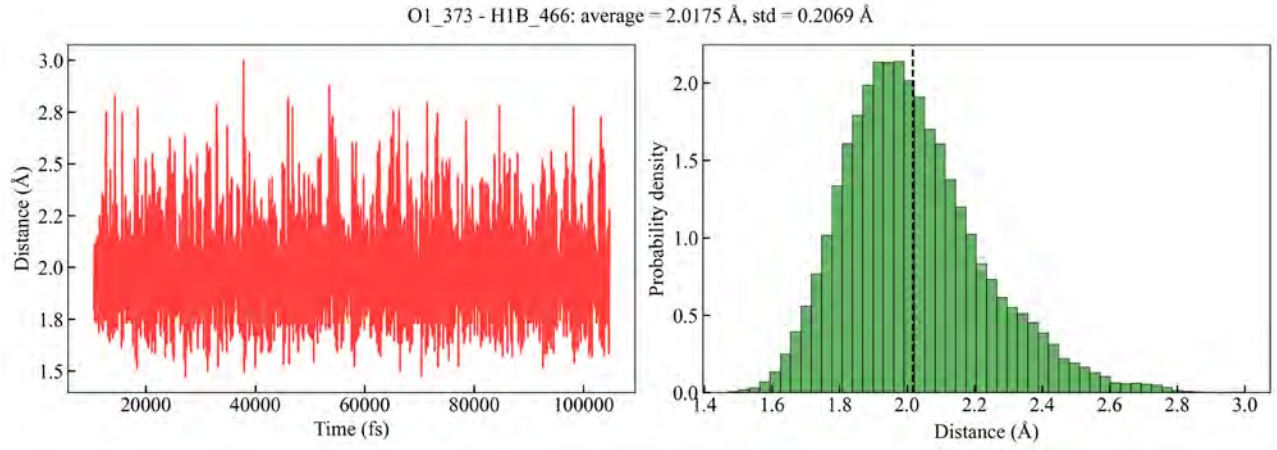
O1_3 - H1B_96

Average distance = 2.0114 Å; standard deviation = 0.1951 Å; number of points = 94257



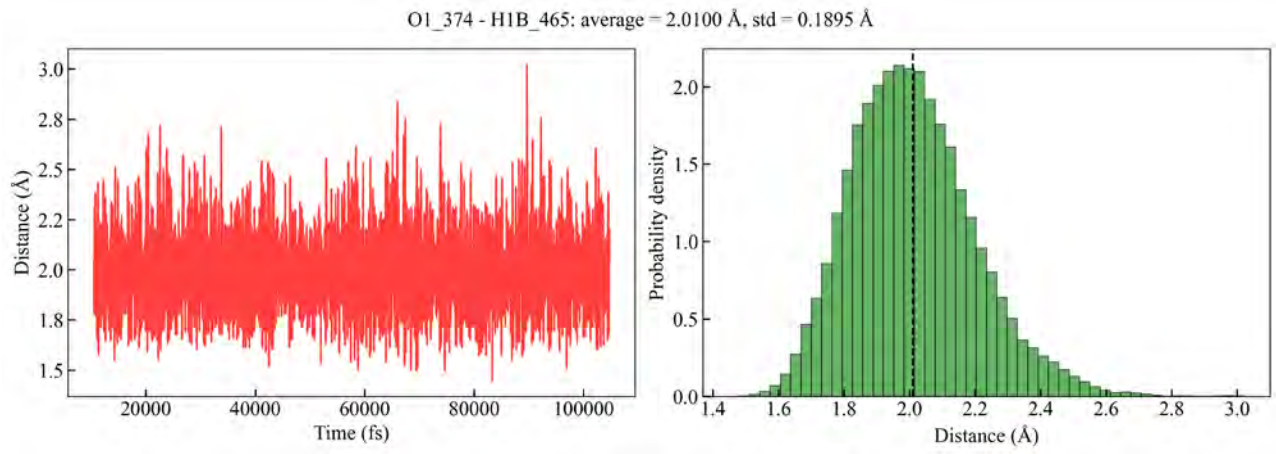
O1_373 - H1B_466

Average distance = 2.0175 Å; standard deviation = 0.2069 Å; number of points = 94257



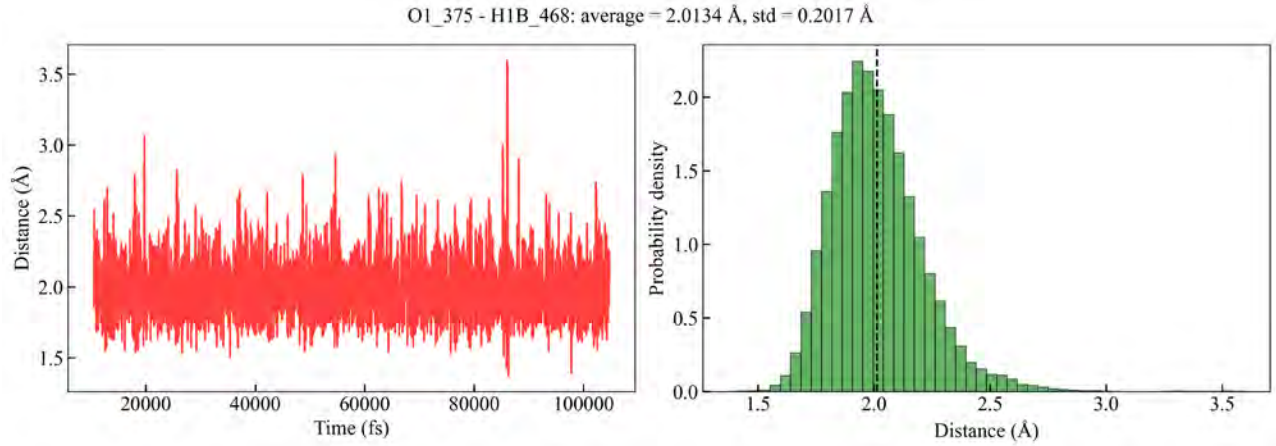
O1_374 - H1B_465

Average distance = 2.0100 Å; standard deviation = 0.1895 Å; number of points = 94257



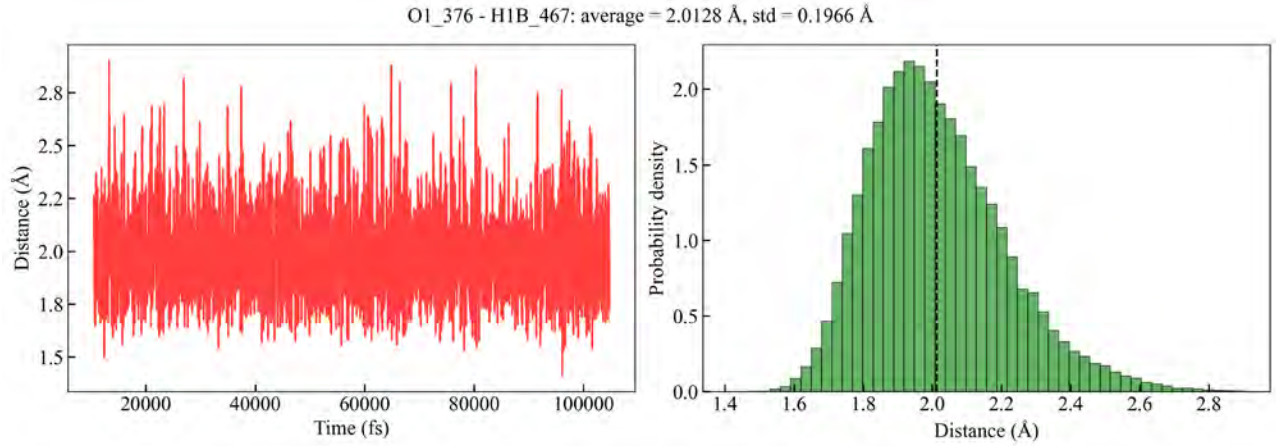
O1_375 - H1B_468

Average distance = 2.0134 Å; standard deviation = 0.2017 Å; number of points = 94257



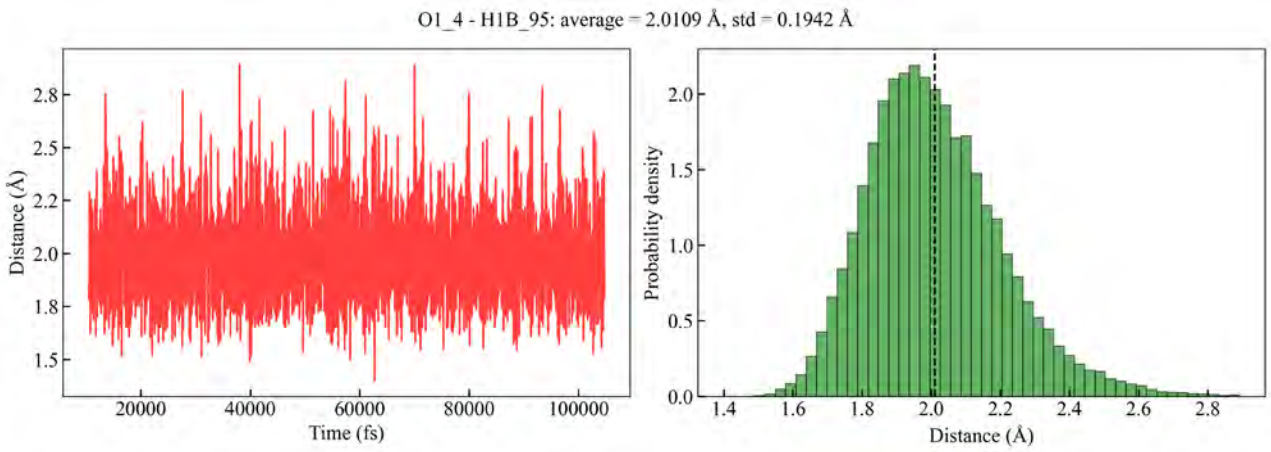
O1_376 - H1B_467

Average distance = 2.0128 Å; standard deviation = 0.1966 Å; number of points = 94257



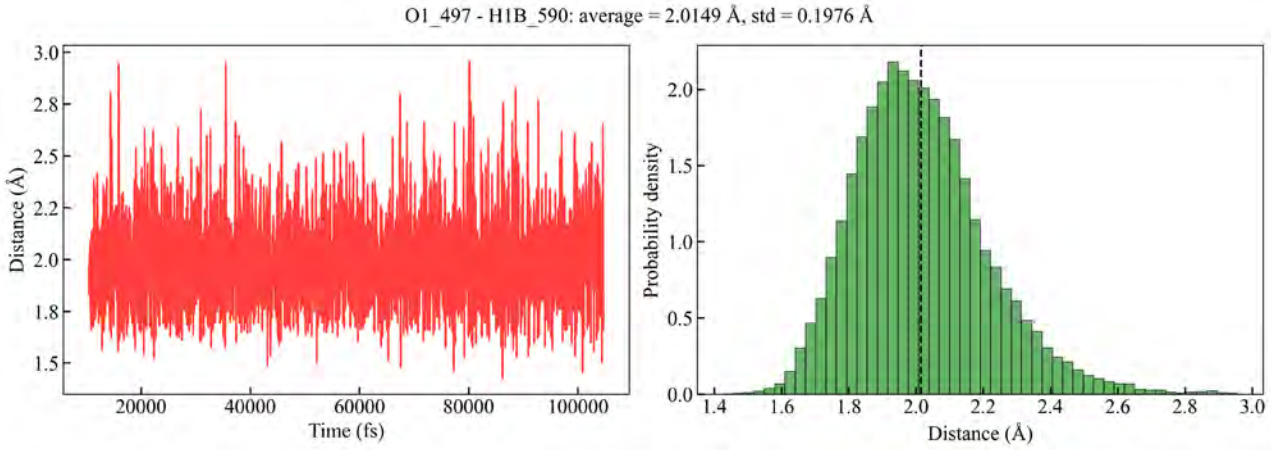
O1_4 - H1B_95

Average distance = 2.0109 Å; standard deviation = 0.1942 Å; number of points = 94257



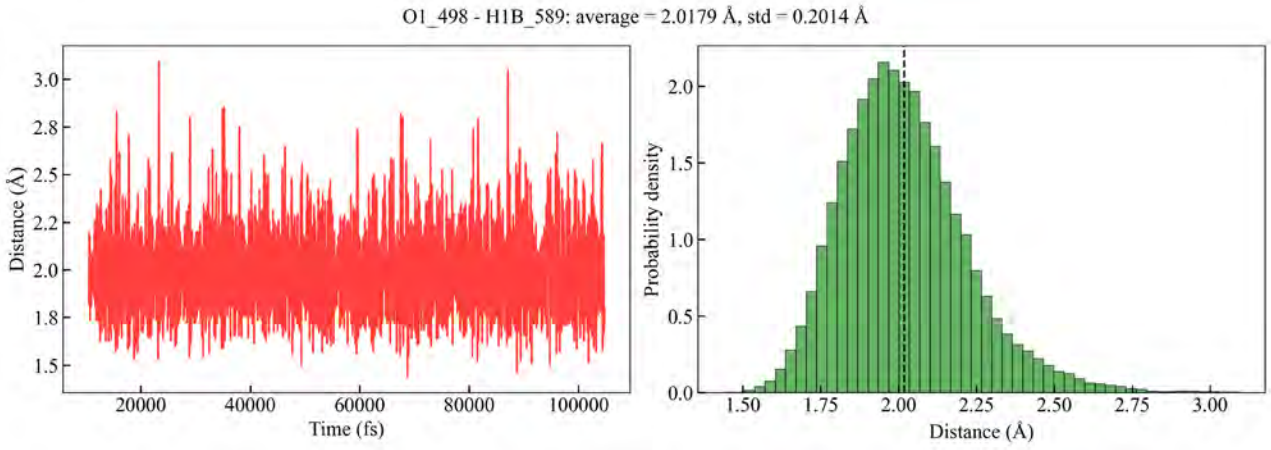
O1_497 - H1B_590

Average distance = 2.0149 Å; standard deviation = 0.1976 Å; number of points = 94257



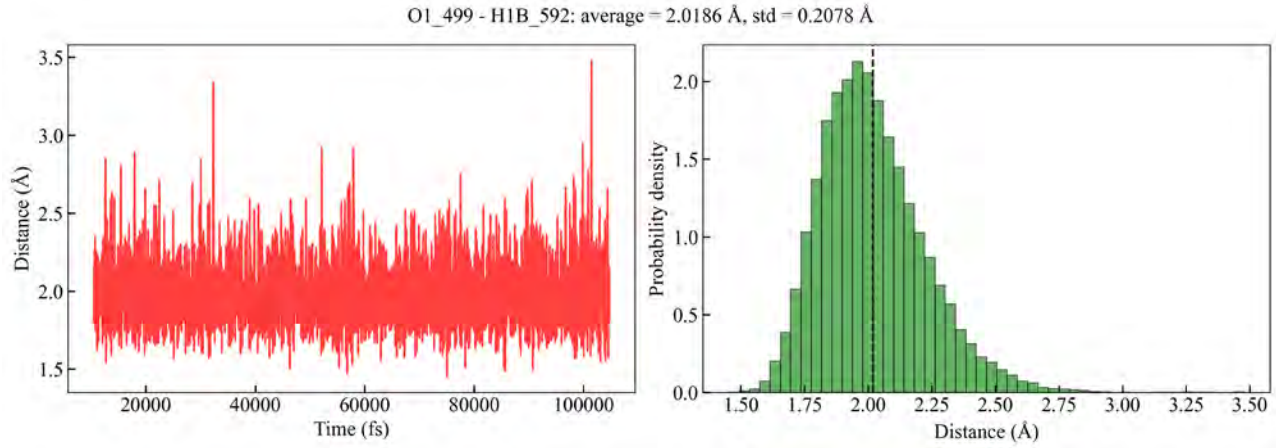
O1_498 - H1B_589

Average distance = 2.0179 Å; standard deviation = 0.2014 Å; number of points = 94257



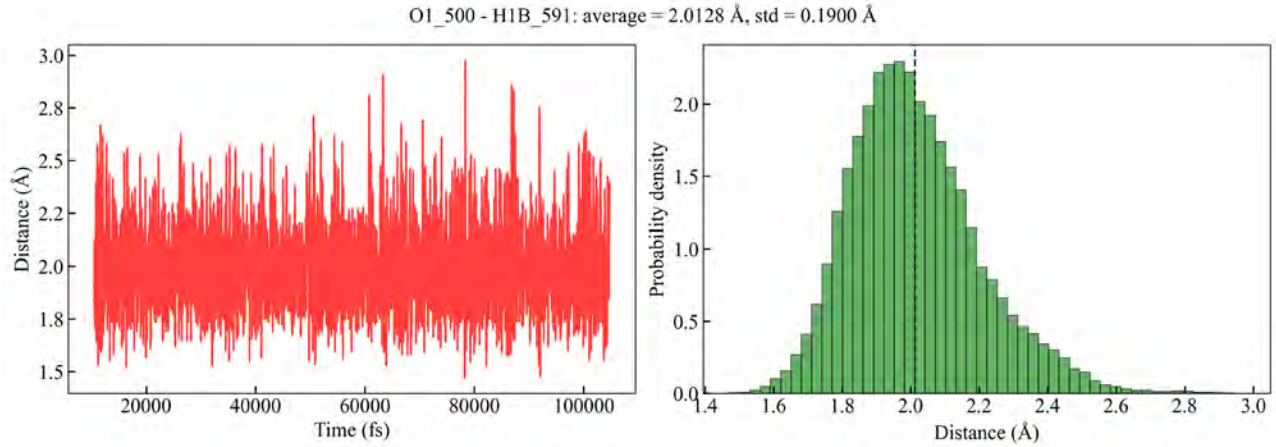
O1_499 - H1B_592

Average distance = 2.0186 Å; standard deviation = 0.2078 Å; number of points = 94257



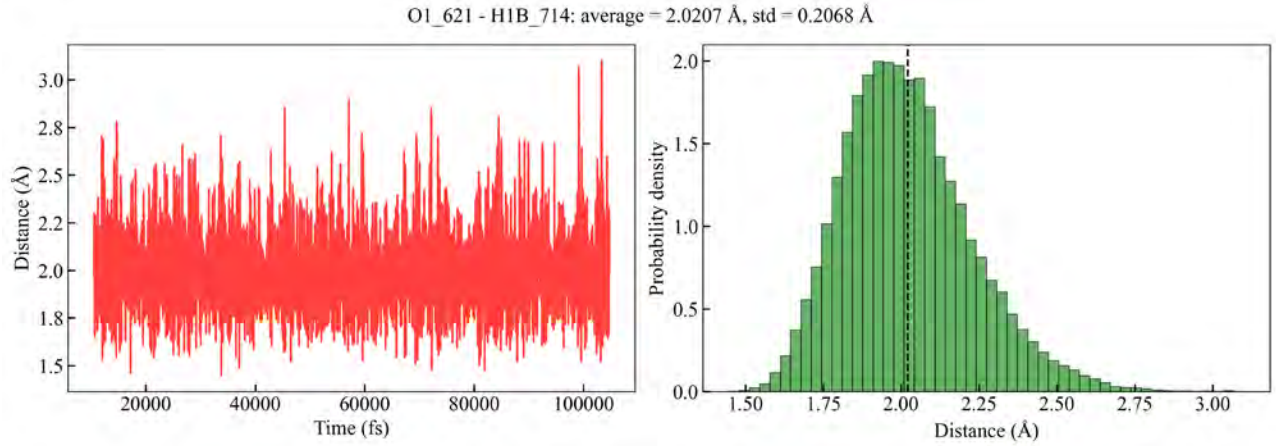
O1_500 - H1B_591

Average distance = 2.0128 Å; standard deviation = 0.1900 Å; number of points = 94257



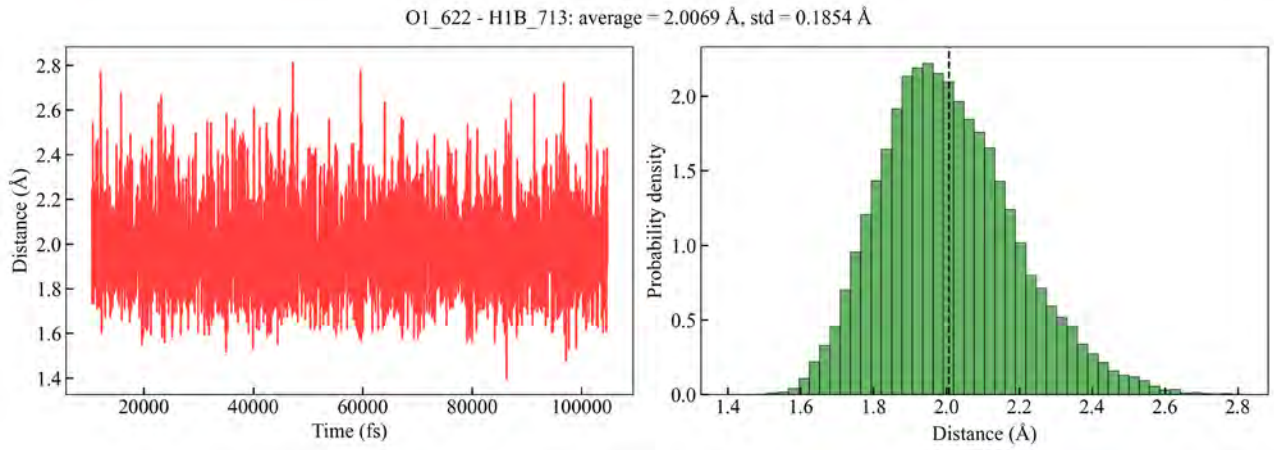
O1_621 - H1B_714

Average distance = 2.0207 Å; standard deviation = 0.2068 Å; number of points = 94257



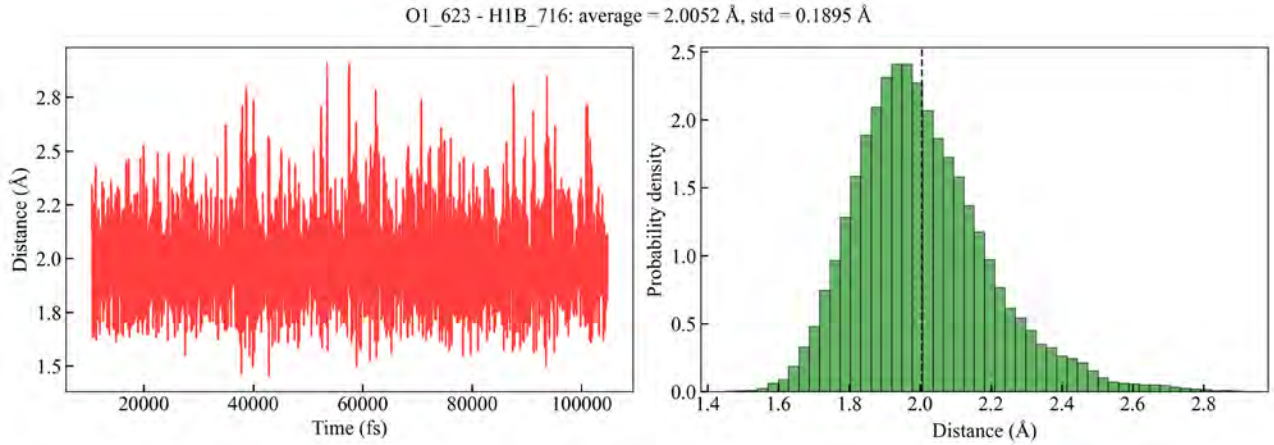
O1_622 - H1B_713

Average distance = 2.0069 Å; standard deviation = 0.1854 Å; number of points = 94257



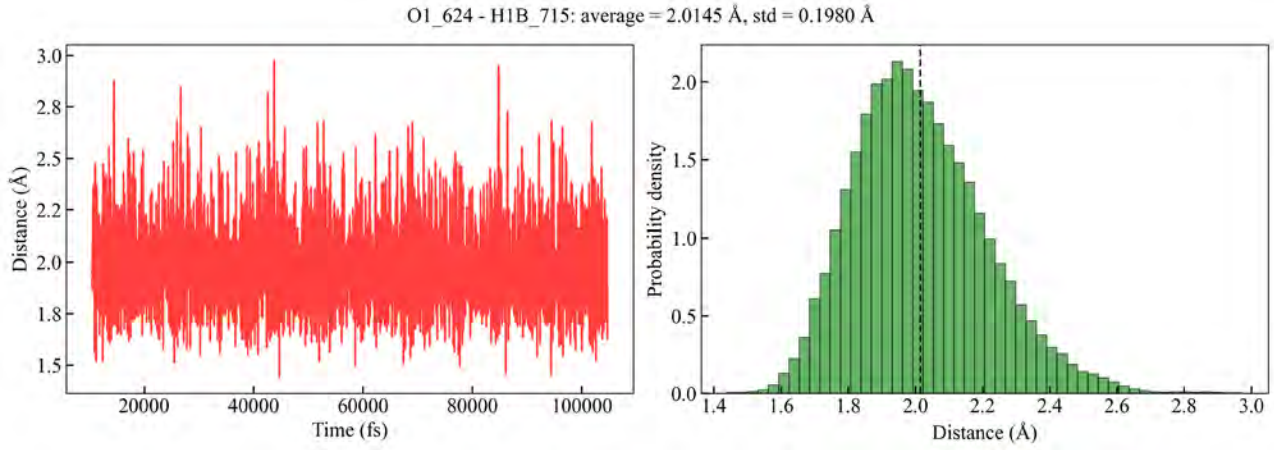
O1_623 - H1B_716

Average distance = 2.0052 Å; standard deviation = 0.1895 Å; number of points = 94257



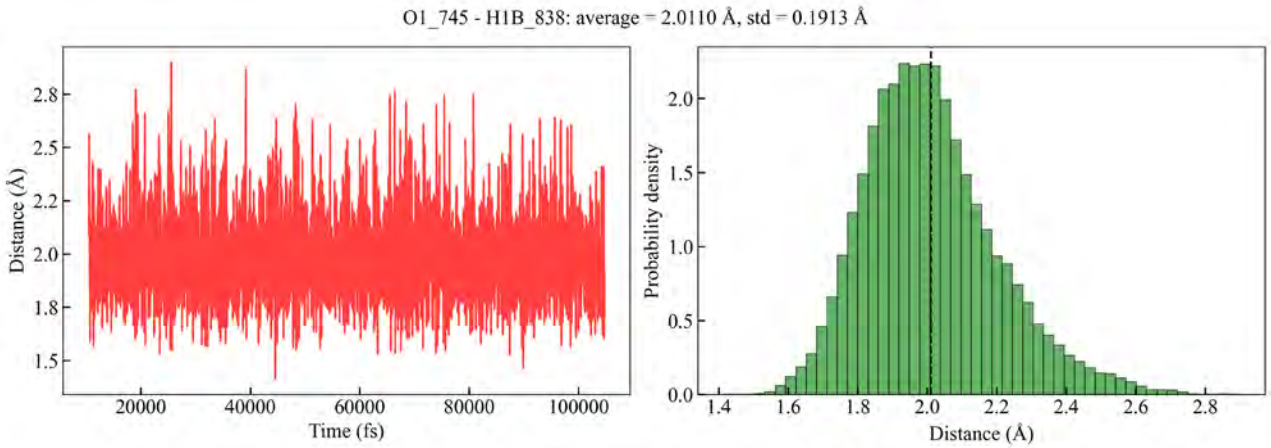
O1_624 - H1B_715

Average distance = 2.0145 Å; standard deviation = 0.1980 Å; number of points = 94257



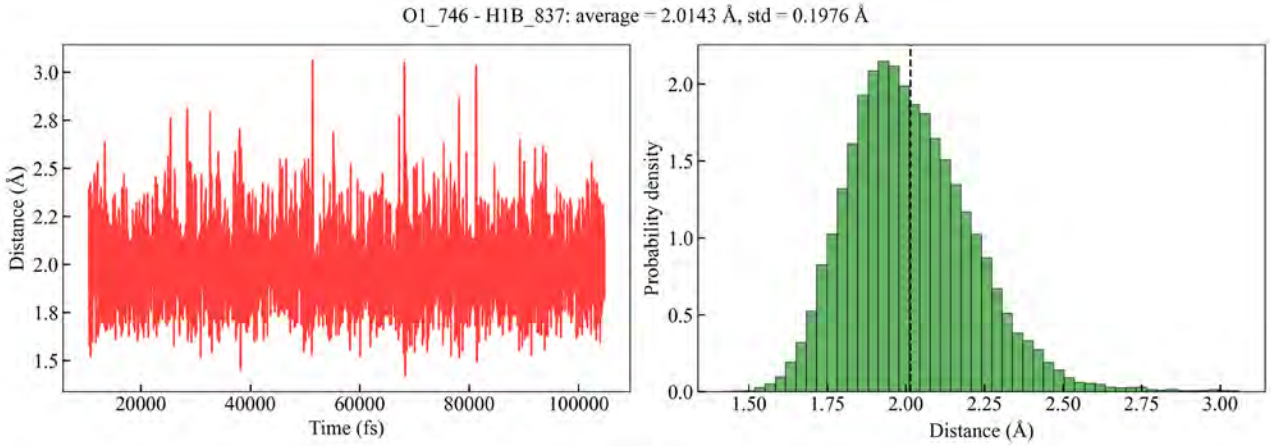
O1_745 - H1B_838

Average distance = 2.0110 Å; standard deviation = 0.1913 Å; number of points = 94257



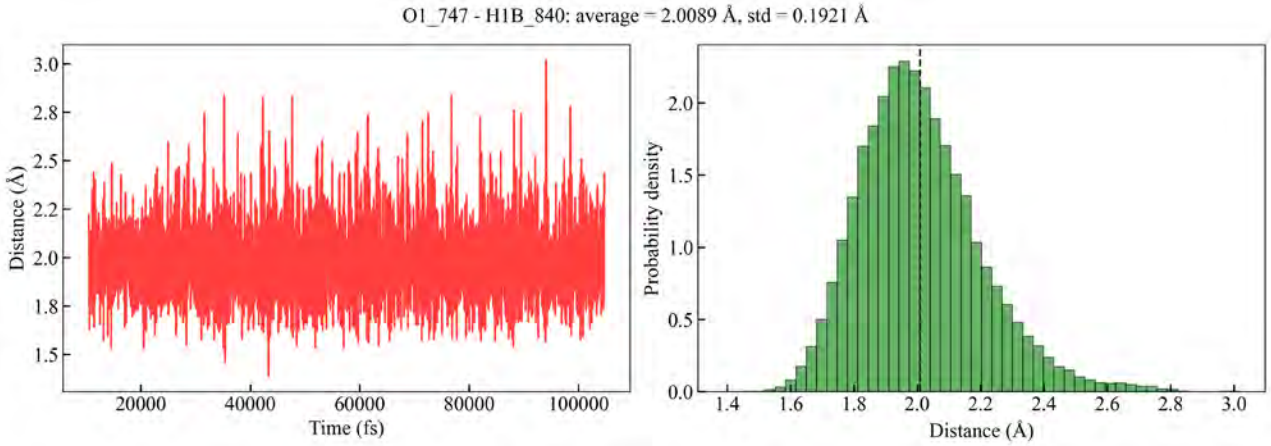
O1_746 - H1B_837

Average distance = 2.0143 Å; standard deviation = 0.1976 Å; number of points = 94257



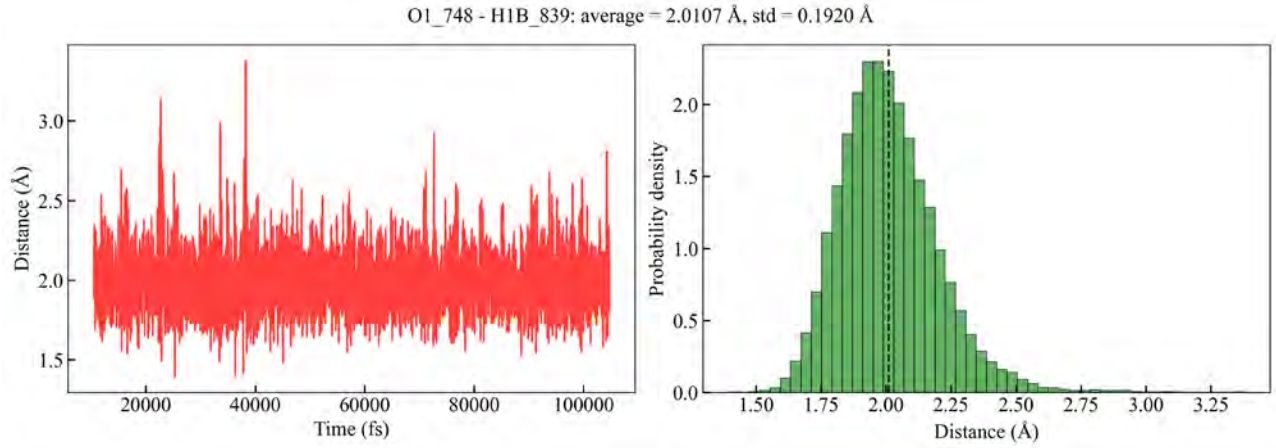
O1_747 - H1B_840

Average distance = 2.0089 Å; standard deviation = 0.1921 Å; number of points = 94257



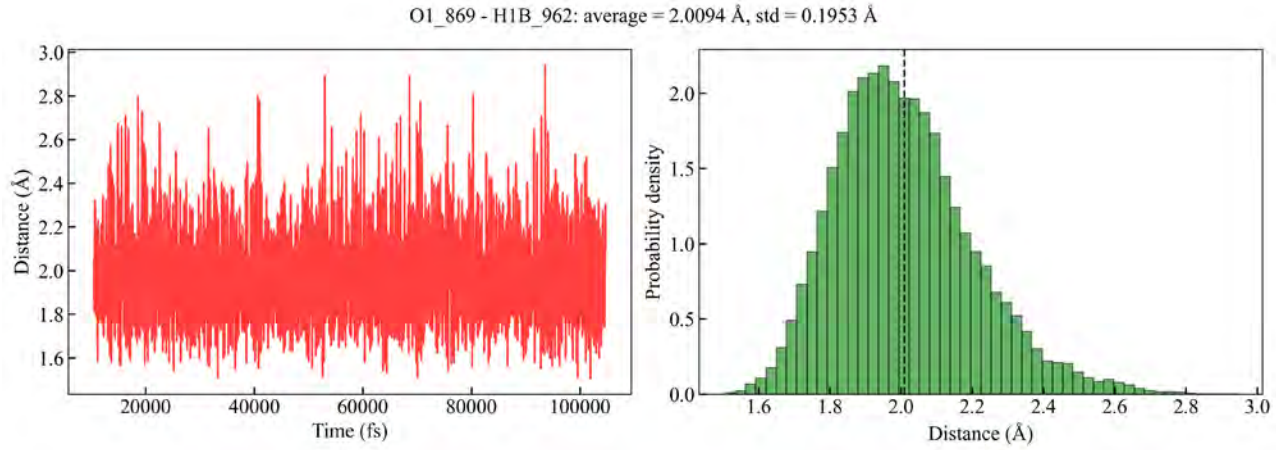
O1_748 - H1B_839

Average distance = 2.0107 Å; standard deviation = 0.1920 Å; number of points = 94257



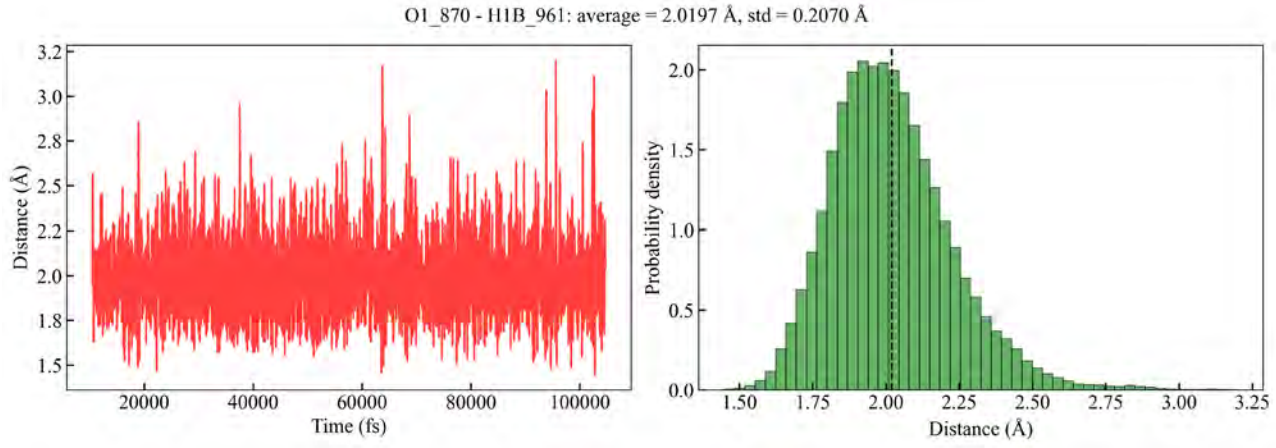
O1_869 - H1B_962

Average distance = 2.0094 Å; standard deviation = 0.1953 Å; number of points = 94257



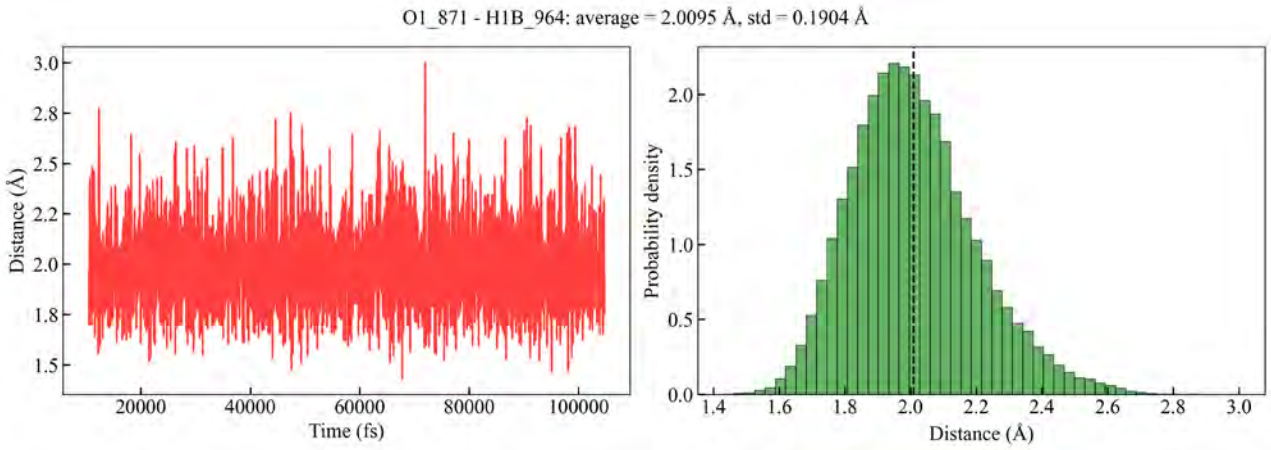
O1_870 - H1B_961

Average distance = 2.0197 Å; standard deviation = 0.2070 Å; number of points = 94257



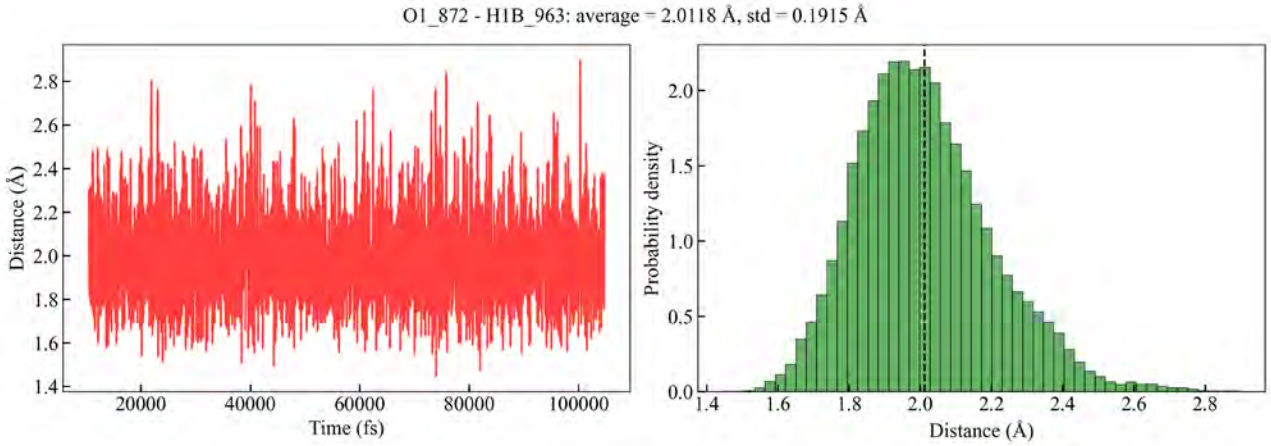
O1_871 - H1B_964

Average distance = 2.0095 Å; standard deviation = 0.1904 Å; number of points = 94257



O1_872 - H1B_963

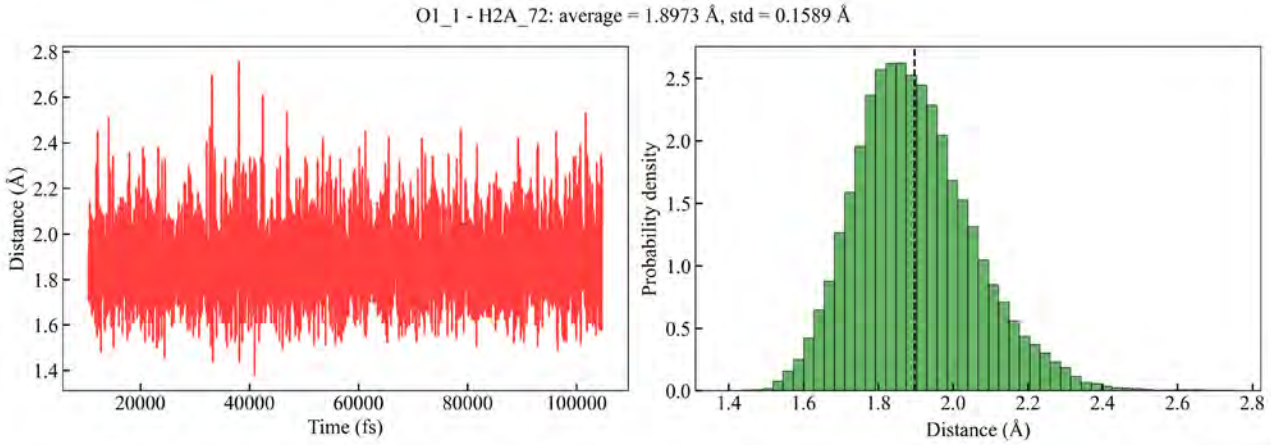
Average distance = 2.0118 Å; standard deviation = 0.1915 Å; number of points = 94257



O1 - H2A

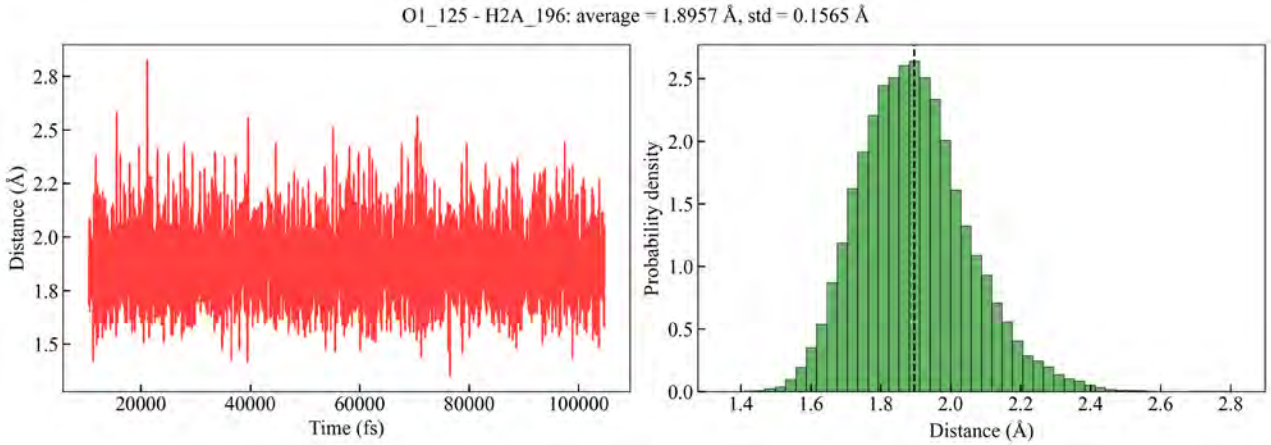
O1_1 - H2A_72

Average distance = 1.8973 Å; standard deviation = 0.1589 Å; number of points = 94257



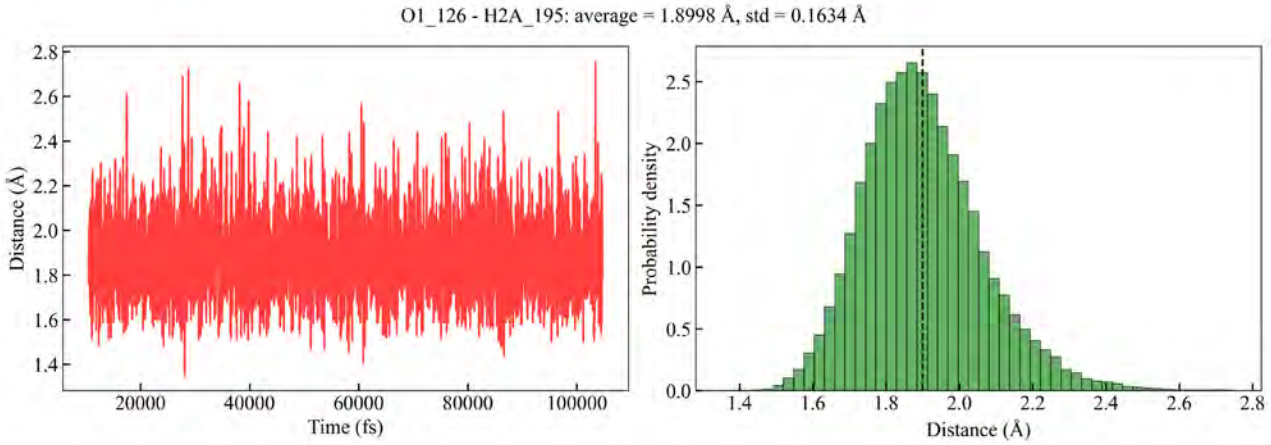
O1_125 - H2A_196

Average distance = 1.8957 Å; standard deviation = 0.1565 Å; number of points = 94257



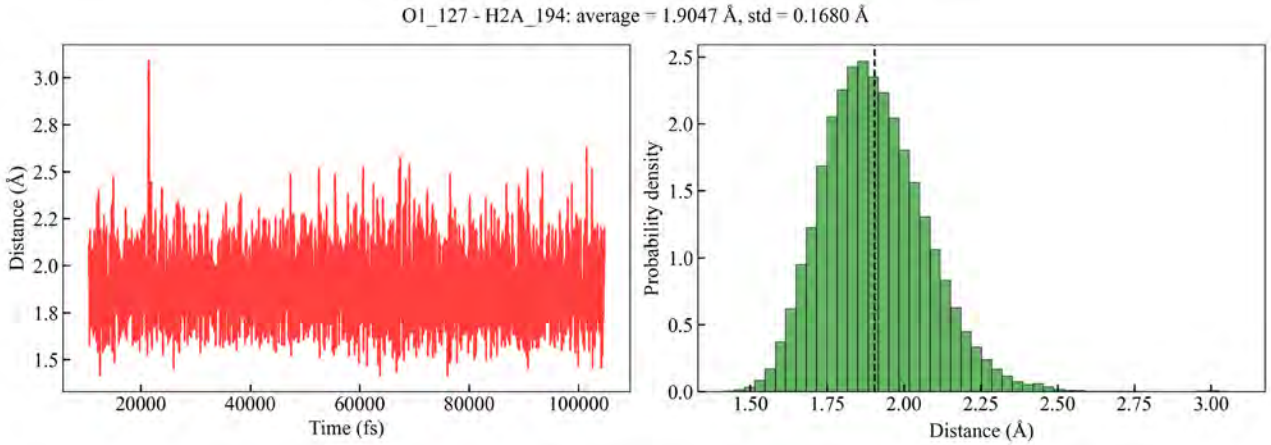
O1_126 - H2A_195

Average distance = 1.8998 Å; standard deviation = 0.1634 Å; number of points = 94257



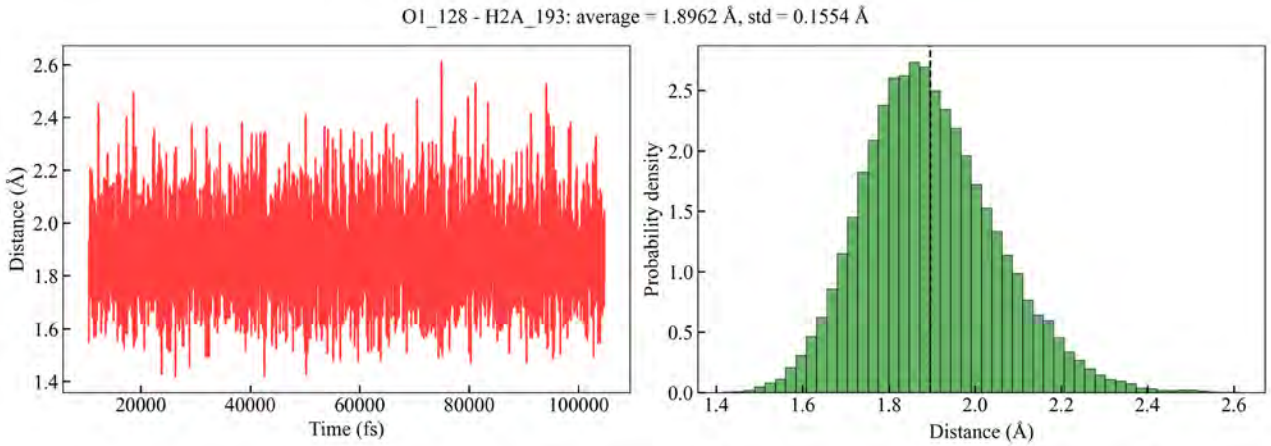
O1_127 - H2A_194

Average distance = 1.9047 Å; standard deviation = 0.1680 Å; number of points = 94257



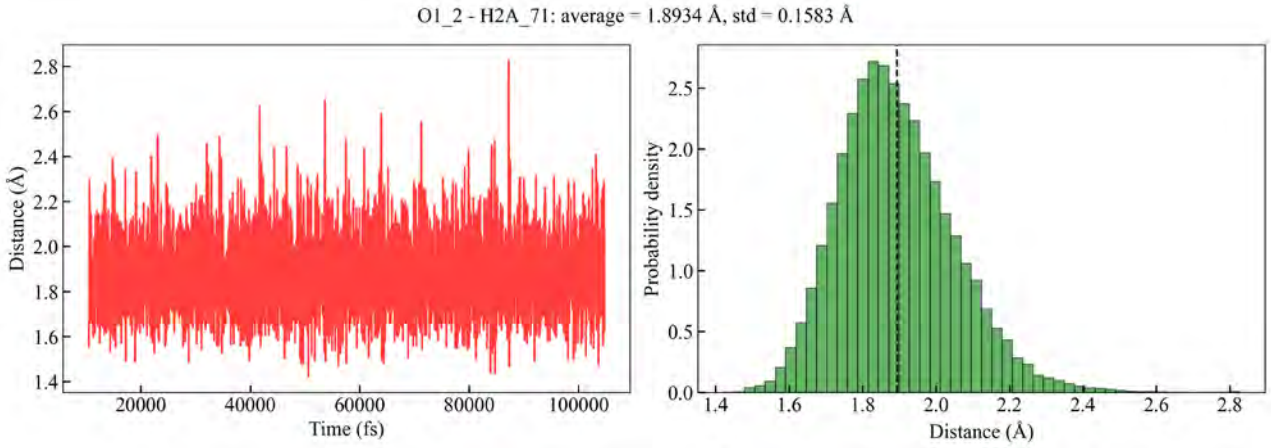
O1_128 - H2A_193

Average distance = 1.8962 Å; standard deviation = 0.1554 Å; number of points = 94257



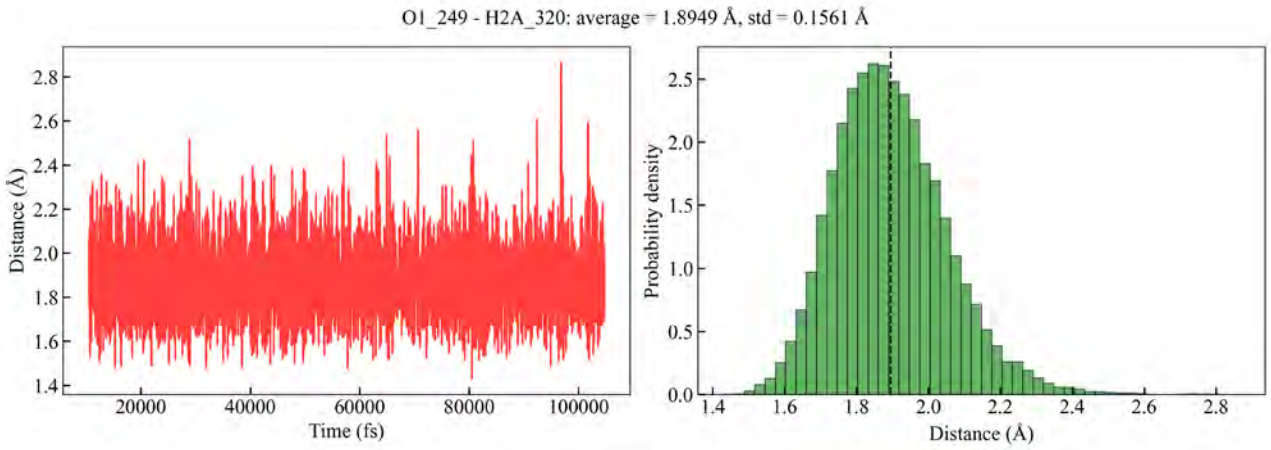
O1_2 - H2A_71

Average distance = 1.8934 Å; standard deviation = 0.1583 Å; number of points = 94257



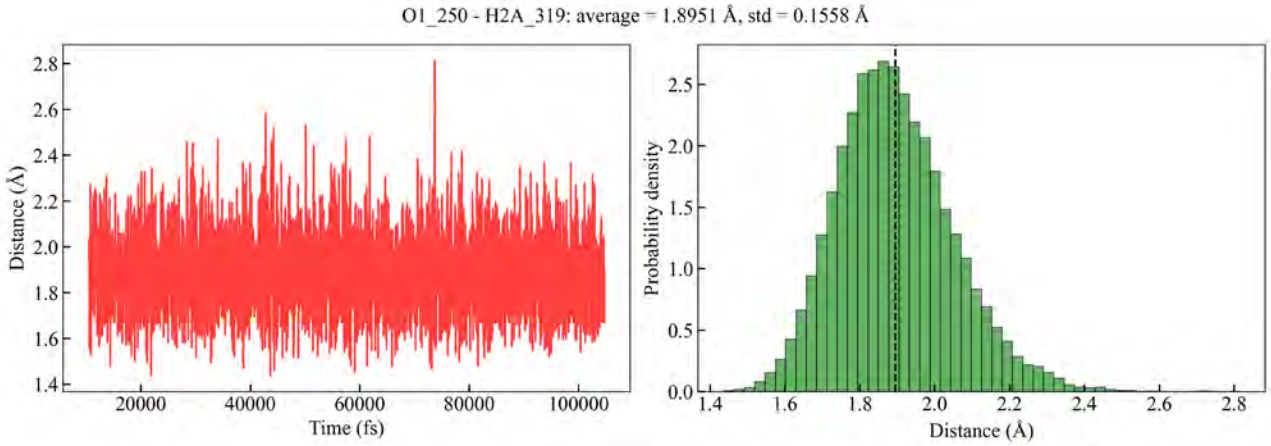
O1_249 - H2A_320

Average distance = 1.8949 Å; standard deviation = 0.1561 Å; number of points = 94257



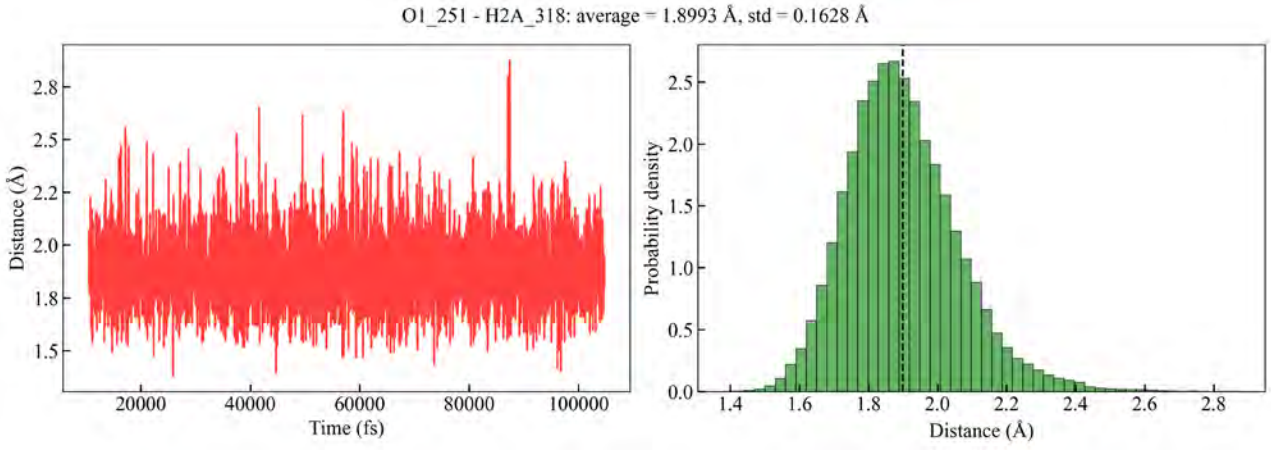
O1_250 - H2A_319

Average distance = 1.8951 Å; standard deviation = 0.1558 Å; number of points = 94257



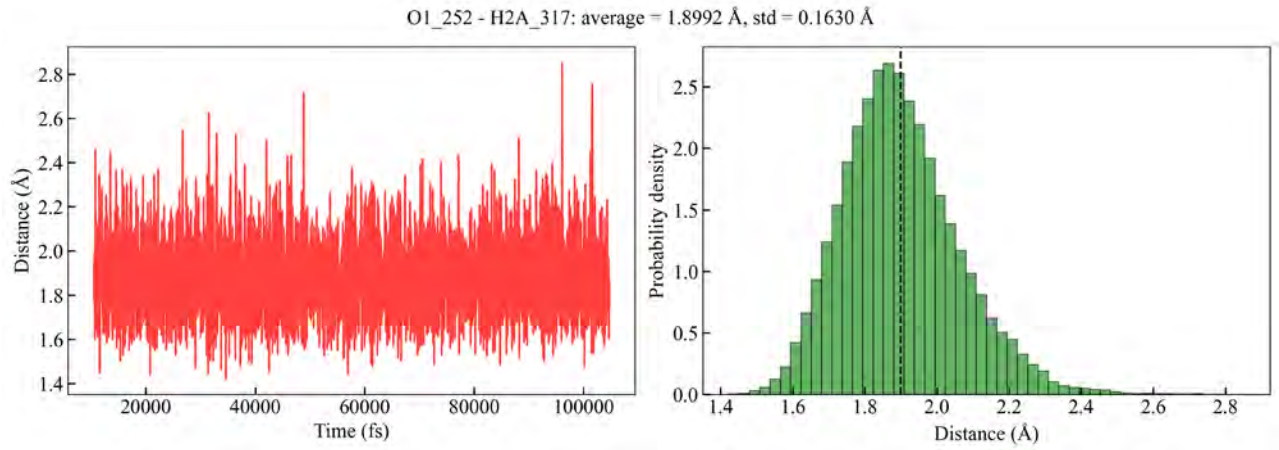
O1_251 - H2A_318

Average distance = 1.8993 Å; standard deviation = 0.1628 Å; number of points = 94257



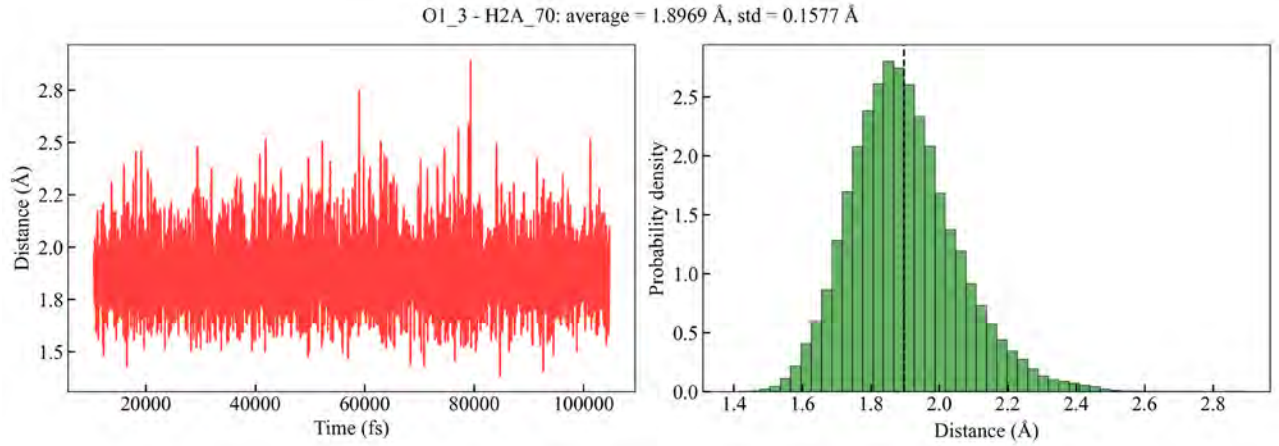
O1_252 - H2A_317

Average distance = 1.8992 Å; standard deviation = 0.1630 Å; number of points = 94257



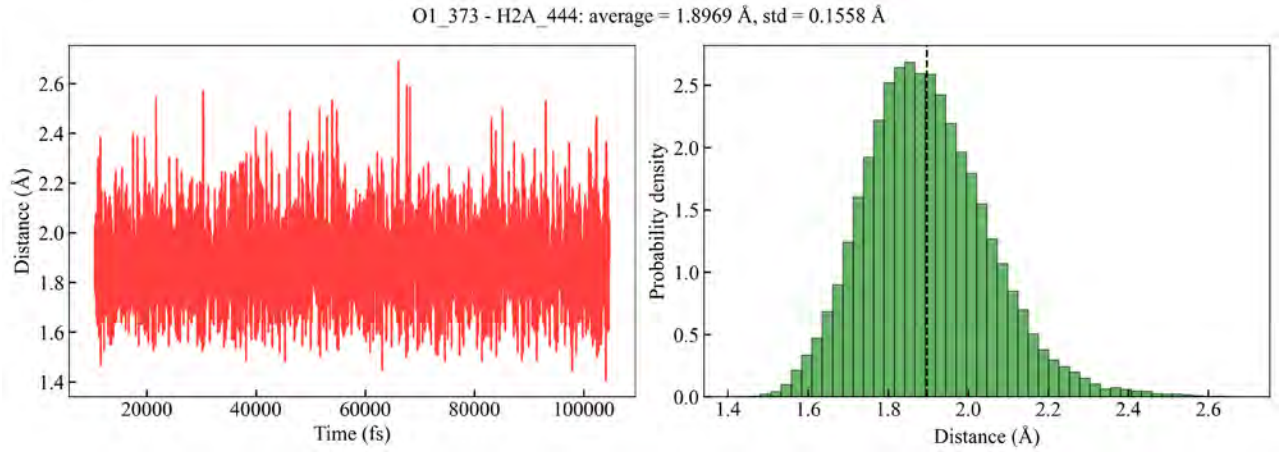
O1_3 - H2A_70

Average distance = 1.8969 Å; standard deviation = 0.1577 Å; number of points = 94257



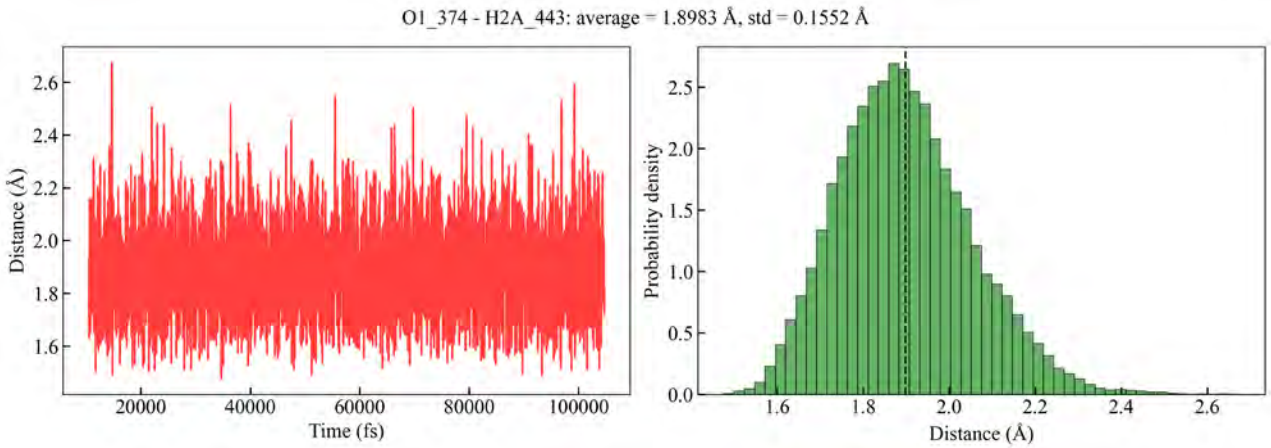
O1_373 - H2A_444

Average distance = 1.8969 Å; standard deviation = 0.1558 Å; number of points = 94257



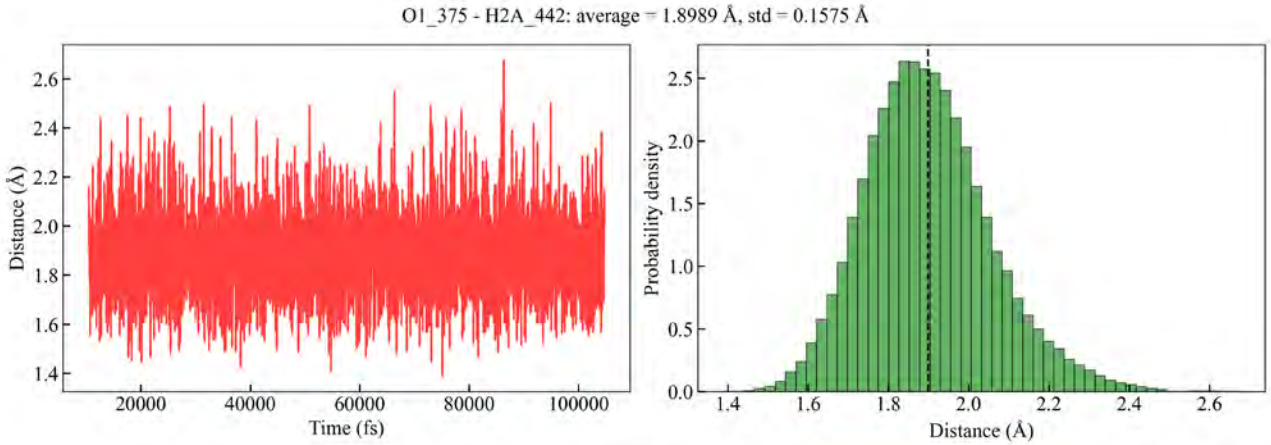
O1_374 - H2A_443

Average distance = 1.8983 Å; standard deviation = 0.1552 Å; number of points = 94257



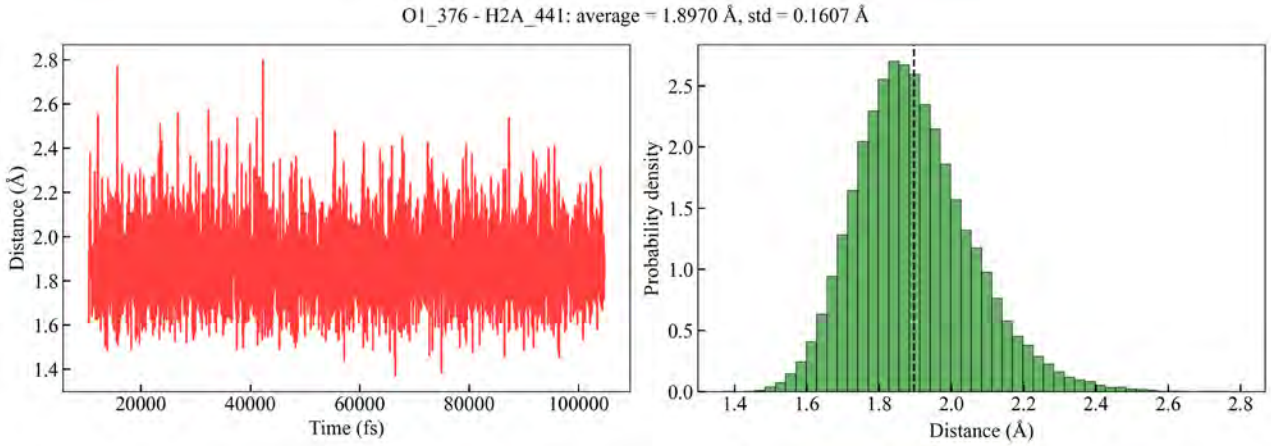
O1_375 - H2A_442

Average distance = 1.8989 Å; standard deviation = 0.1575 Å; number of points = 94257



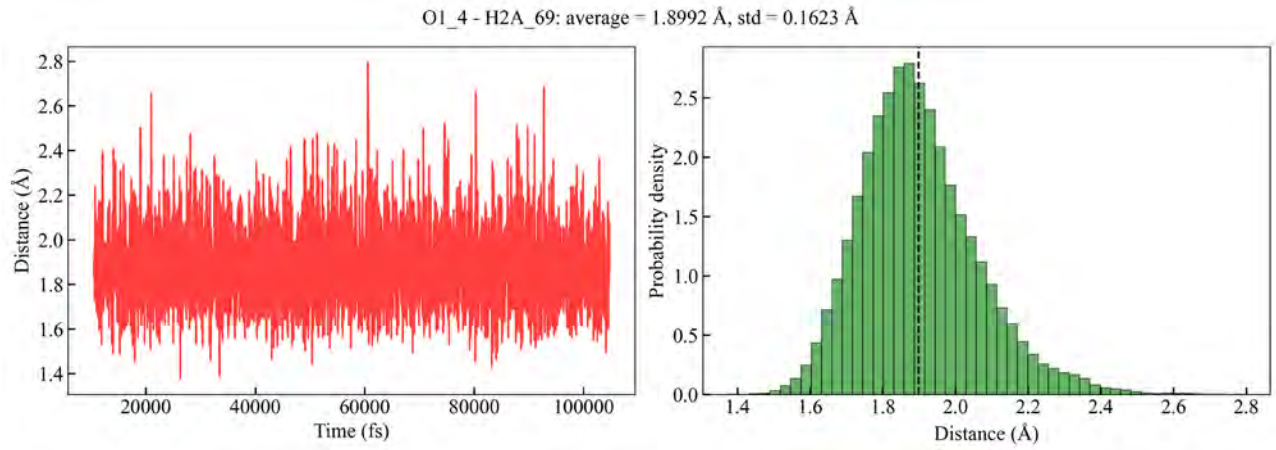
O1_376 - H2A_441

Average distance = 1.8970 Å; standard deviation = 0.1607 Å; number of points = 94257



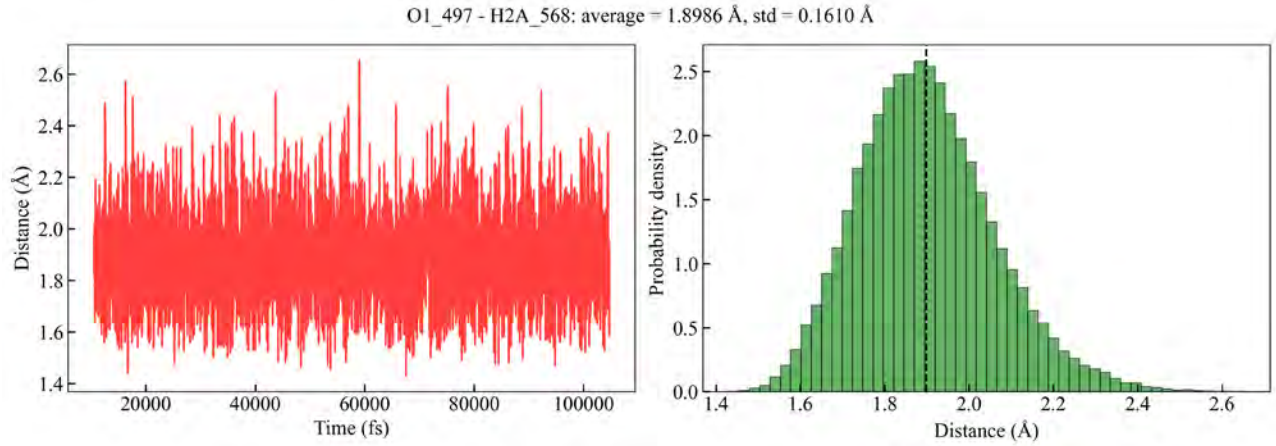
O1_4 - H2A_69

Average distance = 1.8992 Å; standard deviation = 0.1623 Å; number of points = 94257



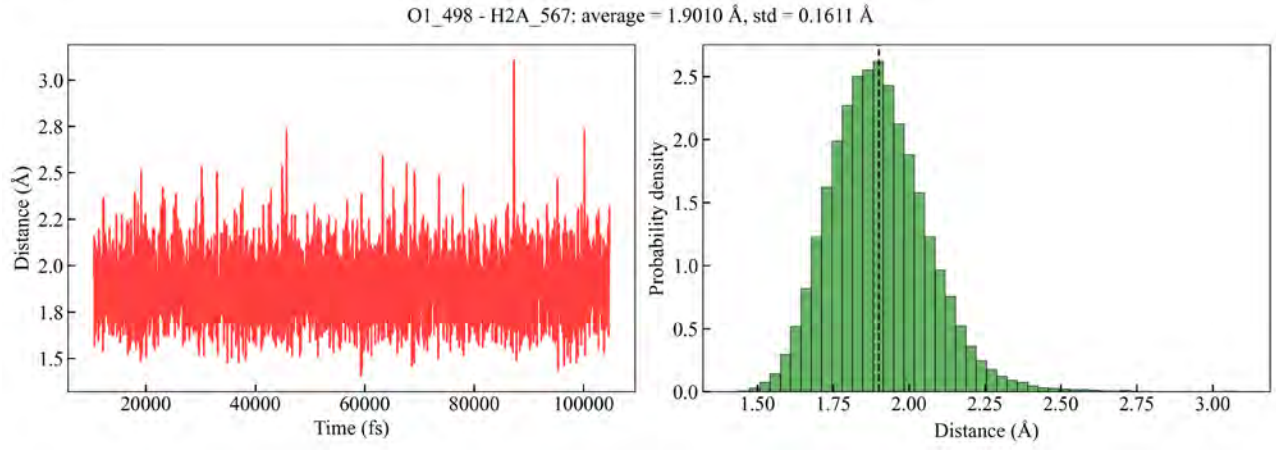
O1_497 - H2A_568

Average distance = 1.8986 Å; standard deviation = 0.1610 Å; number of points = 94257



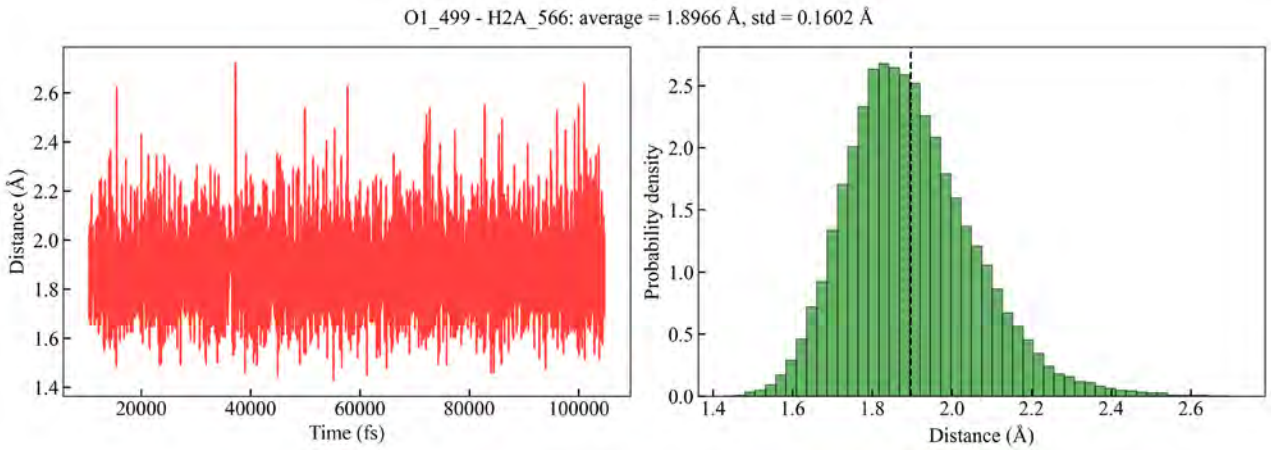
O1_498 - H2A_567

Average distance = 1.9010 Å; standard deviation = 0.1611 Å; number of points = 94257



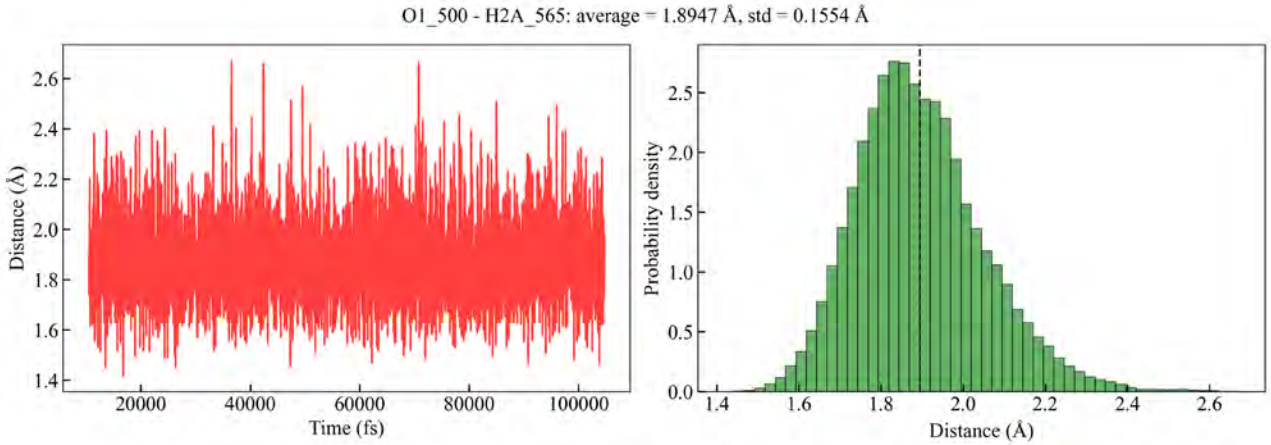
O1_499 - H2A_566

Average distance = 1.8966 Å; standard deviation = 0.1602 Å; number of points = 94257



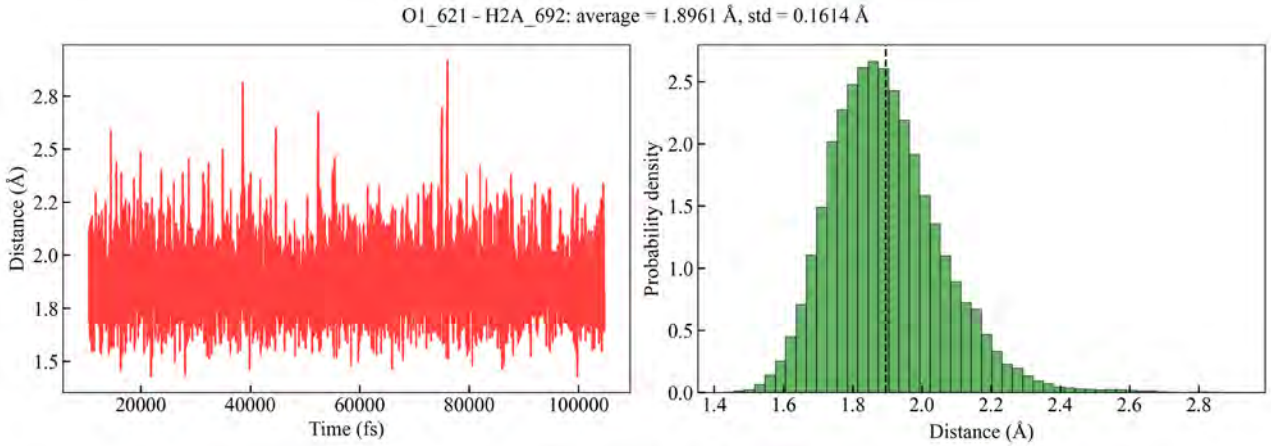
O1_500 - H2A_565

Average distance = 1.8947 Å; standard deviation = 0.1554 Å; number of points = 94257



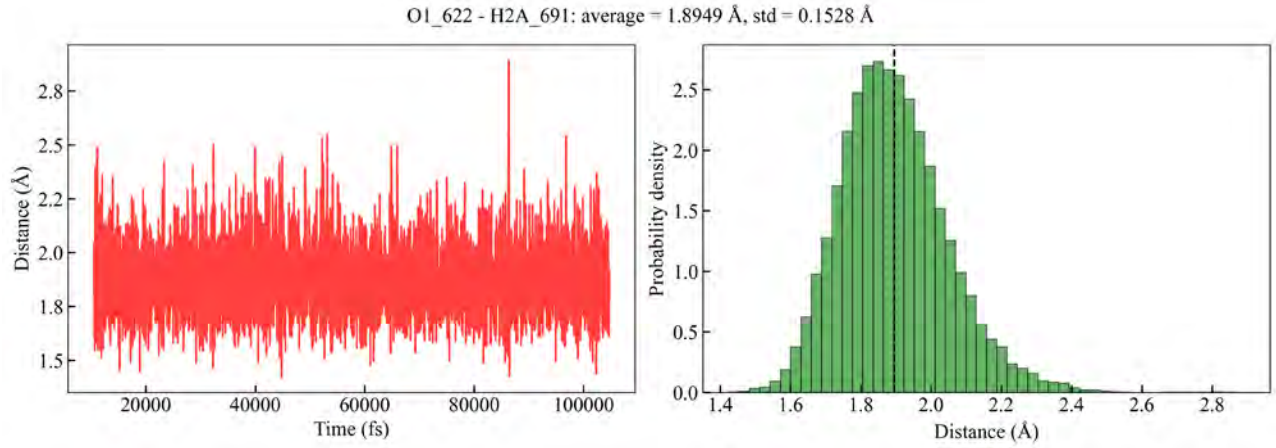
O1_621 - H2A_692

Average distance = 1.8961 Å; standard deviation = 0.1614 Å; number of points = 94257



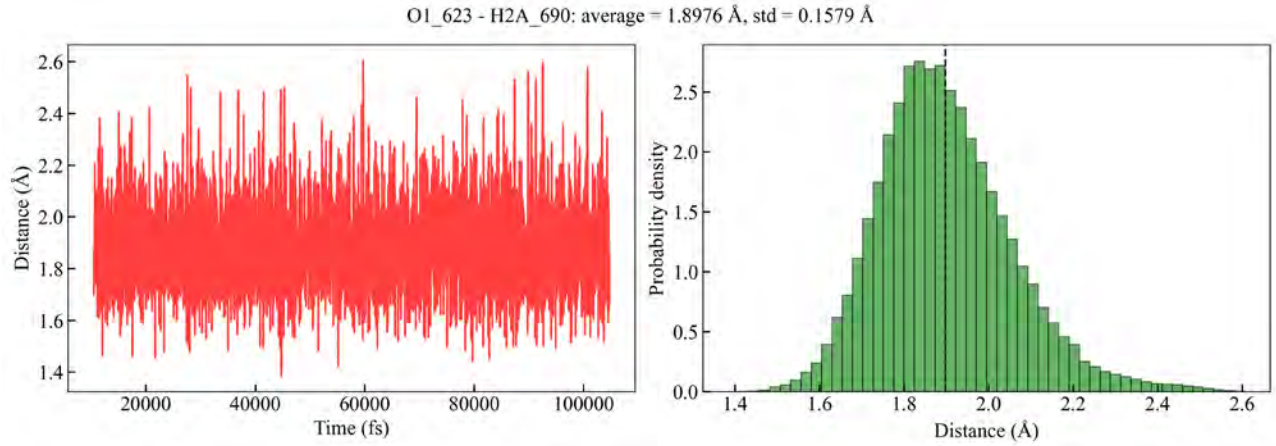
O1_622 - H2A_691

Average distance = 1.8949 Å; standard deviation = 0.1528 Å; number of points = 94257



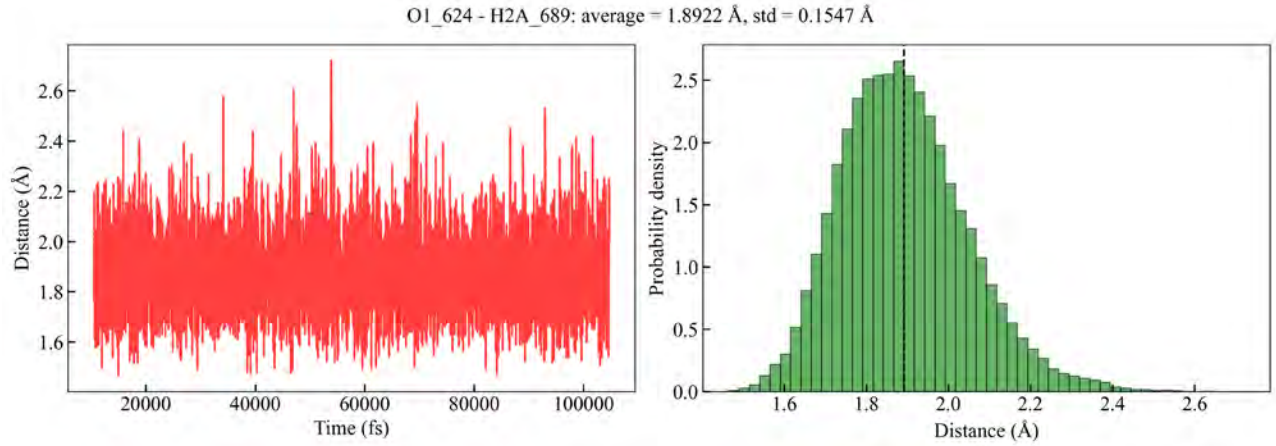
O1_623 - H2A_690

Average distance = 1.8976 Å; standard deviation = 0.1579 Å; number of points = 94257



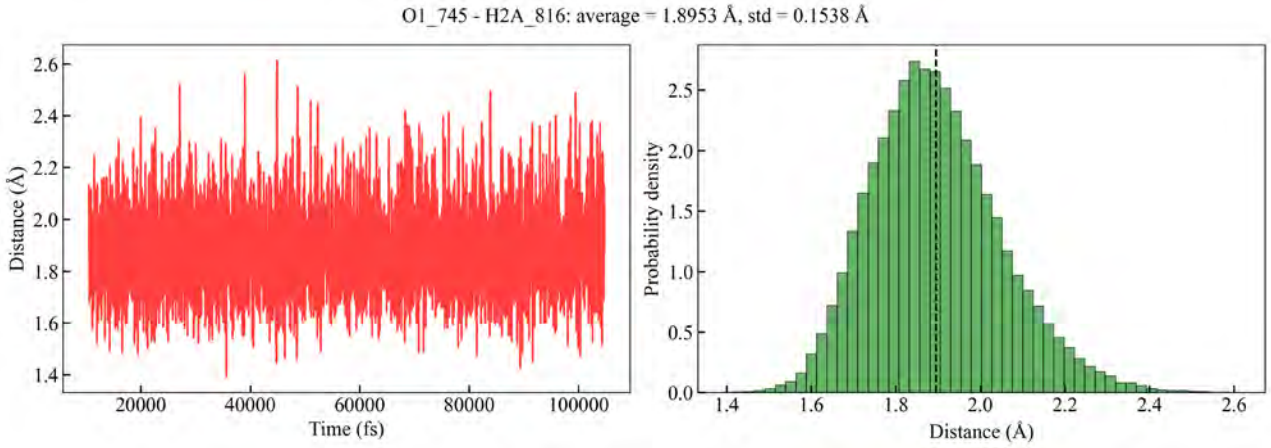
O1_624 - H2A_689

Average distance = 1.8922 Å; standard deviation = 0.1547 Å; number of points = 94257



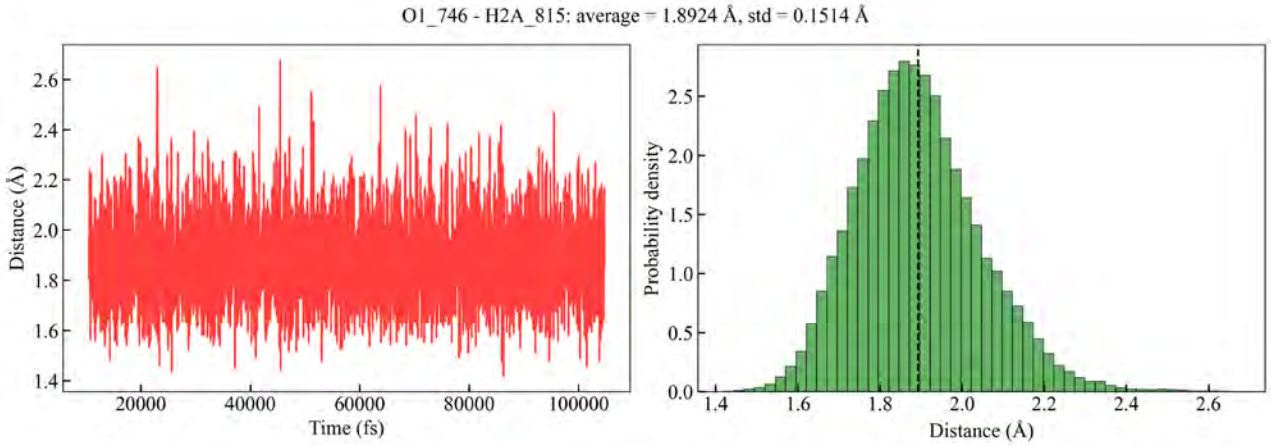
O1_745 - H2A_816

Average distance = 1.8953 Å; standard deviation = 0.1538 Å; number of points = 94257



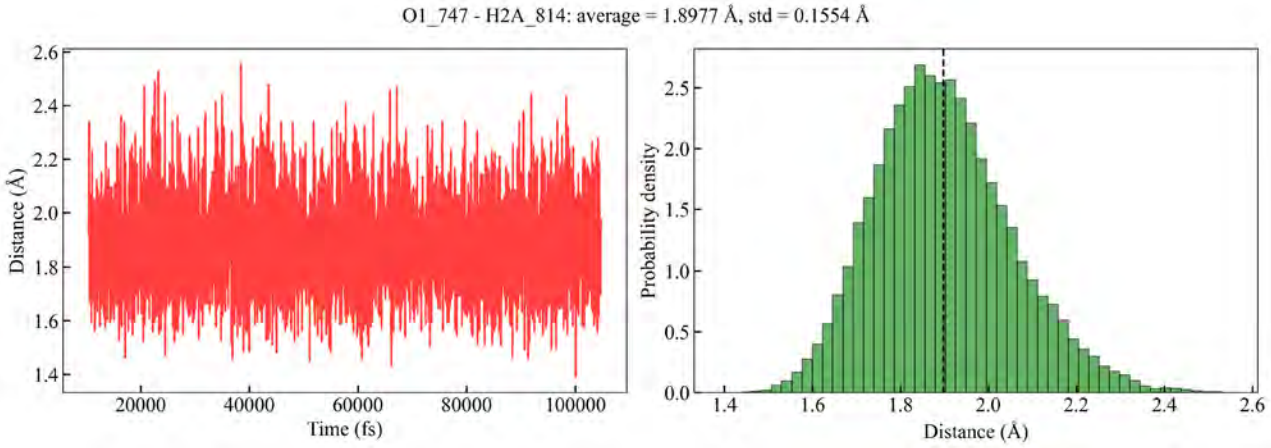
O1_746 - H2A_815

Average distance = 1.8924 Å; standard deviation = 0.1514 Å; number of points = 94257



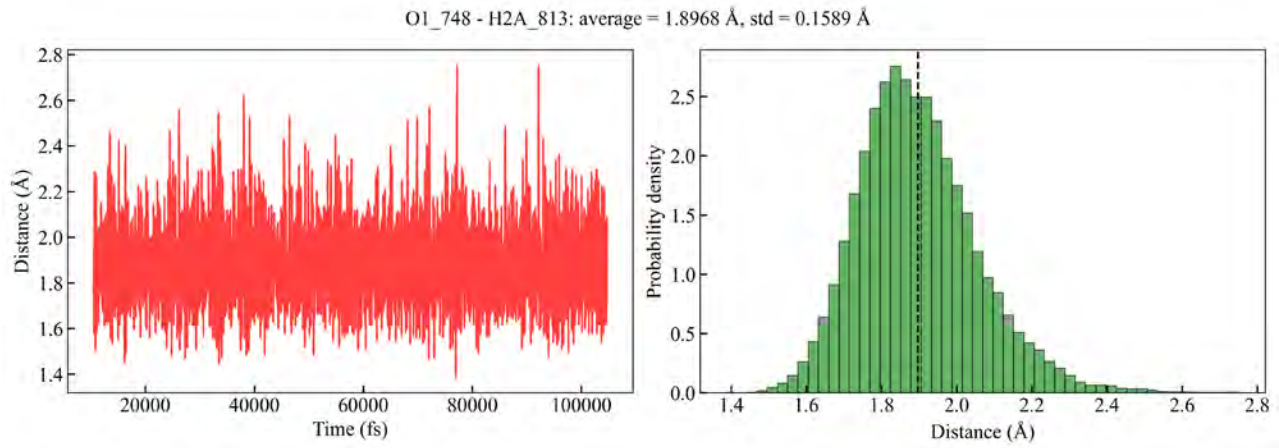
O1_747 - H2A_814

Average distance = 1.8977 Å; standard deviation = 0.1554 Å; number of points = 94257



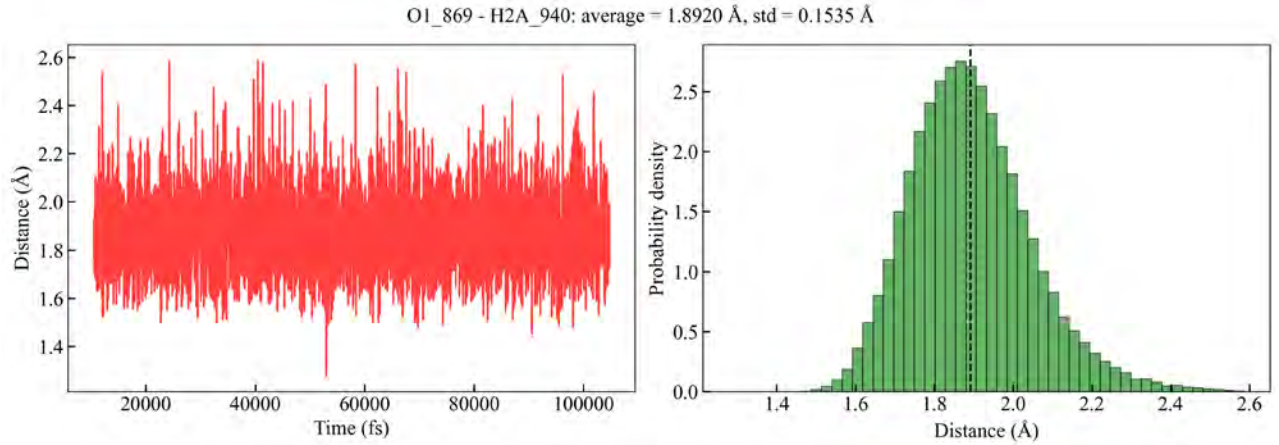
O1_748 - H2A_813

Average distance = 1.8968 Å; standard deviation = 0.1589 Å; number of points = 94257



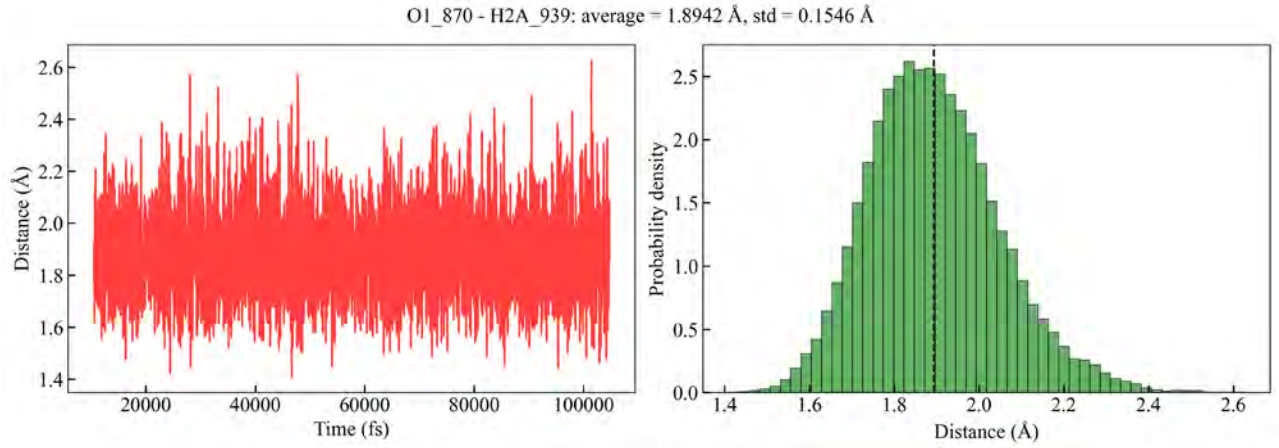
O1_869 - H2A_940

Average distance = 1.8920 Å; standard deviation = 0.1535 Å; number of points = 94257



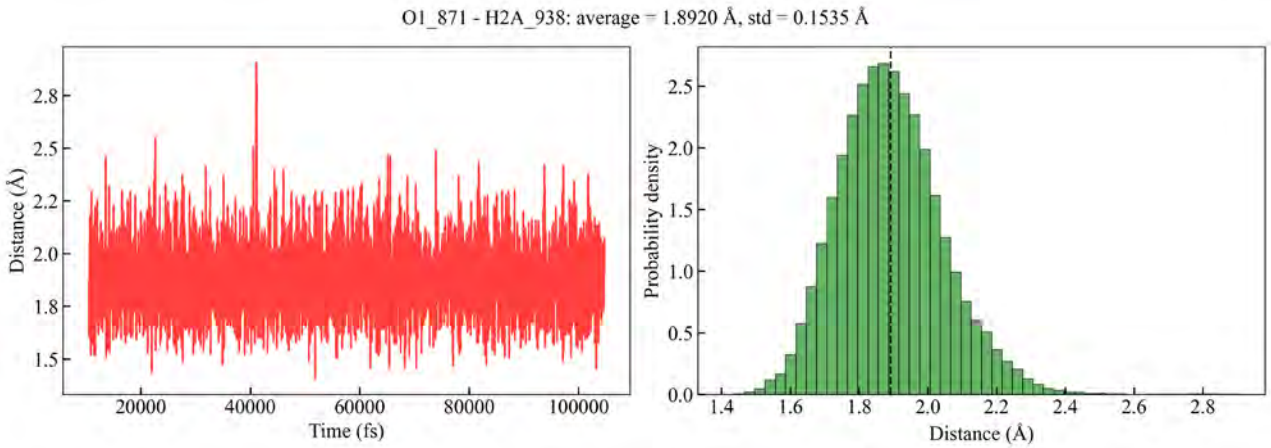
O1_870 - H2A_939

Average distance = 1.8942 Å; standard deviation = 0.1546 Å; number of points = 94257



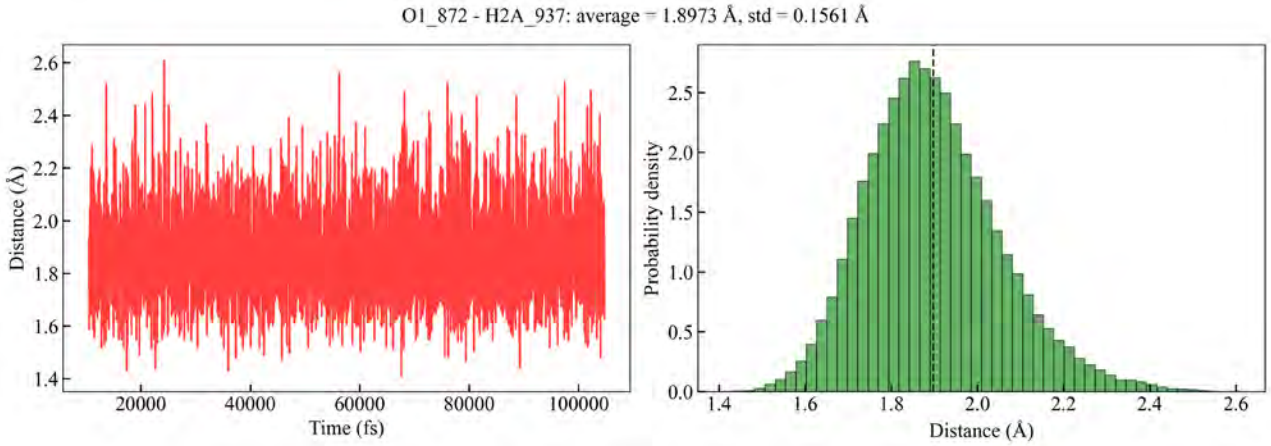
O1_871 - H2A_938

Average distance = 1.8920 Å; standard deviation = 0.1535 Å; number of points = 94257



O1_872 - H2A_937

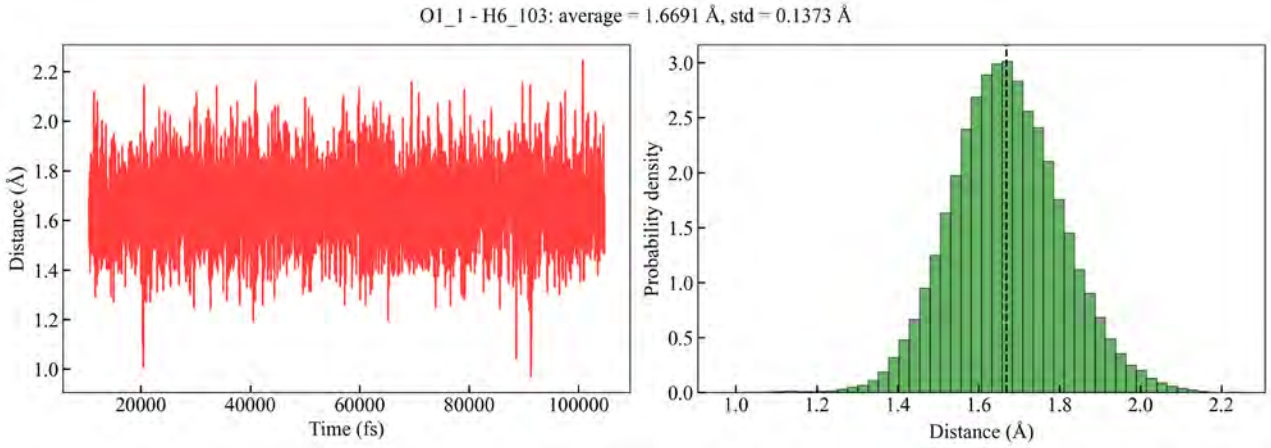
Average distance = 1.8973 Å; standard deviation = 0.1561 Å; number of points = 94257



O1 - H6

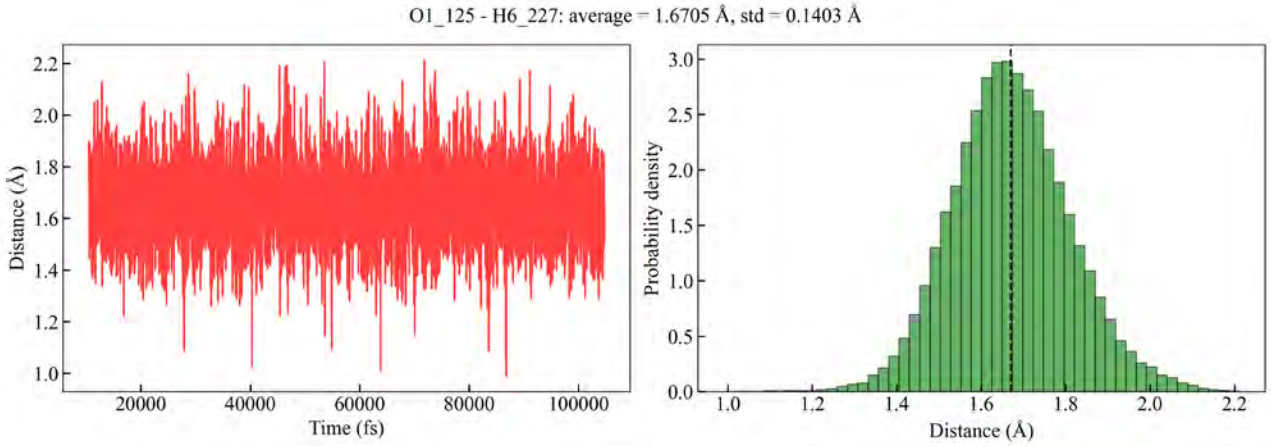
O1_1 - H6_103

Average distance = 1.6691 Å; standard deviation = 0.1373 Å; number of points = 94257



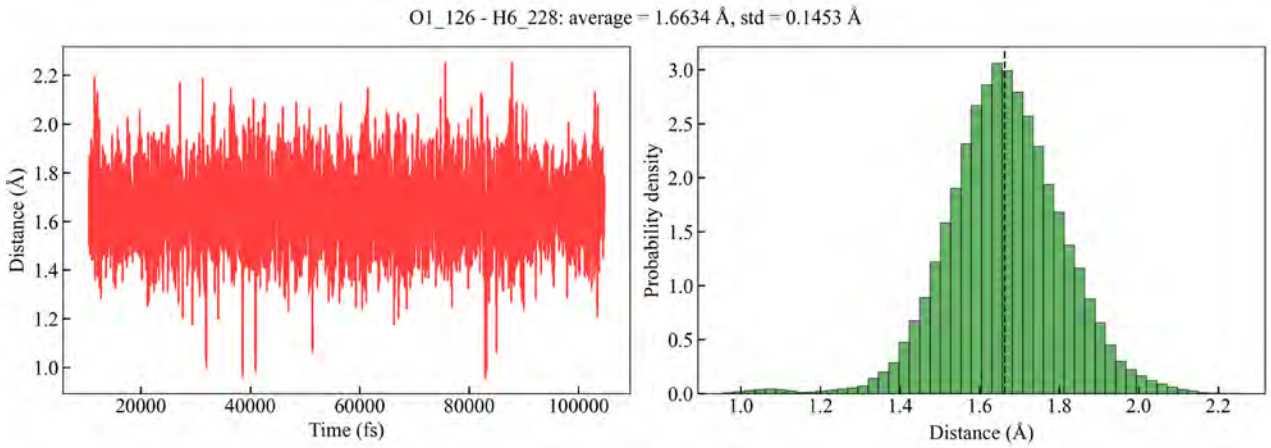
O1_125 - H6_227

Average distance = 1.6705 Å; standard deviation = 0.1403 Å; number of points = 94257



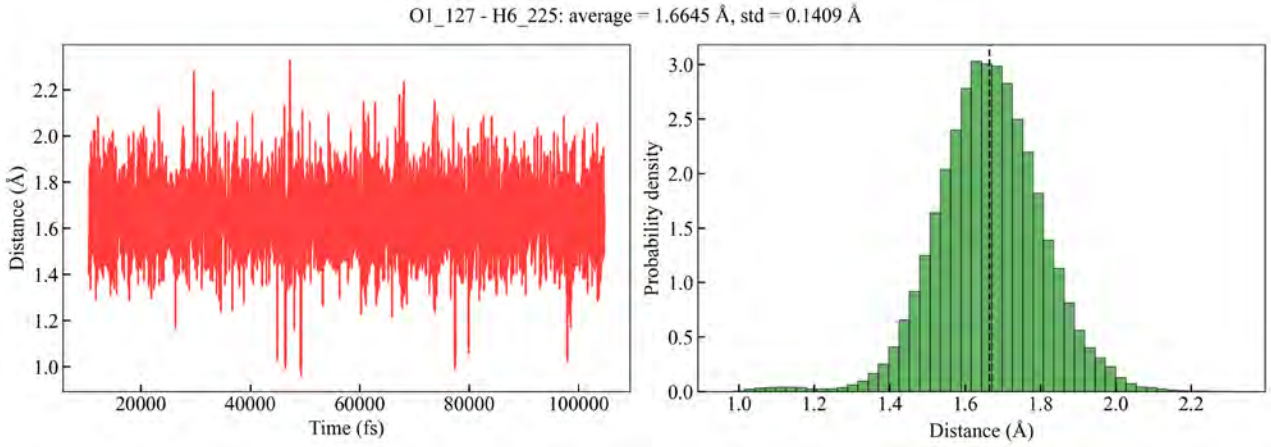
O1_126 - H6_228

Average distance = 1.6634 Å; standard deviation = 0.1453 Å; number of points = 94257



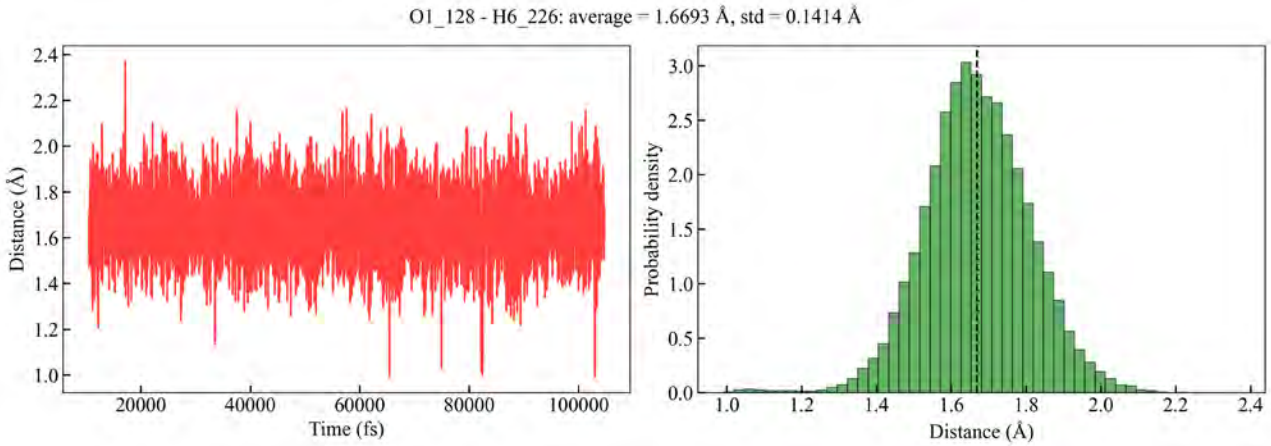
O1_127 - H6_225

Average distance = 1.6645 Å; standard deviation = 0.1409 Å; number of points = 94257



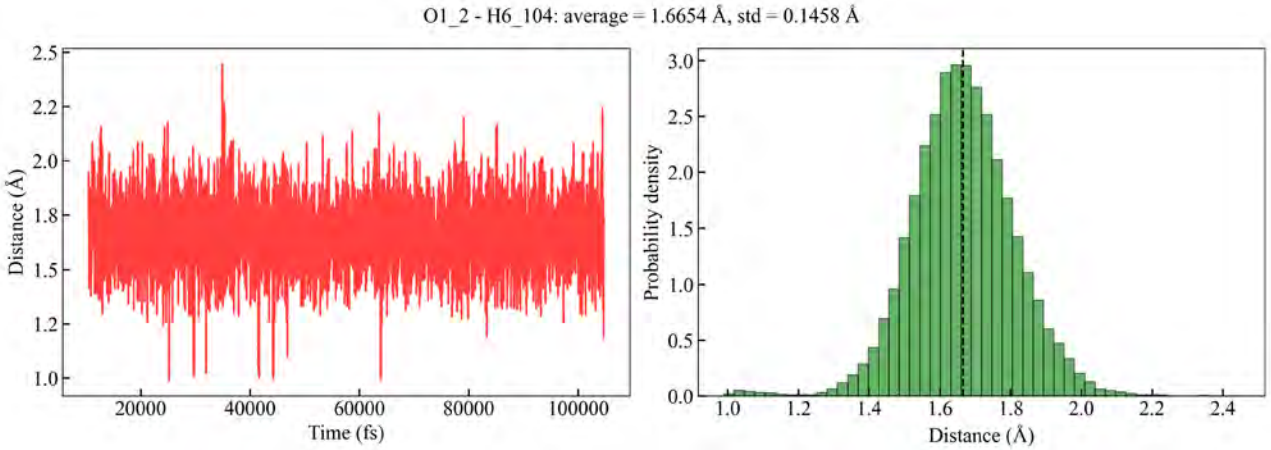
O1_128 - H6_226

Average distance = 1.6693 Å; standard deviation = 0.1414 Å; number of points = 94257



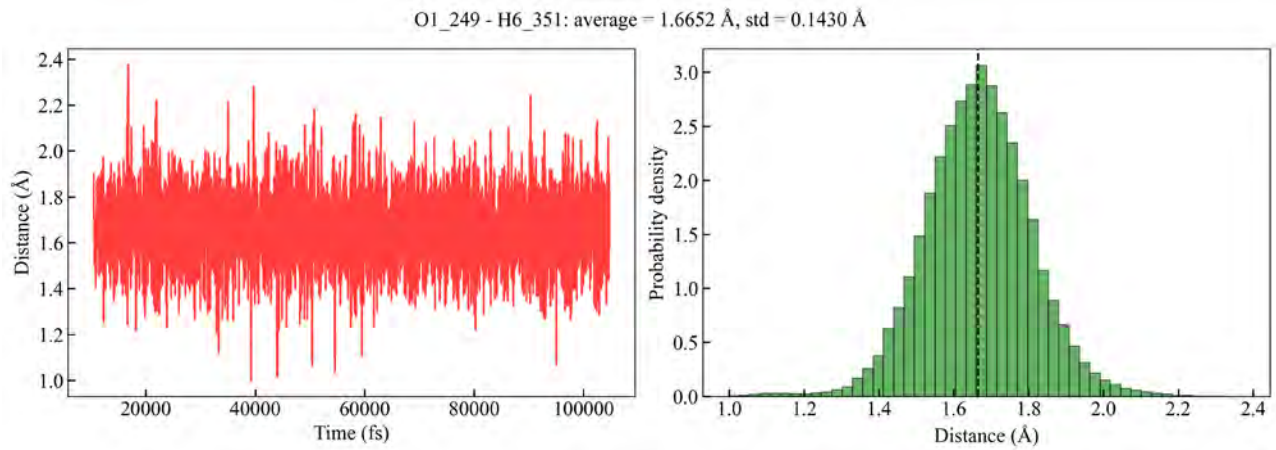
O1_2 - H6_104

Average distance = 1.6654 Å; standard deviation = 0.1458 Å; number of points = 94257



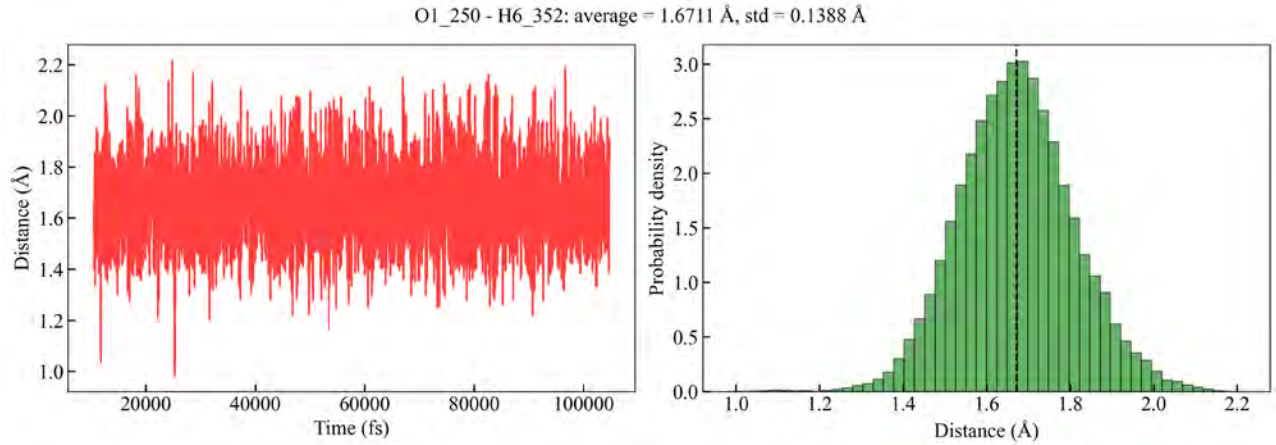
O1_249 - H6_351

Average distance = 1.6652 Å; standard deviation = 0.1430 Å; number of points = 94257



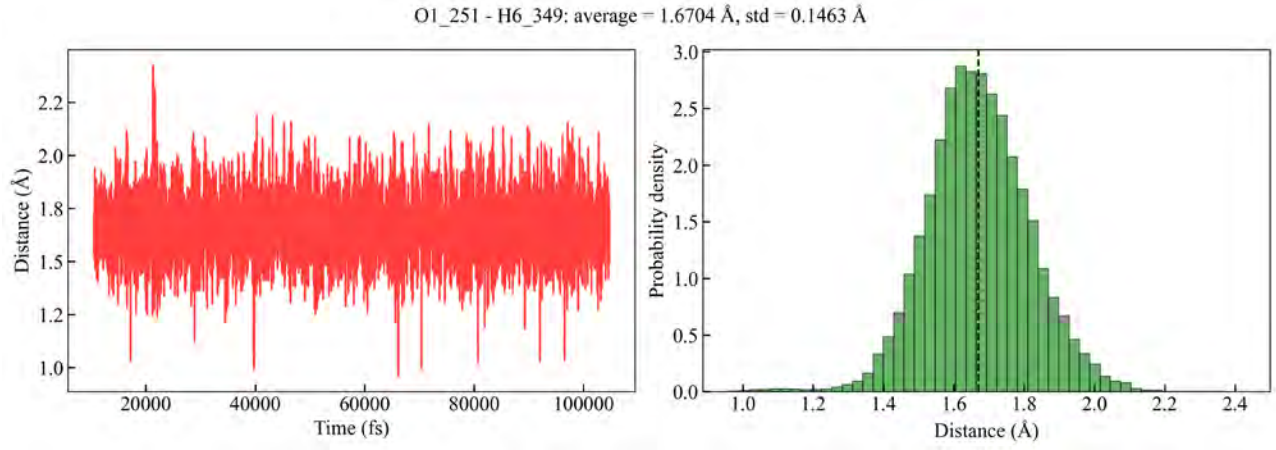
O1_250 - H6_352

Average distance = 1.6711 Å; standard deviation = 0.1388 Å; number of points = 94257



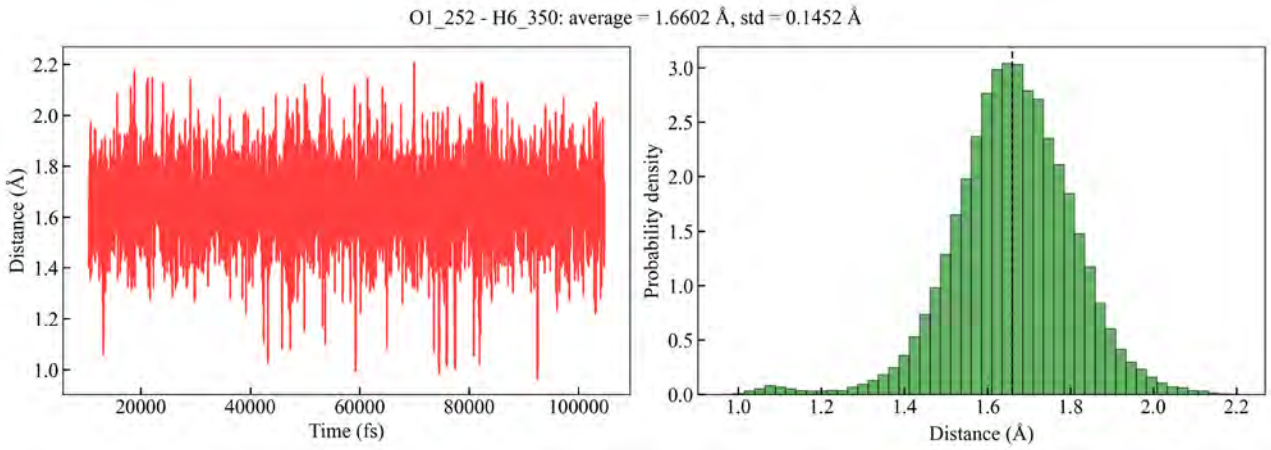
O1_251 - H6_349

Average distance = 1.6704 Å; standard deviation = 0.1463 Å; number of points = 94257



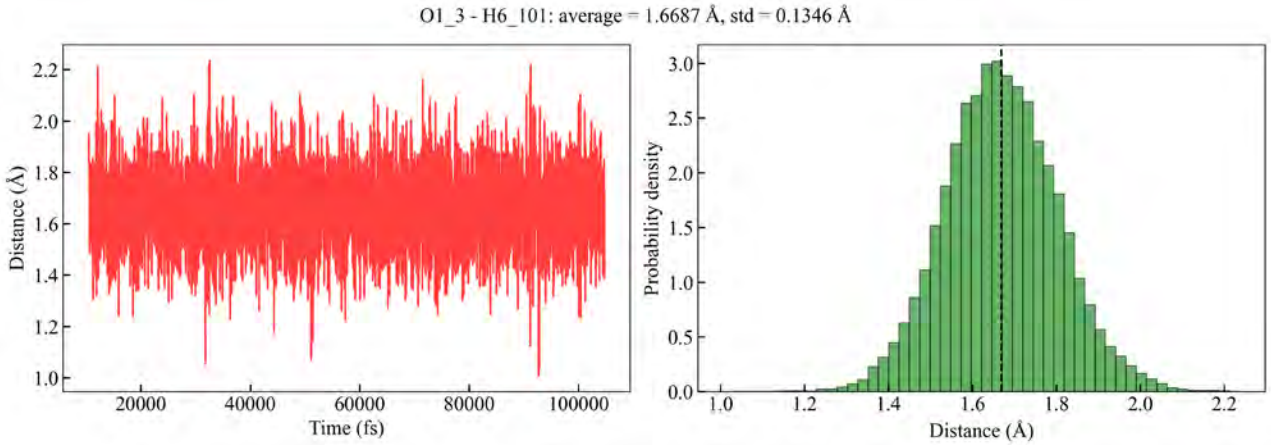
O1_252 - H6_350

Average distance = 1.6602 Å; standard deviation = 0.1452 Å; number of points = 94257



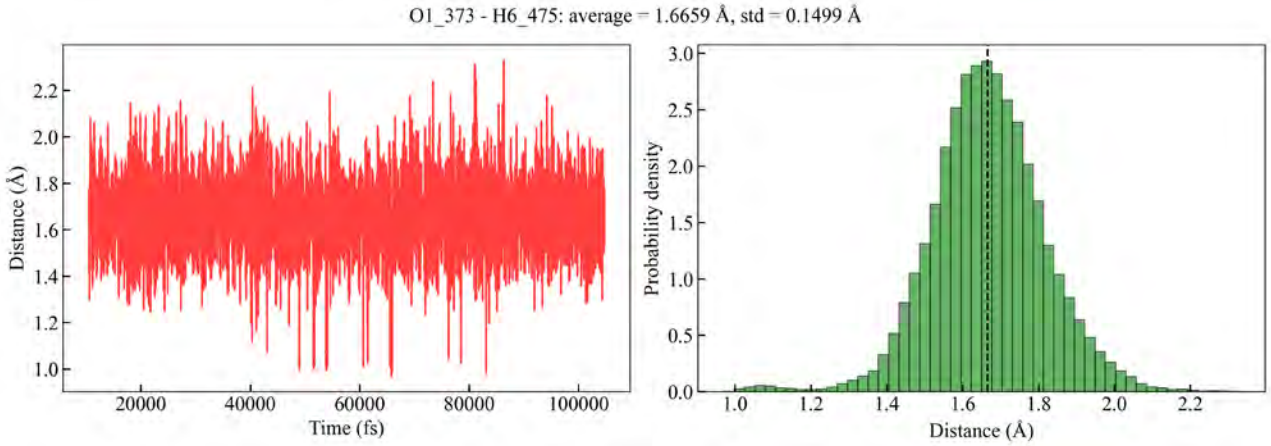
O1_3 - H6_101

Average distance = 1.6687 Å; standard deviation = 0.1346 Å; number of points = 94257



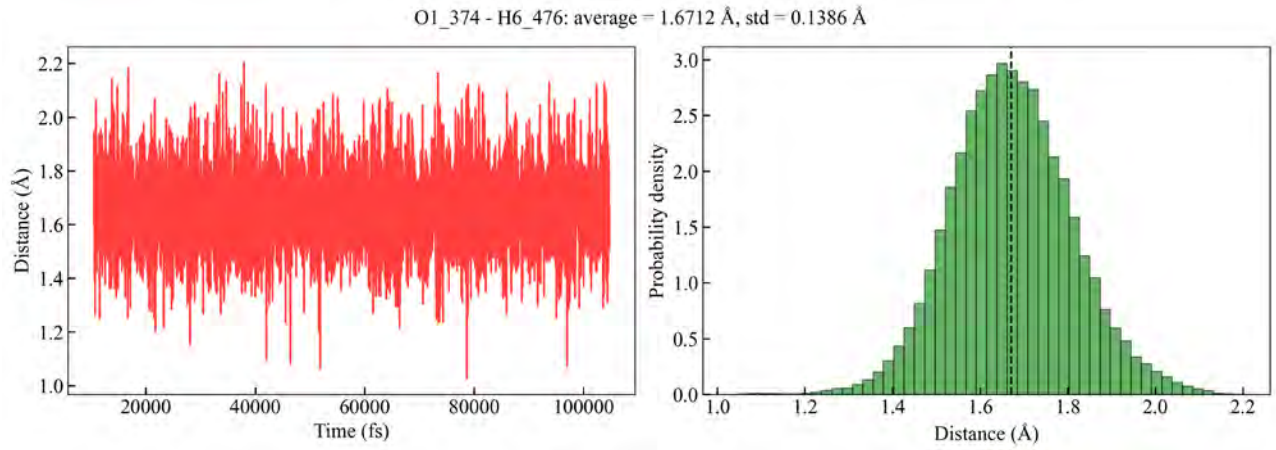
O1_373 - H6_475

Average distance = 1.6659 Å; standard deviation = 0.1499 Å; number of points = 94257



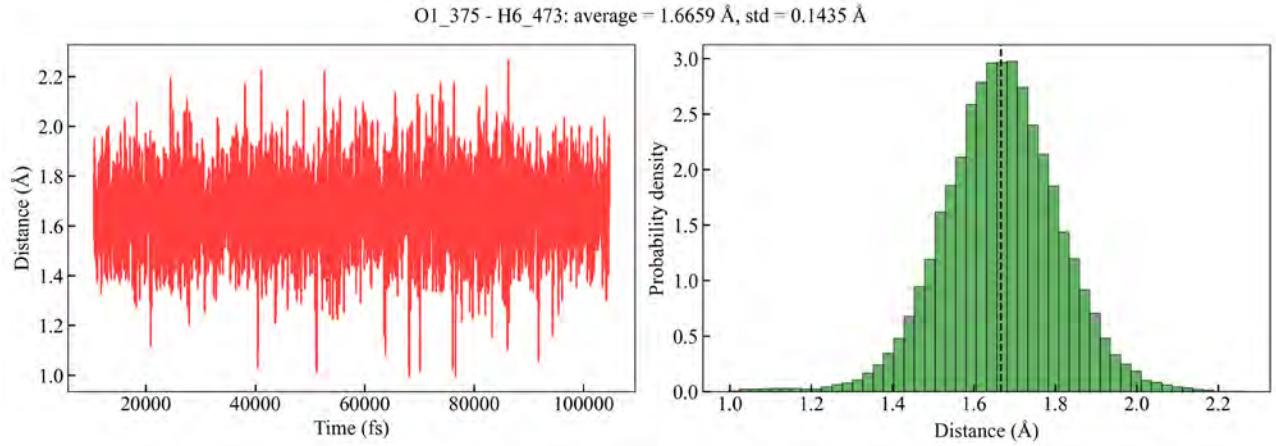
O1_374 - H6_476

Average distance = 1.6712 Å; standard deviation = 0.1386 Å; number of points = 94257



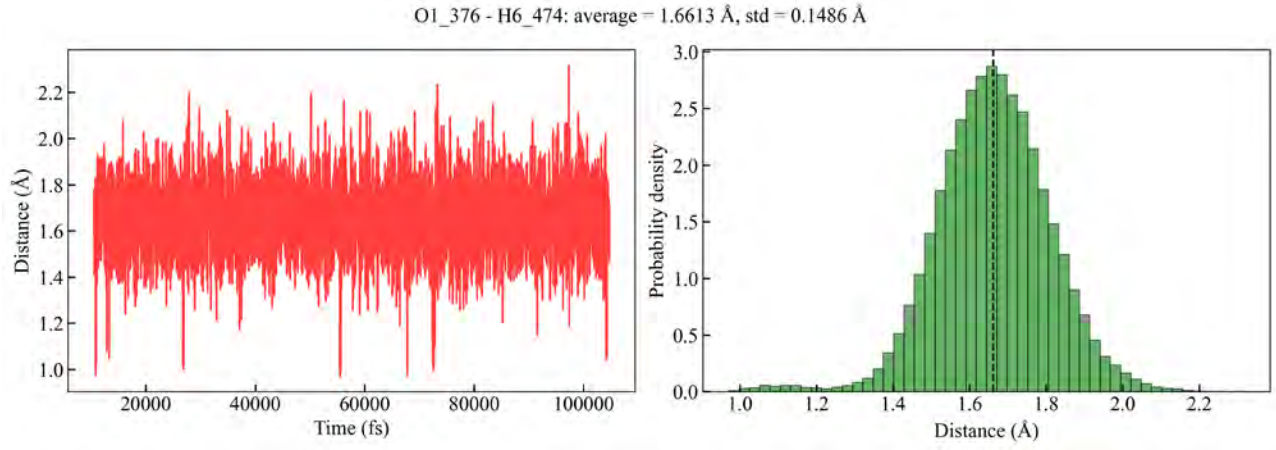
O1_375 - H6_473

Average distance = 1.6659 Å; standard deviation = 0.1435 Å; number of points = 94257



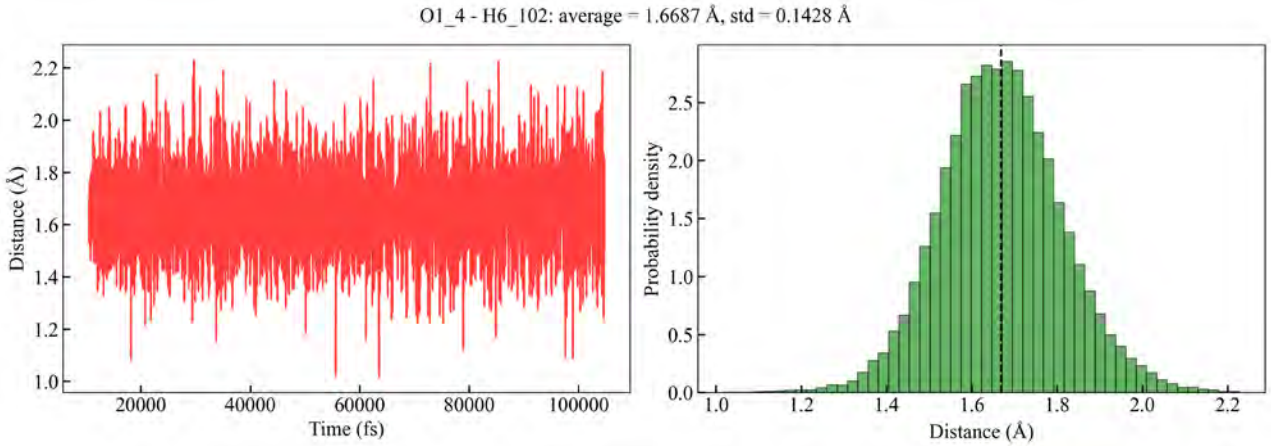
O1_376 - H6_474

Average distance = 1.6613 Å; standard deviation = 0.1486 Å; number of points = 94257



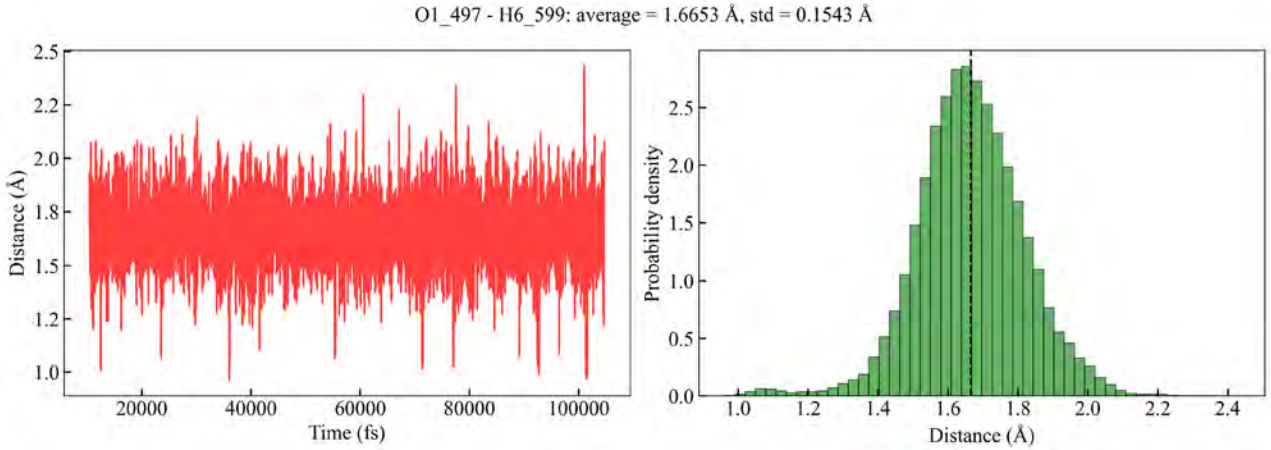
O1_4 - H6_102

Average distance = 1.6687 Å; standard deviation = 0.1428 Å; number of points = 94257



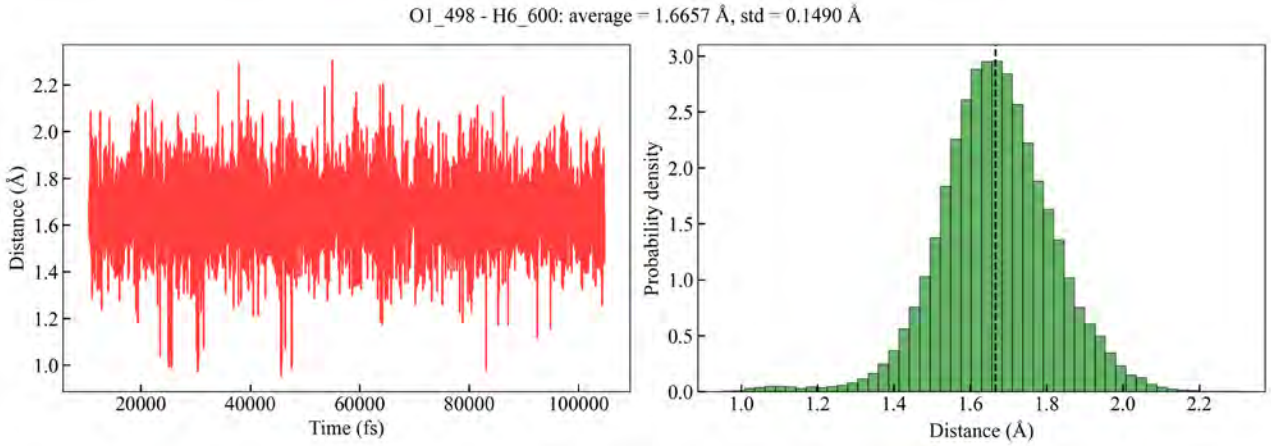
O1_497 - H6_599

Average distance = 1.6653 Å; standard deviation = 0.1543 Å; number of points = 94257



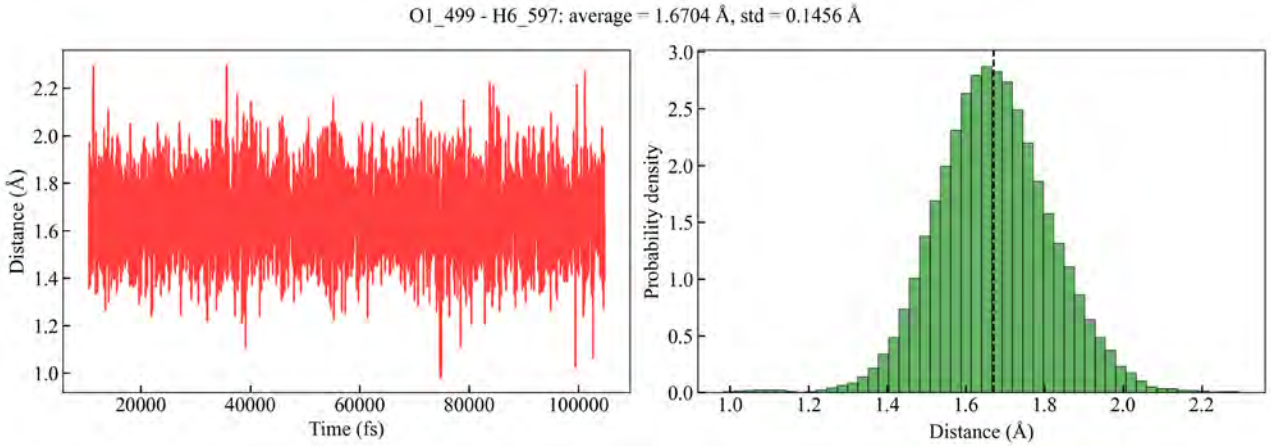
O1_498 - H6_600

Average distance = 1.6657 Å; standard deviation = 0.1490 Å; number of points = 94257



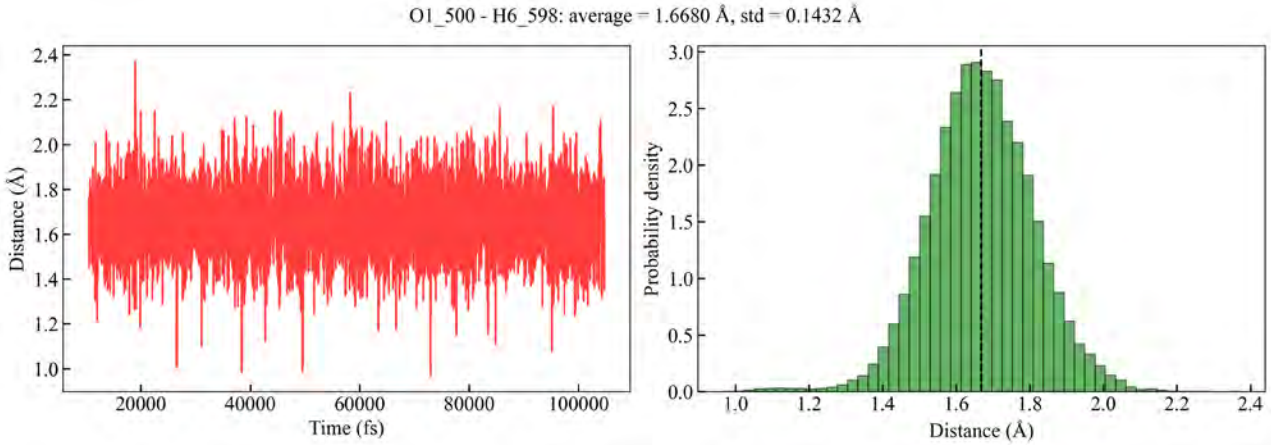
O1_499 - H6_597

Average distance = 1.6704 Å; standard deviation = 0.1456 Å; number of points = 94257



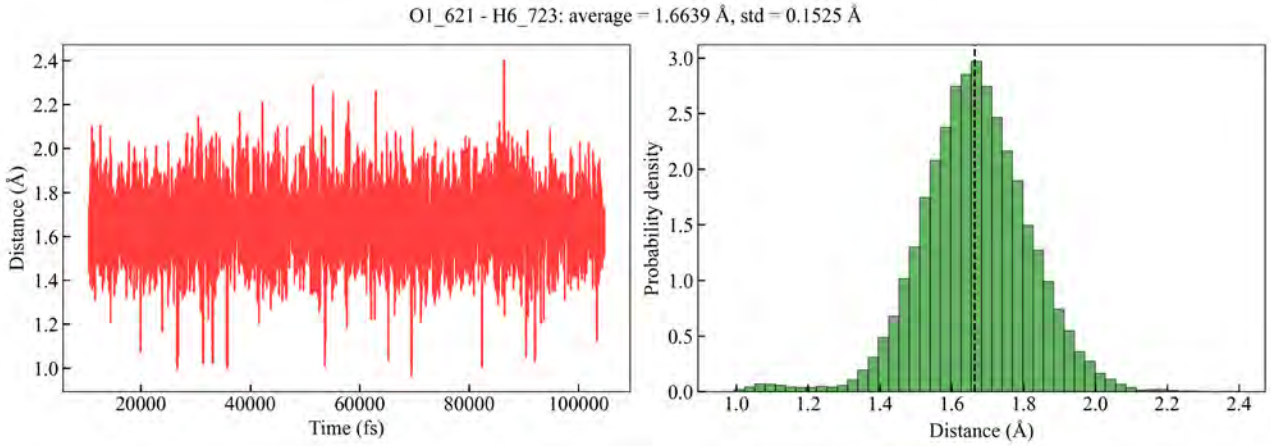
O1_500 - H6_598

Average distance = 1.6680 Å; standard deviation = 0.1432 Å; number of points = 94257



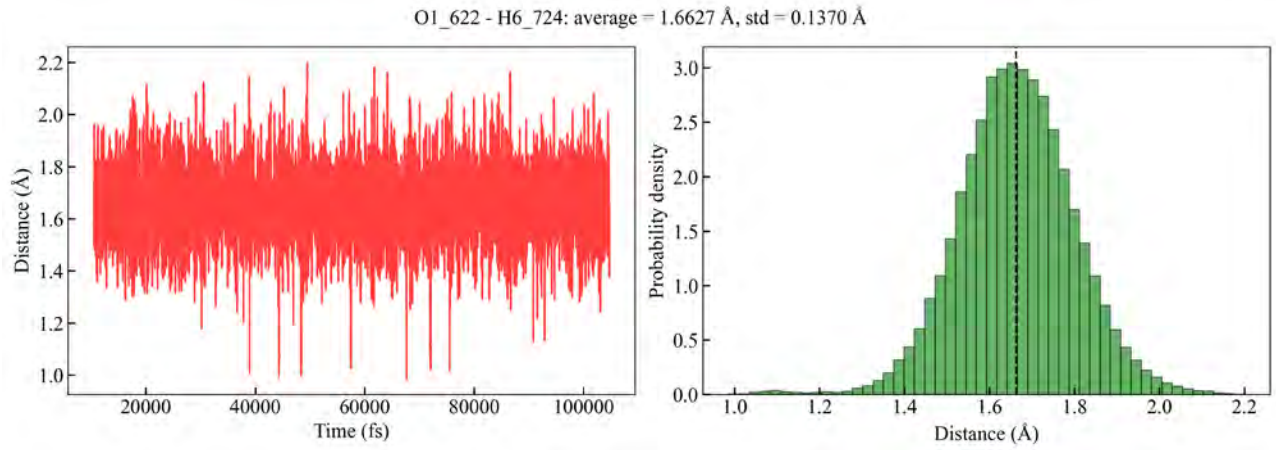
O1_621 - H6_723

Average distance = 1.6639 Å; standard deviation = 0.1525 Å; number of points = 94257



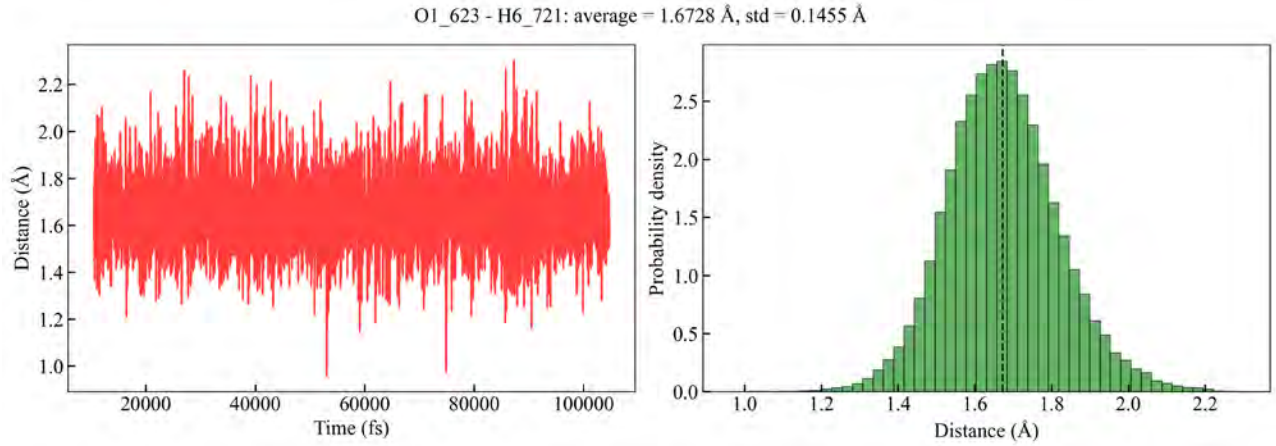
O1_622 - H6_724

Average distance = 1.6627 Å; standard deviation = 0.1370 Å; number of points = 94257



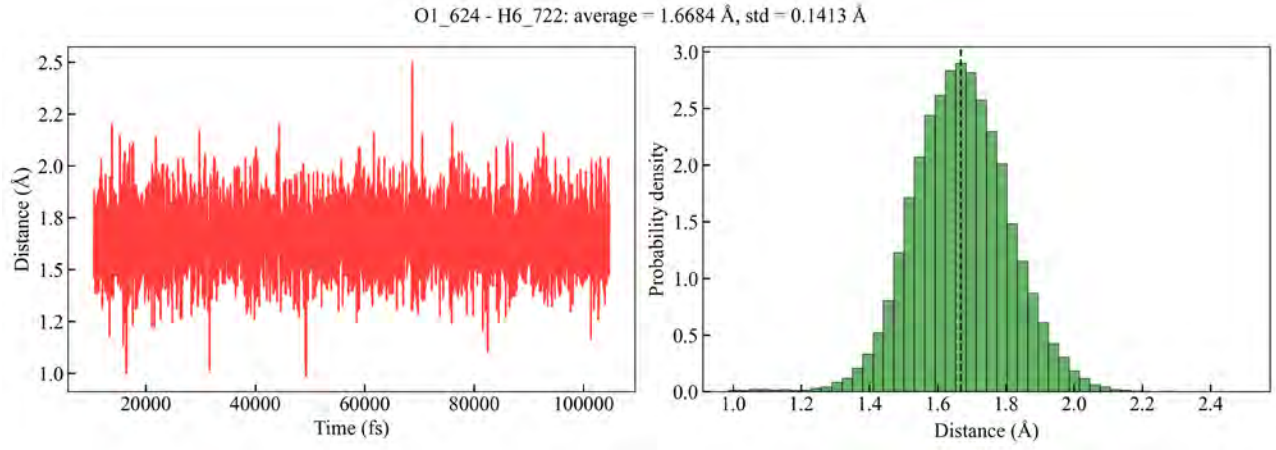
O1_623 - H6_721

Average distance = 1.6728 Å; standard deviation = 0.1455 Å; number of points = 94257



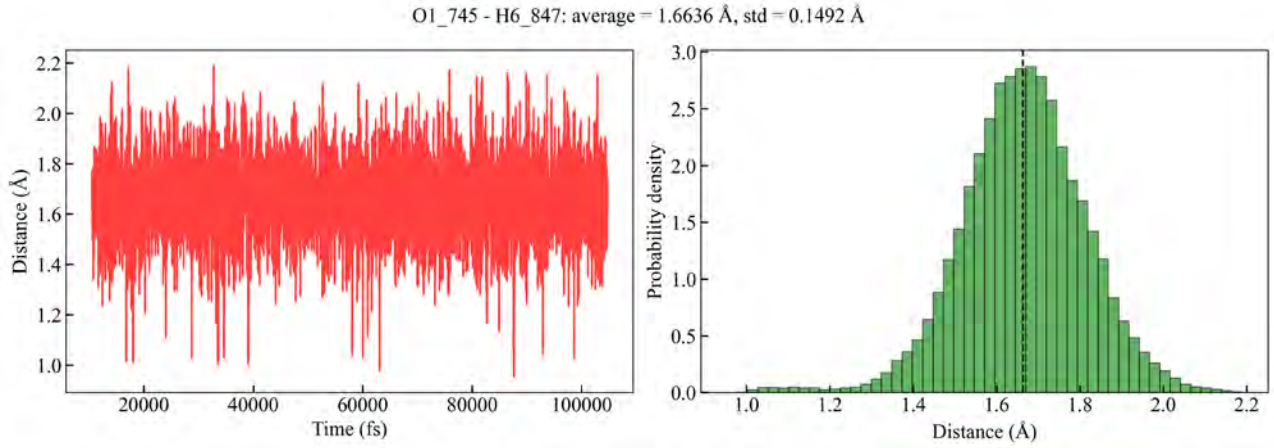
O1_624 - H6_722

Average distance = 1.6684 Å; standard deviation = 0.1413 Å; number of points = 94257



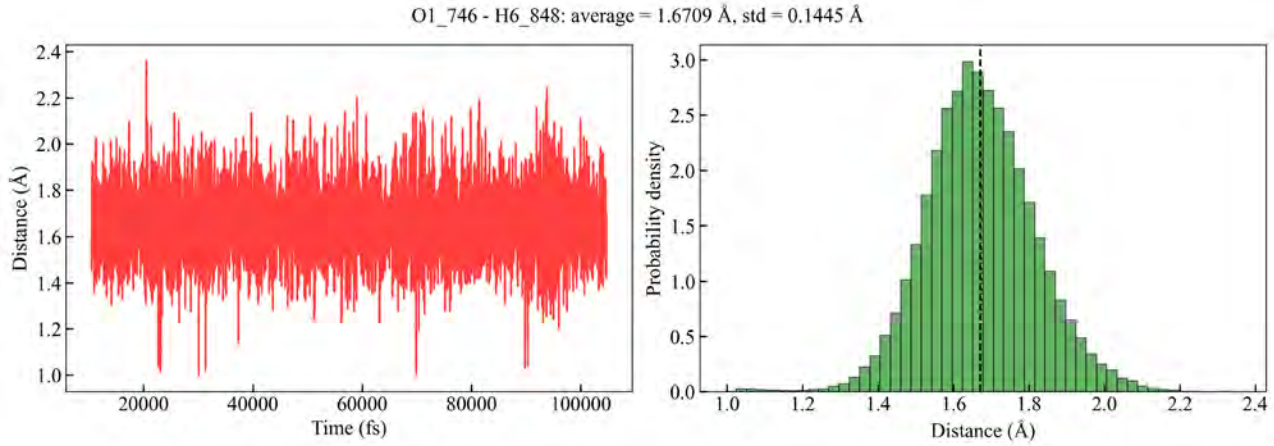
O1_745 - H6_847

Average distance = 1.6636 Å; standard deviation = 0.1492 Å; number of points = 94257



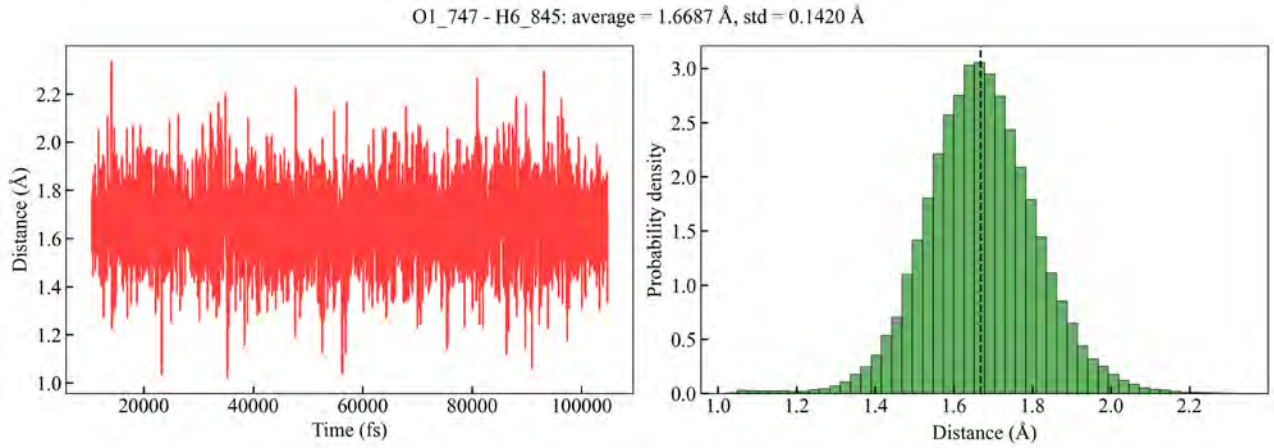
O1_746 - H6_848

Average distance = 1.6709 Å; standard deviation = 0.1445 Å; number of points = 94257



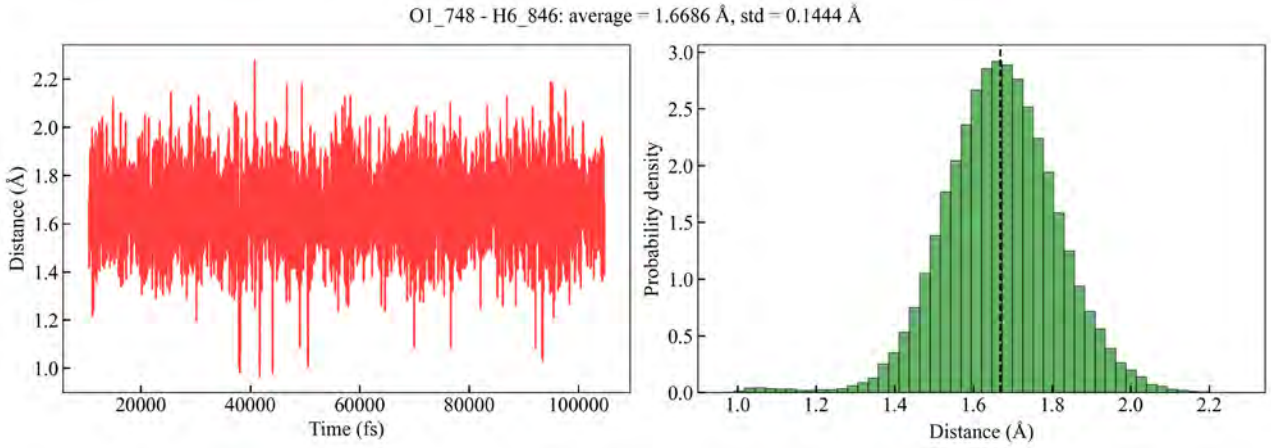
O1_747 - H6_845

Average distance = 1.6687 Å; standard deviation = 0.1420 Å; number of points = 94257



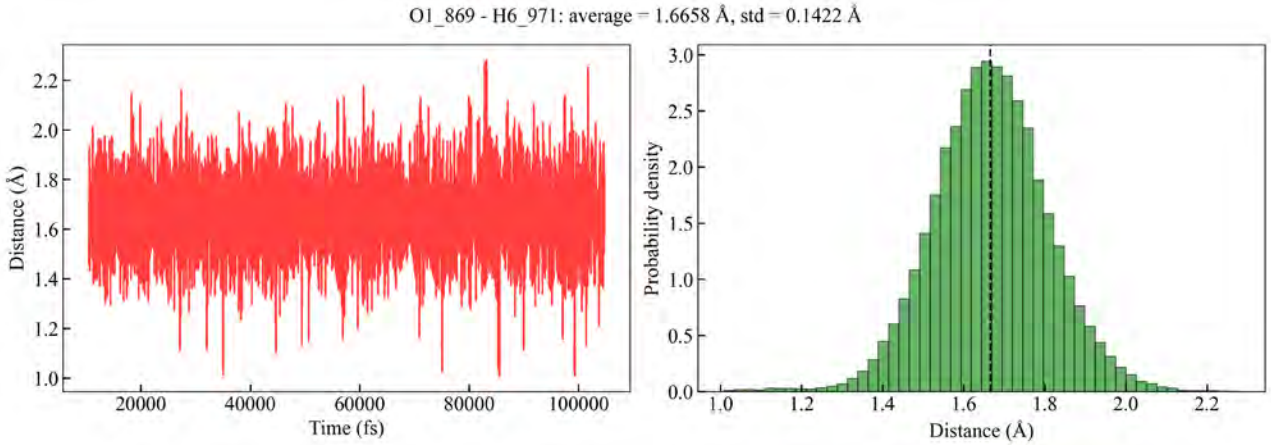
O1_748 - H6_846

Average distance = 1.6686 Å; standard deviation = 0.1444 Å; number of points = 94257



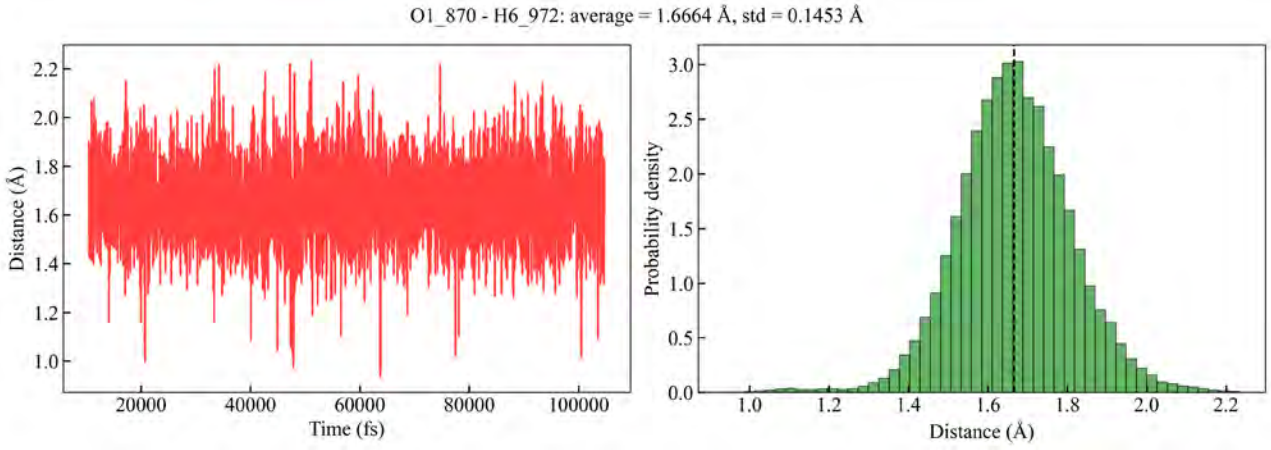
O1_869 - H6_971

Average distance = 1.6658 Å; standard deviation = 0.1422 Å; number of points = 94257



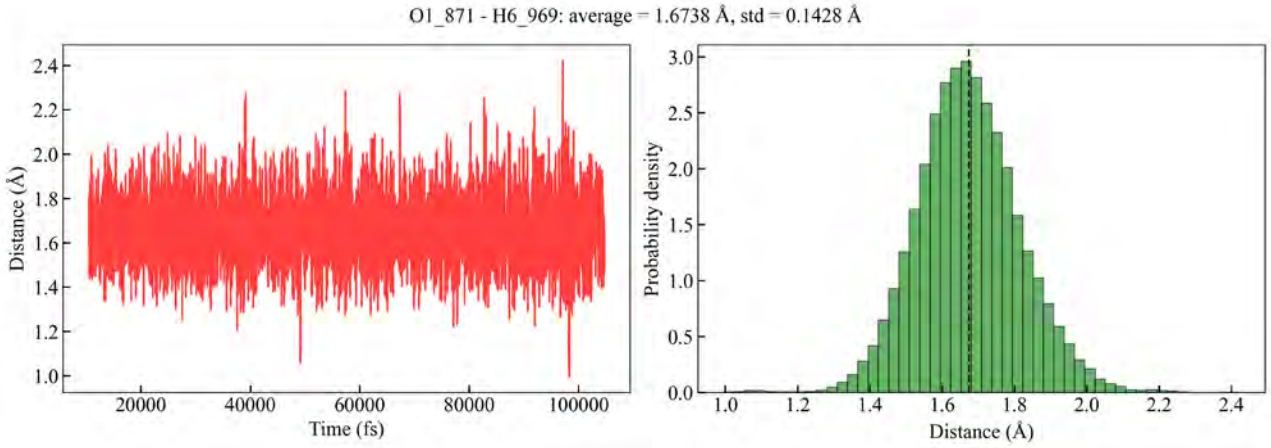
O1_870 - H6_972

Average distance = 1.6664 Å; standard deviation = 0.1453 Å; number of points = 94257



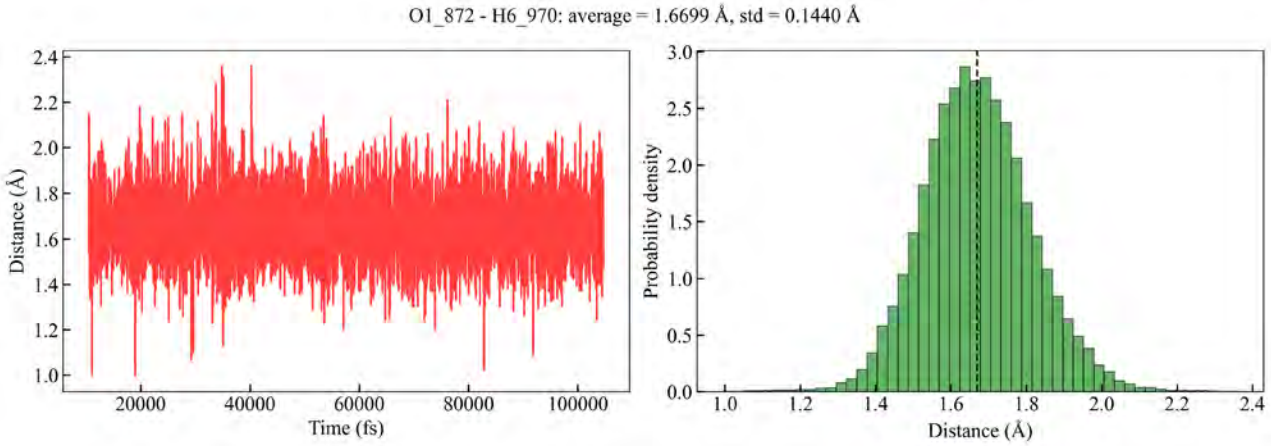
O1_871 - H6_969

Average distance = 1.6738 Å; standard deviation = 0.1428 Å; number of points = 94257



O1_872 - H6_970

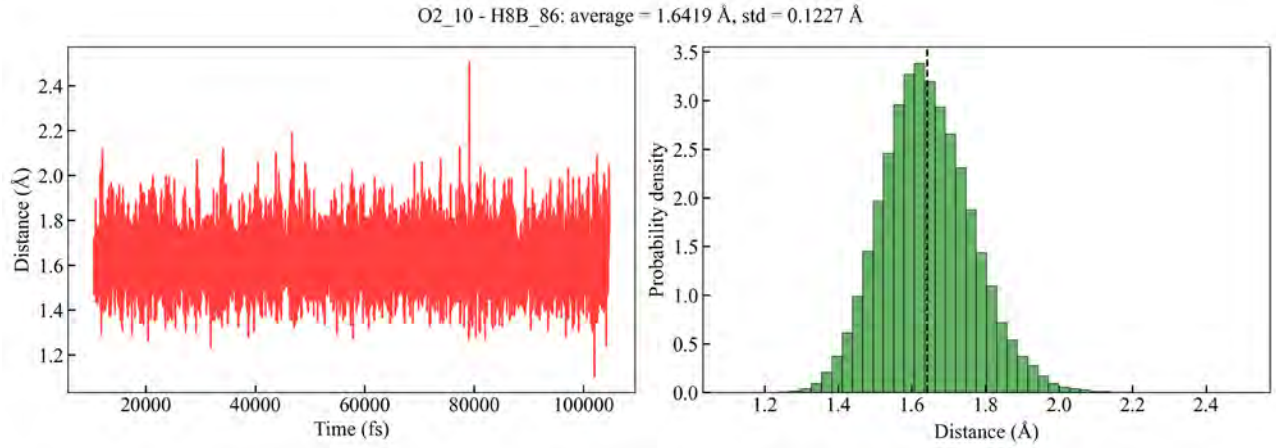
Average distance = 1.6699 Å; standard deviation = 0.1440 Å; number of points = 94257



O2 - H8B

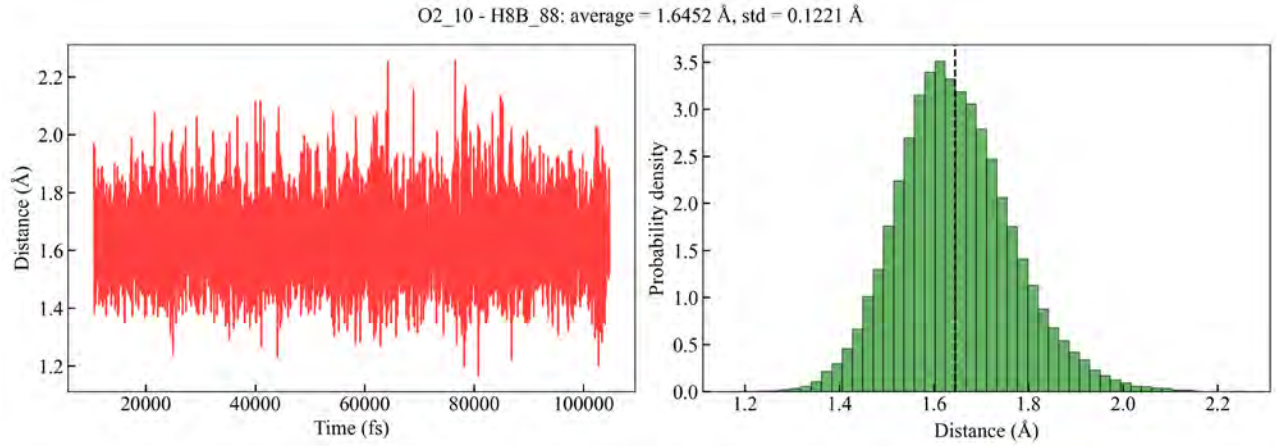
O2_10 - H8B_86

Average distance = 1.6419 Å; standard deviation = 0.1227 Å; number of points = 94257



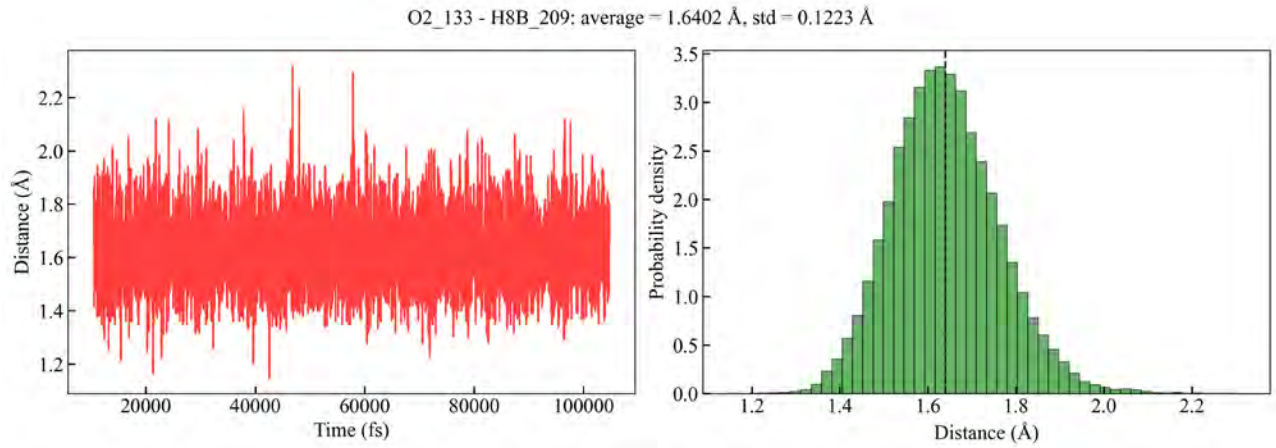
O2_10 - H8B_88

Average distance = 1.6452 Å; standard deviation = 0.1221 Å; number of points = 94257



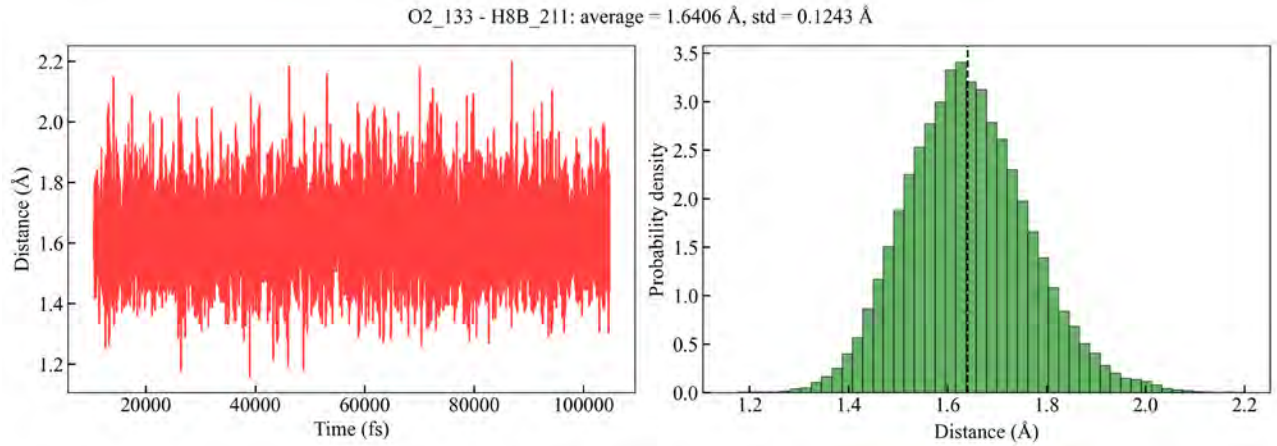
O2_133 - H8B_209

Average distance = 1.6402 Å; standard deviation = 0.1223 Å; number of points = 94257



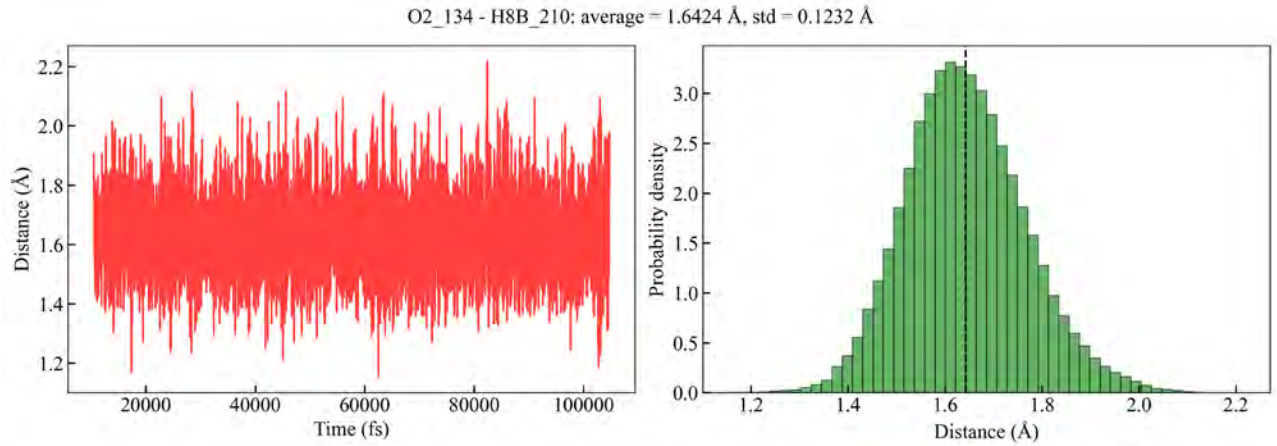
O2_133 - H8B_211

Average distance = 1.6406 Å; standard deviation = 0.1243 Å; number of points = 94257



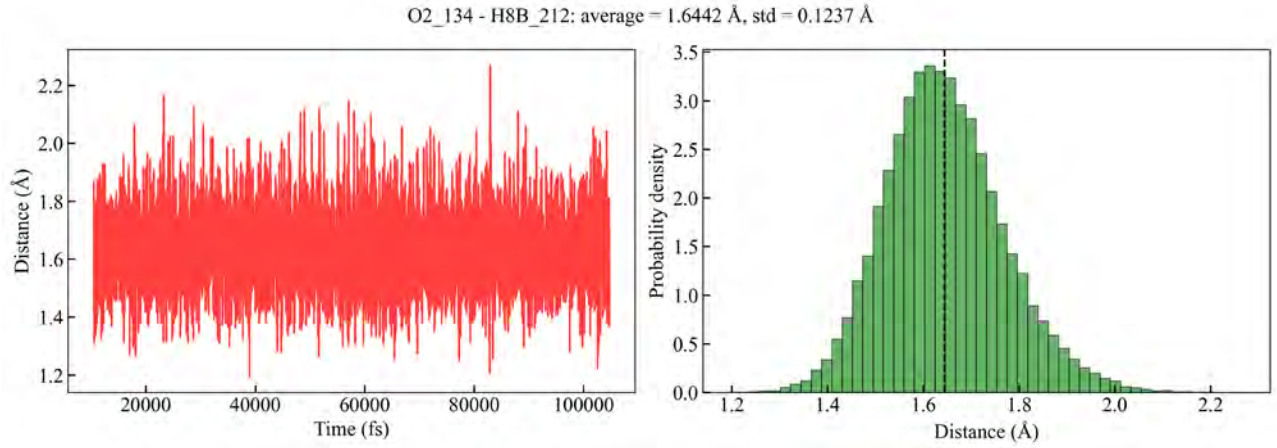
O2_134 - H8B_210

Average distance = 1.6424 Å; standard deviation = 0.1232 Å; number of points = 94257



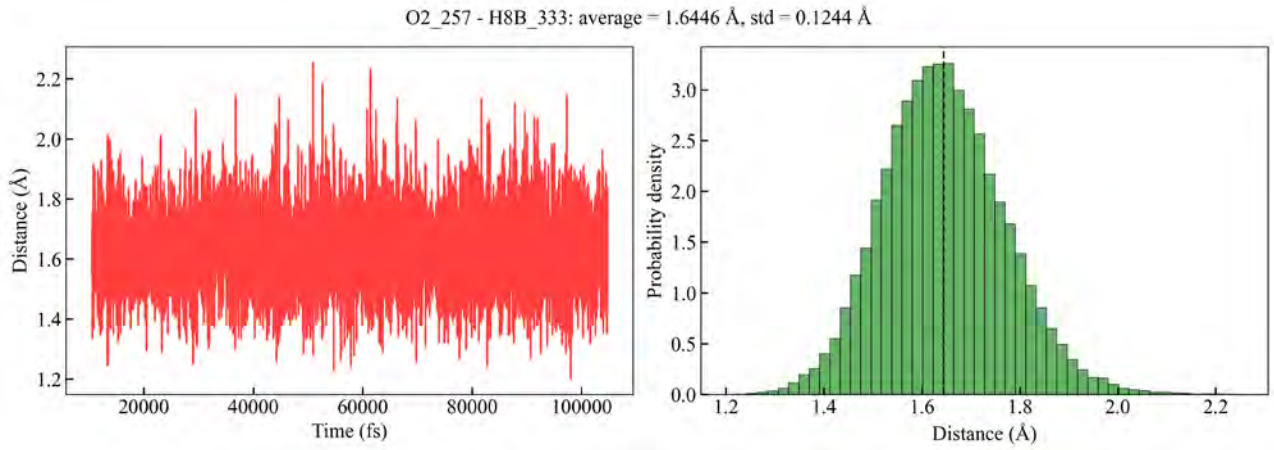
O2_134 - H8B_212

Average distance = 1.6442 Å; standard deviation = 0.1237 Å; number of points = 94257



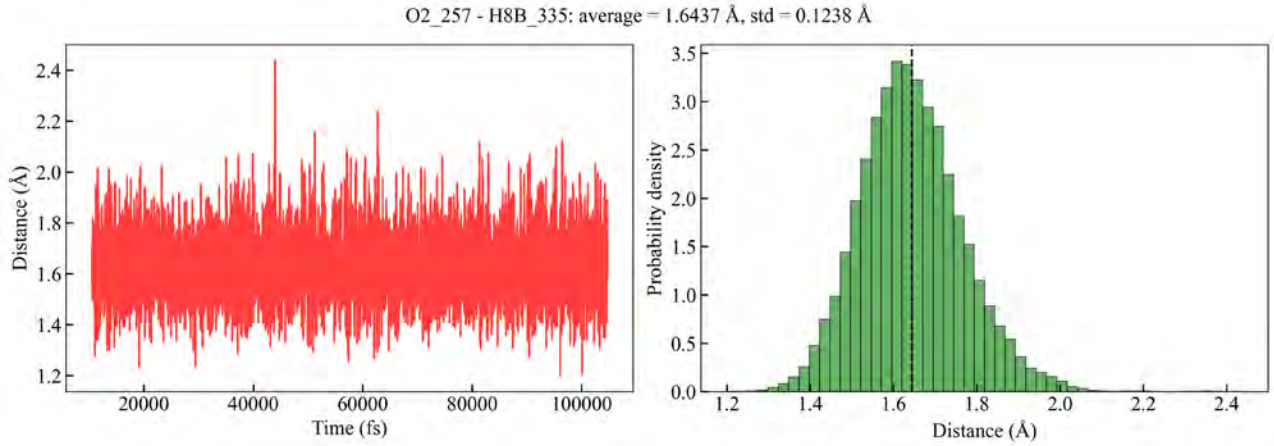
O2_257 - H8B_333

Average distance = 1.6446 Å; standard deviation = 0.1244 Å; number of points = 94257



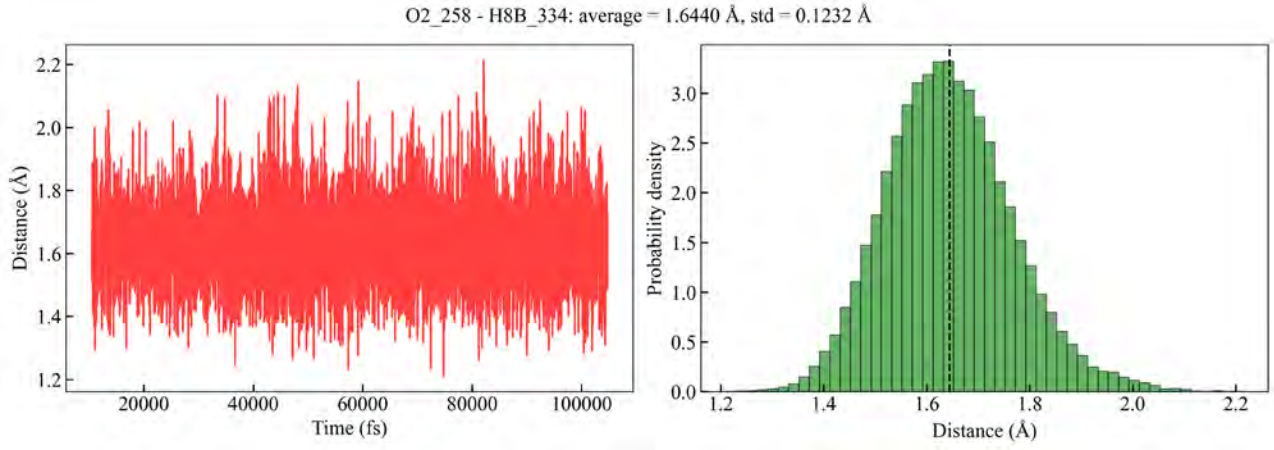
O2_257 - H8B_335

Average distance = 1.6437 Å; standard deviation = 0.1238 Å; number of points = 94257



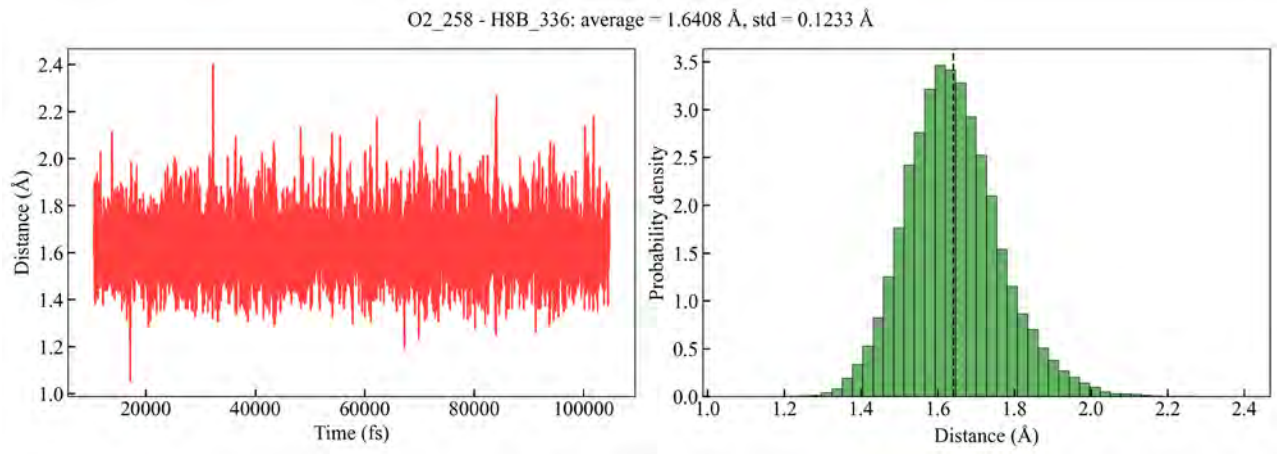
O2_258 - H8B_334

Average distance = 1.6440 Å; standard deviation = 0.1232 Å; number of points = 94257



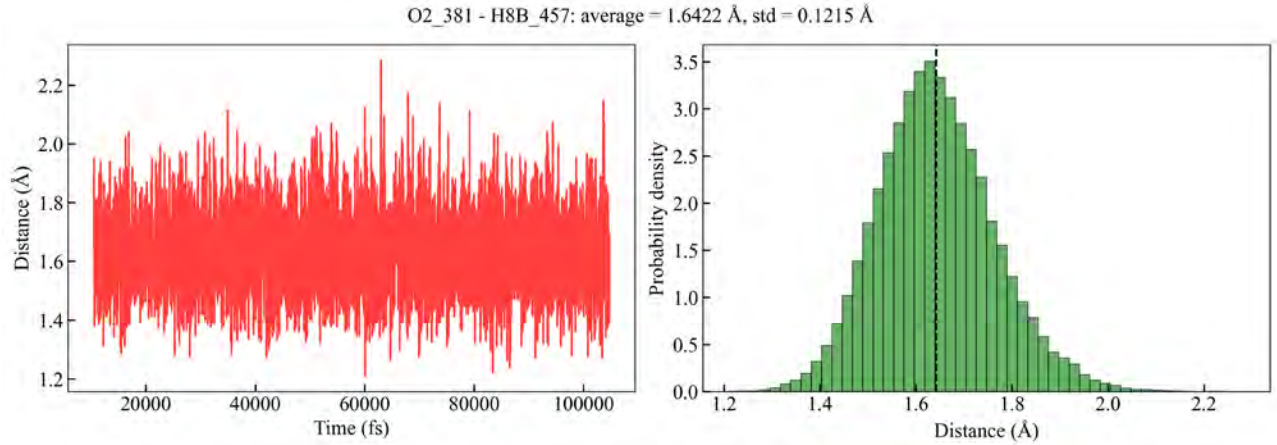
O2_258 - H8B_336

Average distance = 1.6408 Å; standard deviation = 0.1233 Å; number of points = 94257



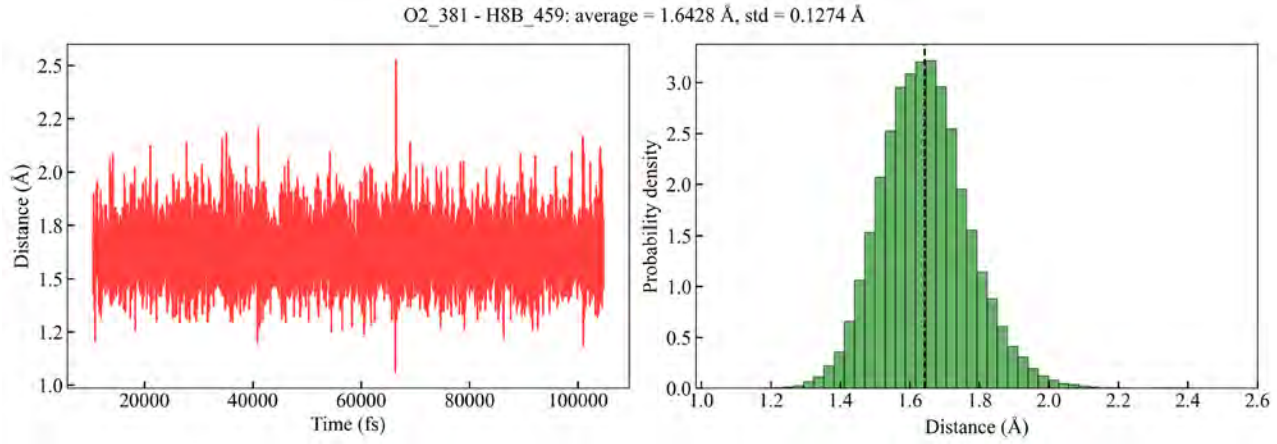
O2_381 - H8B_457

Average distance = 1.6422 Å; standard deviation = 0.1215 Å; number of points = 94257



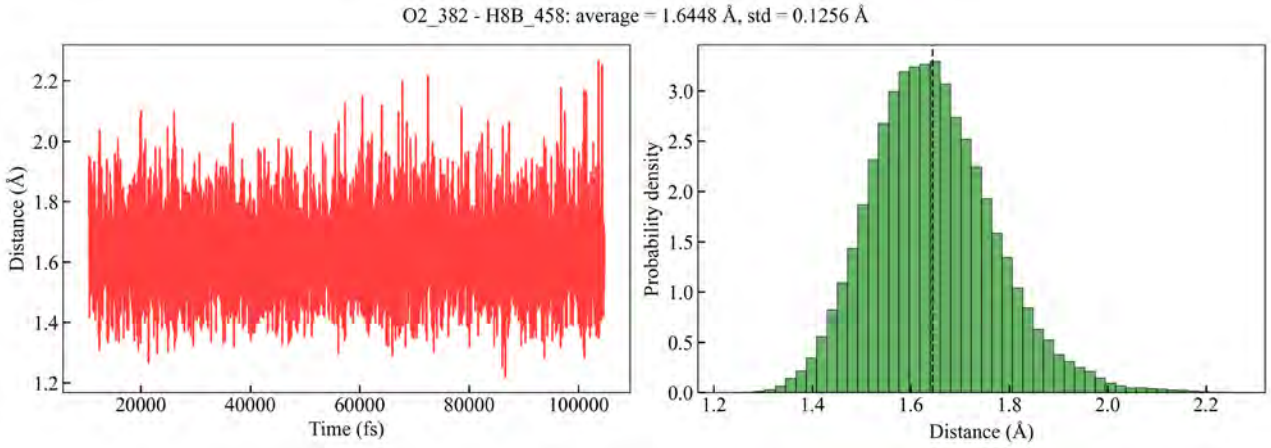
O2_381 - H8B_459

Average distance = 1.6428 Å; standard deviation = 0.1274 Å; number of points = 94257



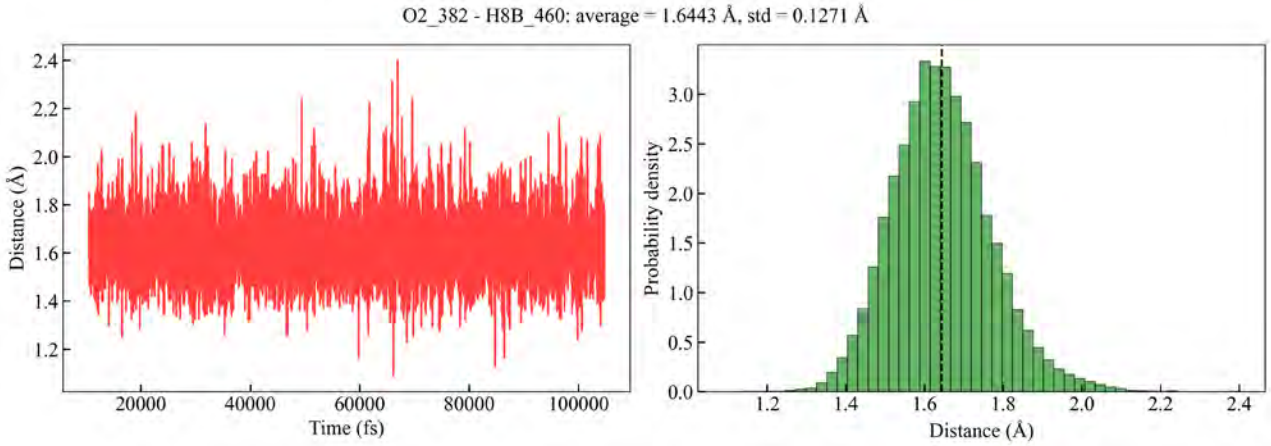
O2_382 - H8B_458

Average distance = 1.6448 Å; standard deviation = 0.1256 Å; number of points = 94257



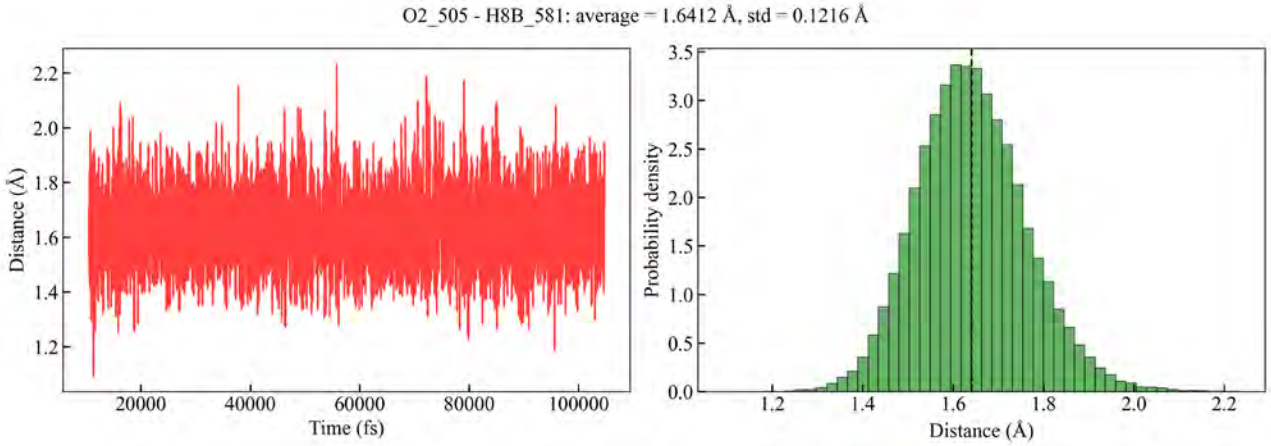
O2_382 - H8B_460

Average distance = 1.6443 Å; standard deviation = 0.1271 Å; number of points = 94257



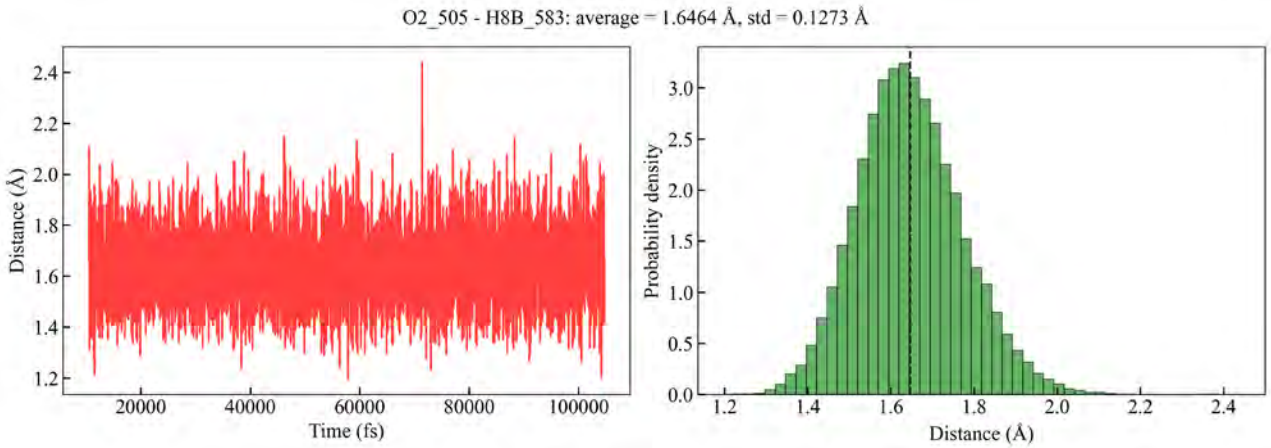
O2_505 - H8B_581

Average distance = 1.6412 Å; standard deviation = 0.1216 Å; number of points = 94257



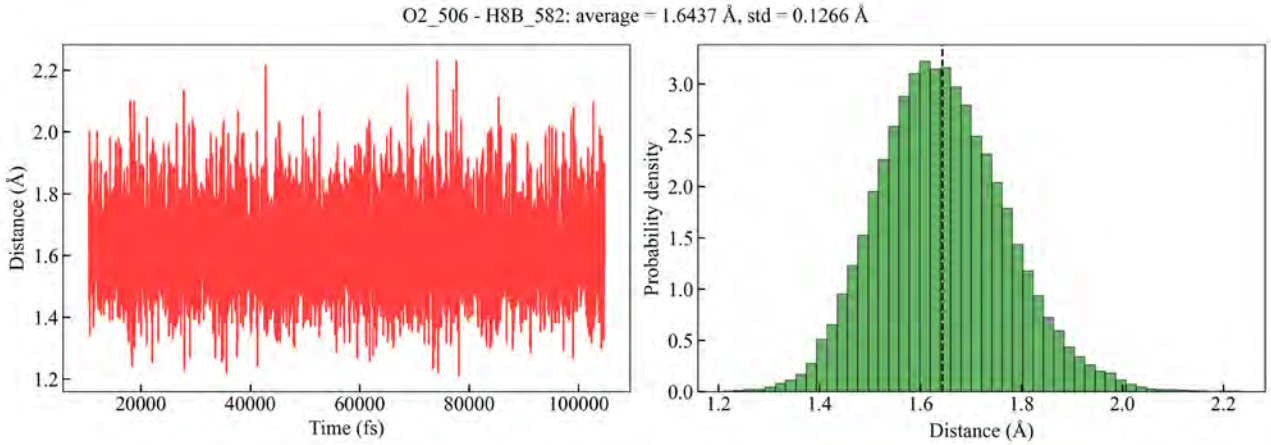
O2_505 - H8B_583

Average distance = 1.6464 Å; standard deviation = 0.1273 Å; number of points = 94257



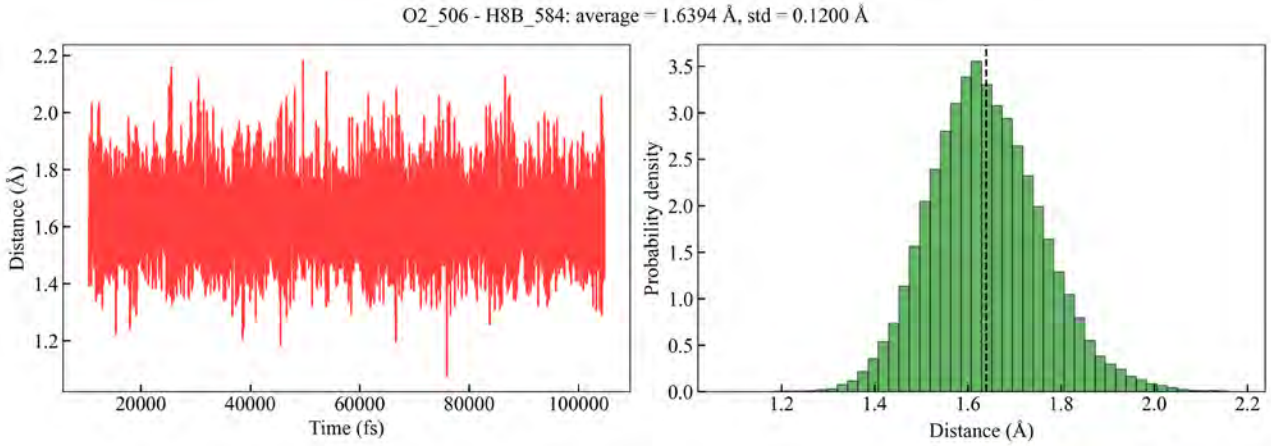
O2_506 - H8B_582

Average distance = 1.6437 Å; standard deviation = 0.1266 Å; number of points = 94257



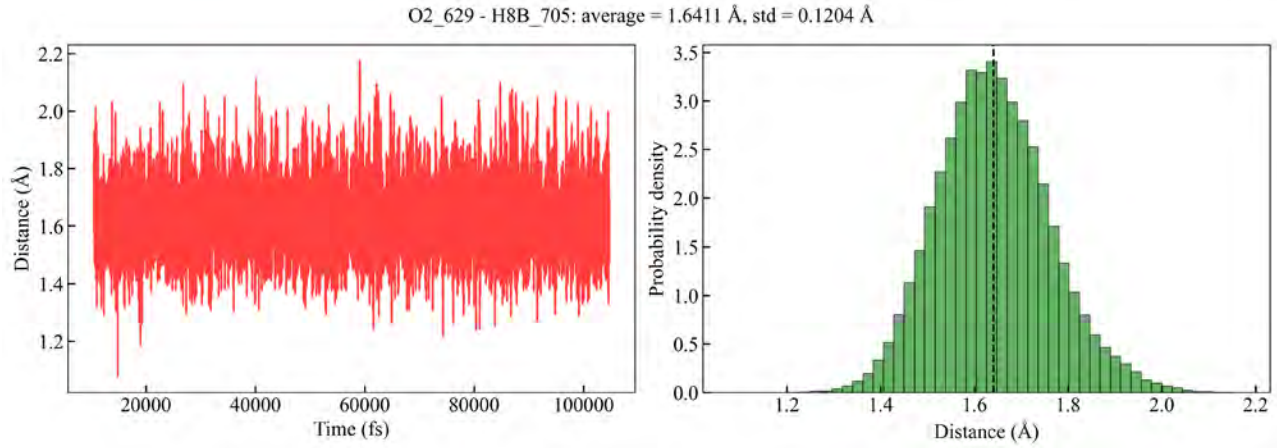
O2_506 - H8B_584

Average distance = 1.6394 Å; standard deviation = 0.1200 Å; number of points = 94257



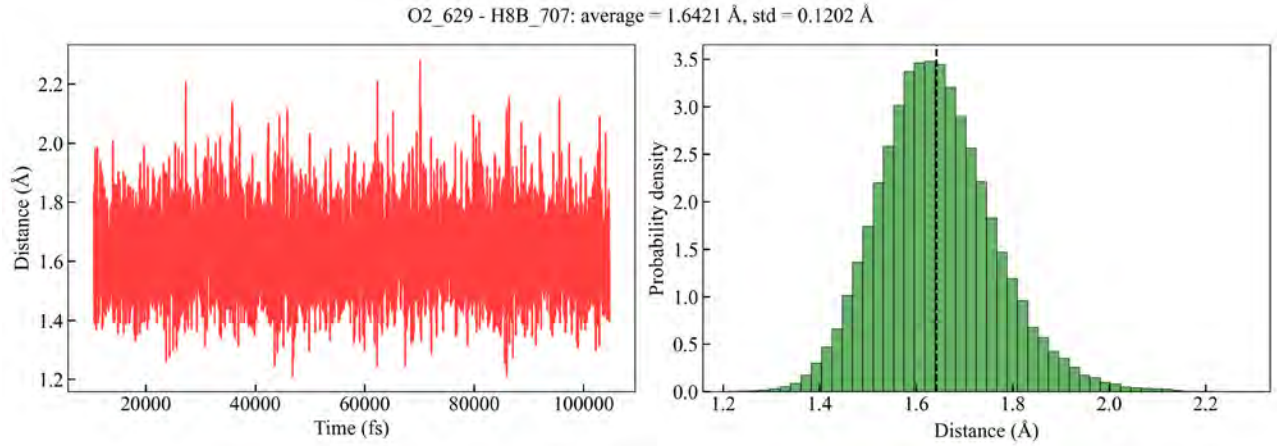
O2_629 - H8B_705

Average distance = 1.6411 Å; standard deviation = 0.1204 Å; number of points = 94257



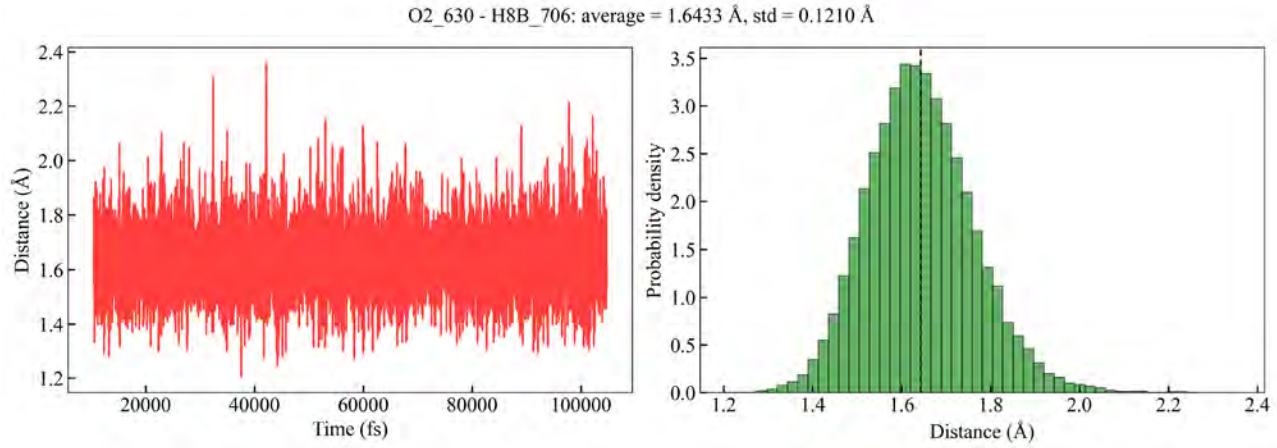
O2_629 - H8B_707

Average distance = 1.6421 Å; standard deviation = 0.1202 Å; number of points = 94257



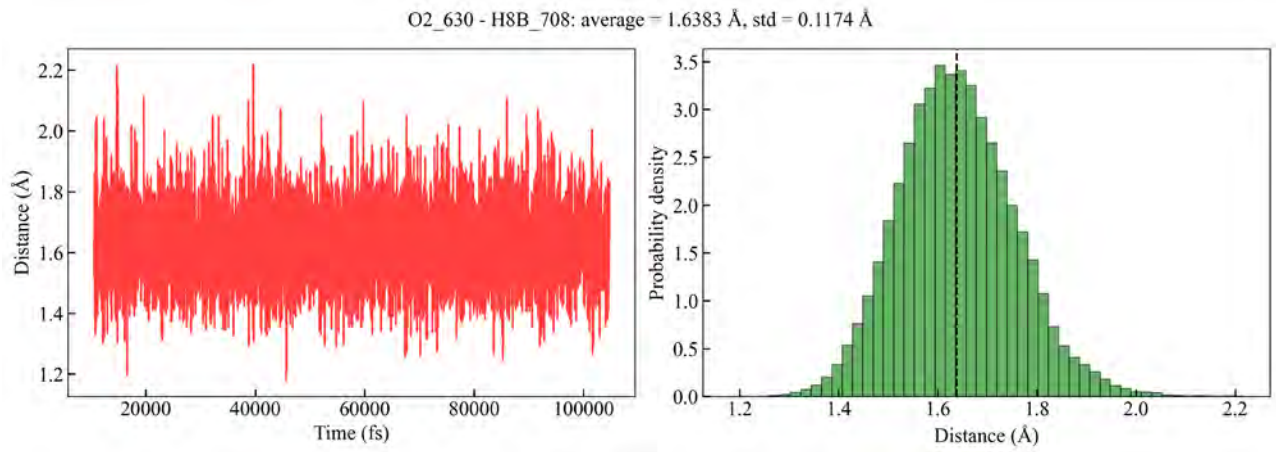
O2_630 - H8B_706

Average distance = 1.6433 Å; standard deviation = 0.1210 Å; number of points = 94257



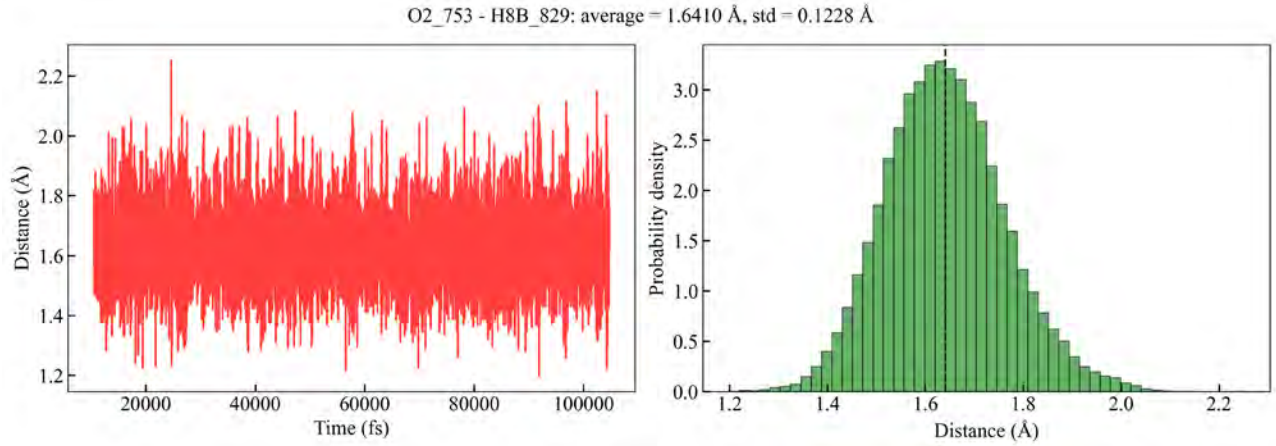
O2_630 - H8B_708

Average distance = 1.6383 Å; standard deviation = 0.1174 Å; number of points = 94257



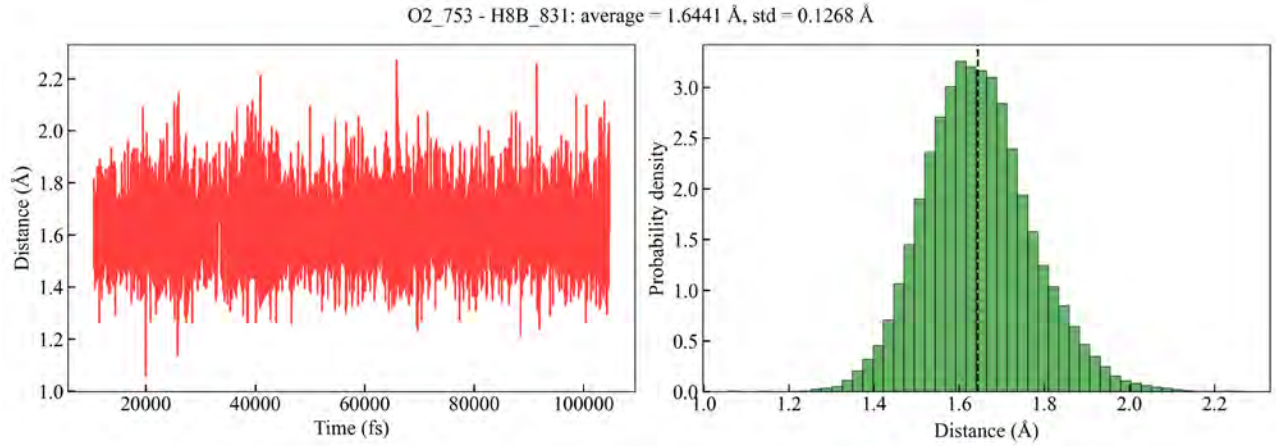
O2_753 - H8B_829

Average distance = 1.6410 Å; standard deviation = 0.1228 Å; number of points = 94257



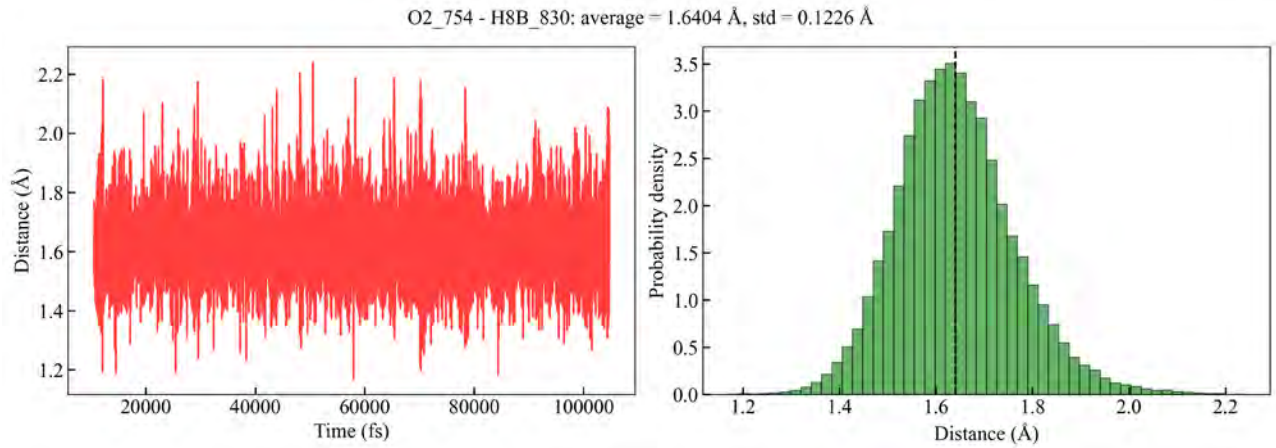
O2_753 - H8B_831

Average distance = 1.6441 Å; standard deviation = 0.1268 Å; number of points = 94257



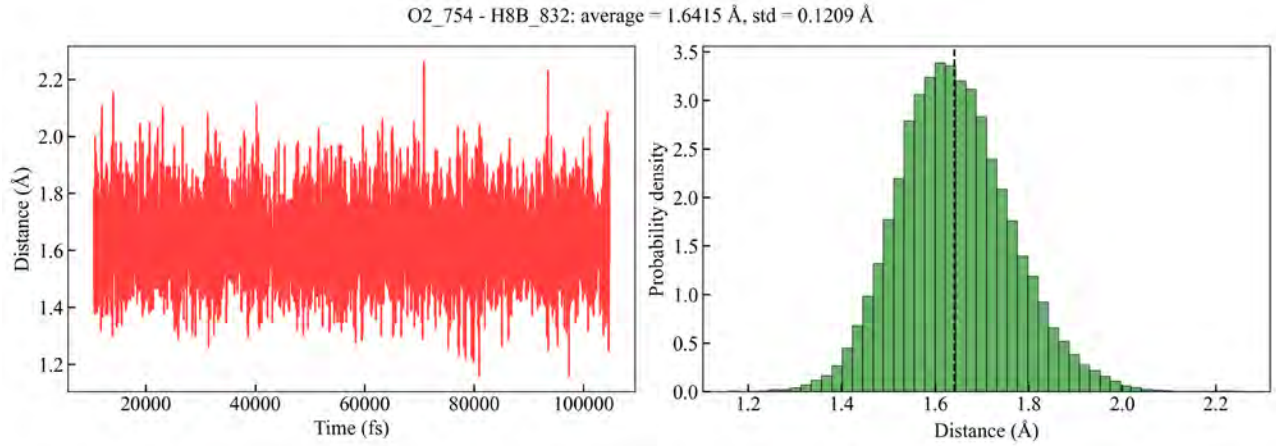
O2_754 - H8B_830

Average distance = 1.6404 Å; standard deviation = 0.1226 Å; number of points = 94257



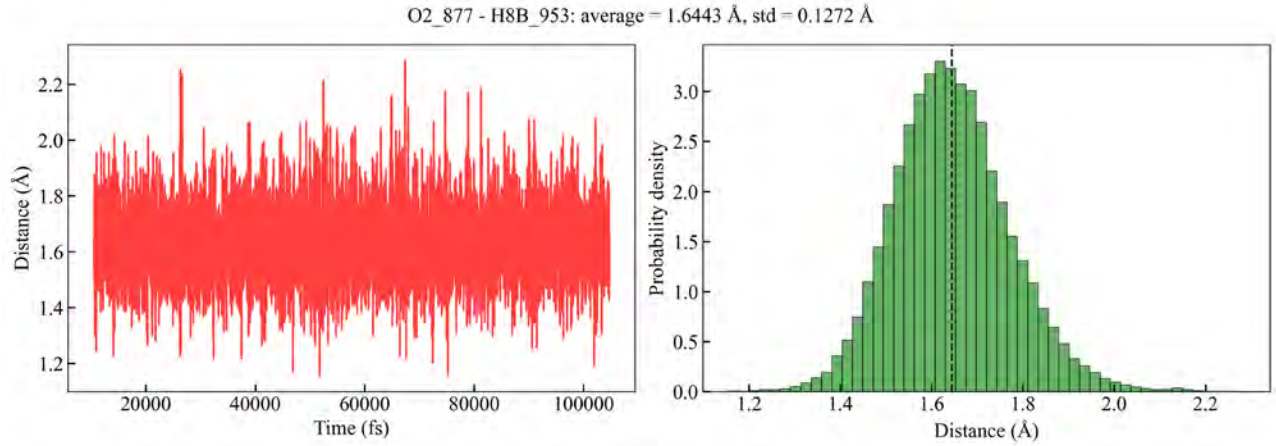
O2_754 - H8B_832

Average distance = 1.6415 Å; standard deviation = 0.1209 Å; number of points = 94257



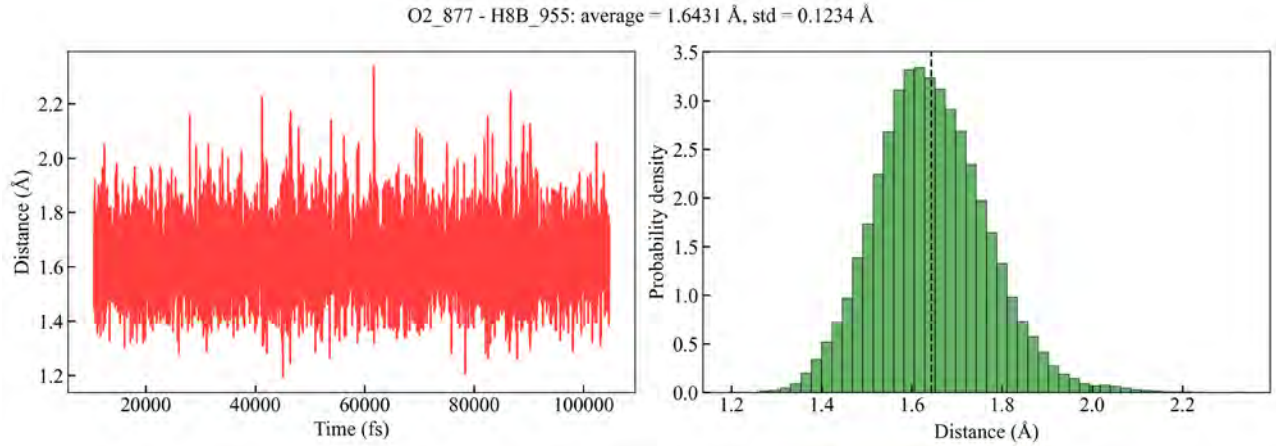
O2_877 - H8B_953

Average distance = 1.6443 Å; standard deviation = 0.1272 Å; number of points = 94257



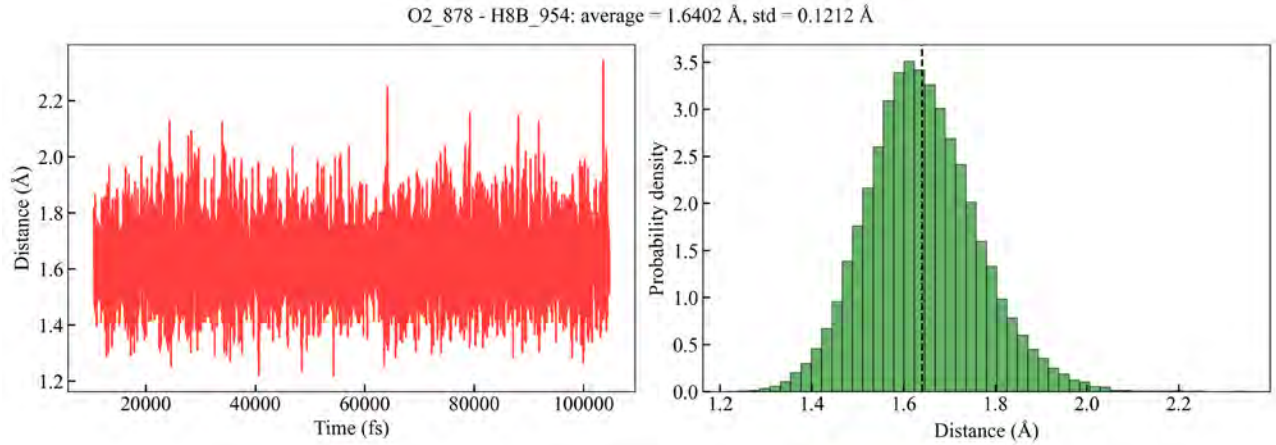
O2_877 - H8B_955

Average distance = 1.6431 Å; standard deviation = 0.1234 Å; number of points = 94257



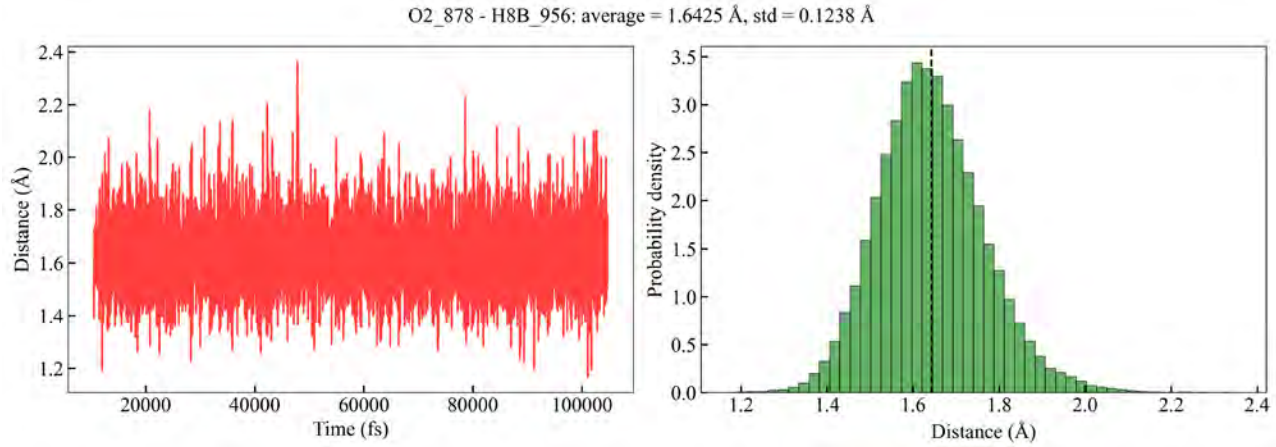
O2_878 - H8B_954

Average distance = 1.6402 Å; standard deviation = 0.1212 Å; number of points = 94257



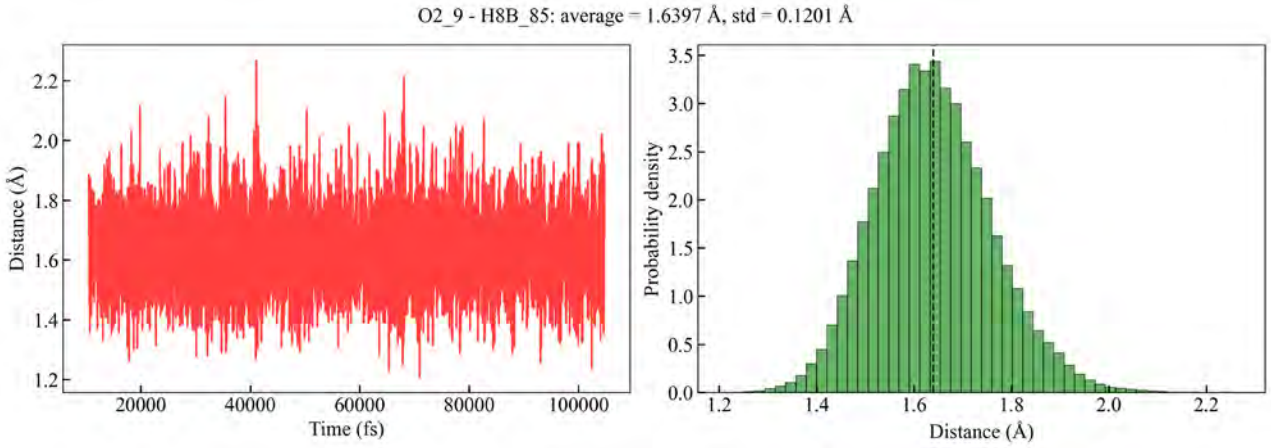
O2_878 - H8B_956

Average distance = 1.6425 Å; standard deviation = 0.1238 Å; number of points = 94257



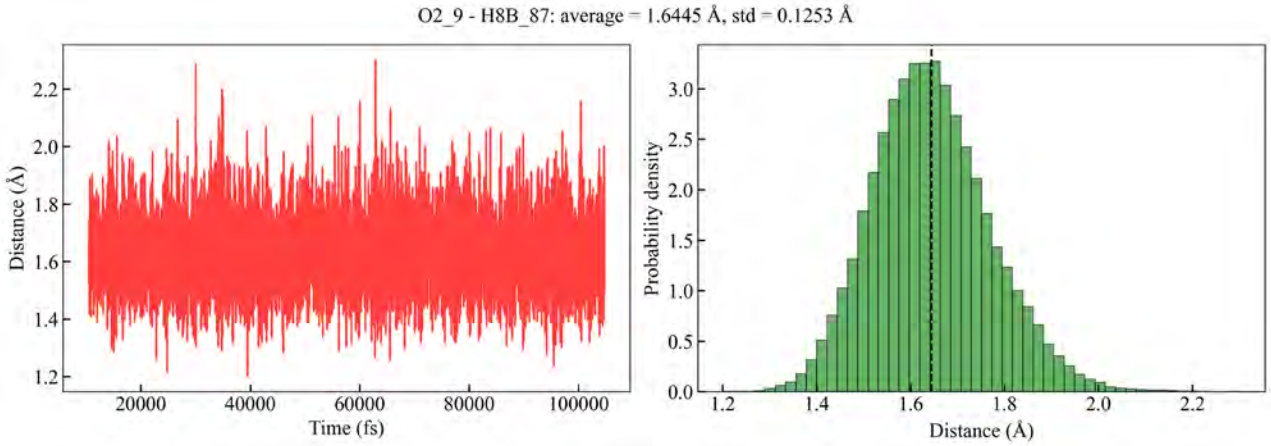
O2_9 - H8B_85

Average distance = 1.6397 Å; standard deviation = 0.1201 Å; number of points = 94257



O2_9 - H8B_87

Average distance = 1.6445 Å; standard deviation = 0.1253 Å; number of points = 94257



3.2.2. P1 at 400 K - Bond Distance Analysis

Table S19. Individual time-averaged hydrogen-involving atomic distances for all equivalent proton environments in the P1 bulk AIMD trajectory at 400 K.

Bond type	Average distance (Å)	Standard dev. σ (Å)	Number of points
N3_143 - H3B_487	2.2576	0.3203	91387
N3_144 - H3B_488	2.2434	0.3151	91387
N3_145 - H3B_485	2.2316	0.3051	91387
N3_146 - H3B_486	2.2488	0.3116	91387
N3_19 - H3B_363	2.2453	0.3199	91387
N3_20 - H3B_364	2.2589	0.3221	91387
N3_22 - H3B_362	2.2922	0.3951	91387
N3_267 - H3B_115	2.2546	0.3213	91387
N3_268 - H3B_116	2.2475	0.3272	91387
N3_269 - H3B_113	2.2471	0.3112	91387
N3_391 - H3B_239	2.2605	0.3211	91387
N3_392 - H3B_240	3.2479	0.6168	91387
N3_393 - H3B_237	2.2606	0.3274	91387
N3_394 - H3B_238	2.2678	0.3295	91387
N3_515 - H3B_859	2.2545	0.3084	91387
N3_516 - H3B_860	2.2387	0.3141	91387
N3_517 - H3B_857	2.2544	0.3185	91387
N3_518 - H3B_858	2.2424	0.3111	91387
N3_639 - H3B_983	2.2498	0.3212	91387
N3_640 - H3B_984	2.2540	0.3189	91387
N3_641 - H3B_981	2.2501	0.3034	91387
N3_642 - H3B_982	2.2562	0.3233	91387
N3_763 - H3B_611	2.2555	0.3086	91387
N3_765 - H3B_609	2.2254	0.2982	91387
N3_766 - H3B_610	2.2557	0.3119	91387
N3_887 - H3B_735	2.2478	0.3162	91387
N3_888 - H3B_736	2.2592	0.3130	91387
N3_889 - H3B_733	2.2505	0.3255	91387
N4_147 - H3A_229	1.9369	0.2029	91387
N4_148 - H3A_230	1.9348	0.2083	91387
N4_149 - H3A_231	1.9402	0.2081	91387
N4_150 - H3A_232	1.9288	0.1901	91387
N4_24 - H3A_106	1.9825	0.3196	91387
N4_25 - H3A_107	1.9448	0.2176	91387
N4_26 - H3A_108	1.9397	0.2146	91387
N4_271 - H3A_353	1.9368	0.2043	91387
N4_273 - H3A_355	1.9304	0.1978	91387
N4_274 - H3A_356	1.9334	0.1937	91387
N4_395 - H3A_477	1.9585	0.2941	91387
N4_396 - H3A_478	1.9384	0.2209	91387
N4_397 - H3A_479	1.9355	0.2090	91387
N4_398 - H3A_480	2.9761	0.6103	91387
N4_519 - H3A_601	1.9404	0.2043	91387
N4_520 - H3A_602	1.9342	0.1974	91387
N4_521 - H3A_603	1.9380	0.1968	91387
N4_522 - H3A_604	1.9254	0.1911	91387
N4_643 - H3A_725	1.9263	0.1869	91387
N4_644 - H3A_726	1.9264	0.1878	91387
N4_645 - H3A_727	1.9294	0.1990	91387

N4_646 - H3A_728	1.9308	0.1991	91387
N4_767 - H3A_849	1.9451	0.2139	91387
N4_768 - H3A_850	1.9302	0.1937	91387
N4_769 - H3A_851	1.9219	0.1788	91387
N4_891 - H3A_973	1.9434	0.2142	91387
N4_893 - H3A_975	1.9431	0.2058	91387
N4_894 - H3A_976	1.9266	0.1884	91387
O1_1 - H1B_94	2.0502	0.2410	91387
O1_125 - H1B_218	2.0508	0.2474	91387
O1_126 - H1B_217	2.0577	0.2558	91387
O1_127 - H1B_220	2.0398	0.2240	91387
O1_128 - H1B_219	2.0655	0.2529	91387
O1_2 - H1B_93	2.0520	0.2346	91387
O1_249 - H1B_342	2.0474	0.2384	91387
O1_250 - H1B_341	2.0515	0.2418	91387
O1_251 - H1B_344	2.0548	0.2410	91387
O1_252 - H1B_343	2.0483	0.2382	91387
O1_3 - H1B_96	2.0478	0.2403	91387
O1_373 - H1B_466	2.0492	0.2413	91387
O1_374 - H1B_465	2.0484	0.2372	91387
O1_375 - H1B_468	2.0456	0.2334	91387
O1_376 - H1B_467	2.0445	0.2338	91387
O1_4 - H1B_95	2.0474	0.2384	91387
O1_497 - H1B_590	2.0348	0.2207	91387
O1_498 - H1B_589	2.0314	0.2157	91387
O1_499 - H1B_592	2.0577	0.2544	91387
O1_500 - H1B_591	2.0574	0.2492	91387
O1_621 - H1B_714	2.0511	0.2359	91387
O1_622 - H1B_713	2.0436	0.2289	91387
O1_623 - H1B_716	2.0478	0.2401	91387
O1_624 - H1B_715	2.0581	0.2495	91387
O1_745 - H1B_838	2.0474	0.2397	91387
O1_746 - H1B_837	2.0456	0.2364	91387
O1_747 - H1B_840	2.0585	0.2525	91387
O1_748 - H1B_839	2.0591	0.2446	91387
O1_869 - H1B_962	2.0401	0.2307	91387
O1_870 - H1B_961	2.0527	0.2452	91387
O1_871 - H1B_964	2.0493	0.2374	91387
O1_872 - H1B_963	2.0470	0.2314	91387
O1_1 - H2A_72	1.9191	0.1842	91387
O1_125 - H2A_196	1.9256	0.1875	91387
O1_126 - H2A_195	1.9403	0.2081	91387
O1_127 - H2A_194	1.9212	0.1863	91387
O1_128 - H2A_193	1.9317	0.1974	91387
O1_2 - H2A_71	1.9174	0.1787	91387
O1_249 - H2A_320	1.9236	0.1928	91387
O1_250 - H2A_319	1.9254	0.1919	91387
O1_251 - H2A_318	1.9298	0.1914	91387
O1_252 - H2A_317	1.9279	0.1910	91387
O1_3 - H2A_70	1.9246	0.1877	91387
O1_373 - H2A_444	1.9170	0.1792	91387
O1_374 - H2A_443	1.9260	0.1937	91387
O1_375 - H2A_442	1.9238	0.1918	91387

O1_376 - H2A_441	1.9294	0.1918	91387
O1_4 - H2A_69	1.9270	0.1930	91387
O1_497 - H2A_568	1.9332	0.2006	91387
O1_498 - H2A_567	1.9320	0.1917	91387
O1_499 - H2A_566	1.9240	0.1891	91387
O1_500 - H2A_565	1.9174	0.1850	91387
O1_621 - H2A_692	1.9254	0.1877	91387
O1_622 - H2A_691	1.9299	0.1981	91387
O1_623 - H2A_690	1.9244	0.1888	91387
O1_624 - H2A_689	1.9237	0.1918	91387
O1_745 - H2A_816	1.9290	0.1972	91387
O1_746 - H2A_815	1.9303	0.1971	91387
O1_747 - H2A_814	1.9264	0.1946	91387
O1_748 - H2A_813	1.9274	0.1884	91387
O1_869 - H2A_940	1.9238	0.1939	91387
O1_870 - H2A_939	1.9150	0.1778	91387
O1_871 - H2A_938	1.9145	0.1849	91387
O1_872 - H2A_937	1.9263	0.1899	91387
O1_1 - H6_103	1.6672	0.1798	91387
O1_125 - H6_227	1.6653	0.1867	91387
O1_126 - H6_228	1.6651	0.1870	91387
O1_127 - H6_225	1.6667	0.1860	91387
O1_128 - H6_226	1.6548	0.1830	91387
O1_2 - H6_104	1.6652	0.1824	91387
O1_249 - H6_351	1.6562	0.1949	91387
O1_250 - H6_352	1.6666	0.1781	91387
O1_251 - H6_349	1.6592	0.1770	91387
O1_252 - H6_350	1.6579	0.1776	91387
O1_3 - H6_101	1.6607	0.1738	91387
O1_373 - H6_475	1.6670	0.1713	91387
O1_374 - H6_476	1.6631	0.1701	91387
O1_375 - H6_473	1.6642	0.1756	91387
O1_376 - H6_474	1.6642	0.1711	91387
O1_4 - H6_102	1.6577	0.1908	91387
O1_497 - H6_599	1.6626	0.1660	91387
O1_498 - H6_600	1.6670	0.1786	91387
O1_499 - H6_597	1.6615	0.1833	91387
O1_500 - H6_598	1.6620	0.1807	91387
O1_621 - H6_723	1.6651	0.1802	91387
O1_622 - H6_724	1.6623	0.1858	91387
O1_623 - H6_721	1.6628	0.1757	91387
O1_624 - H6_722	1.6580	0.1854	91387
O1_745 - H6_847	1.6682	0.1805	91387
O1_746 - H6_848	1.6663	0.1898	91387
O1_747 - H6_845	1.6634	0.1808	91387
O1_748 - H6_846	1.6554	0.1970	91387
O1_869 - H6_971	1.6563	0.1825	91387
O1_870 - H6_972	1.6671	0.1670	91387
O1_871 - H6_969	1.6702	0.1777	91387
O1_872 - H6_970	1.6568	0.1823	91387
O2_10 - H8B_86	1.6631	0.1519	91387
O2_10 - H8B_88	1.6621	0.1523	91387
O2_133 - H8B_209	1.6643	0.1494	91387

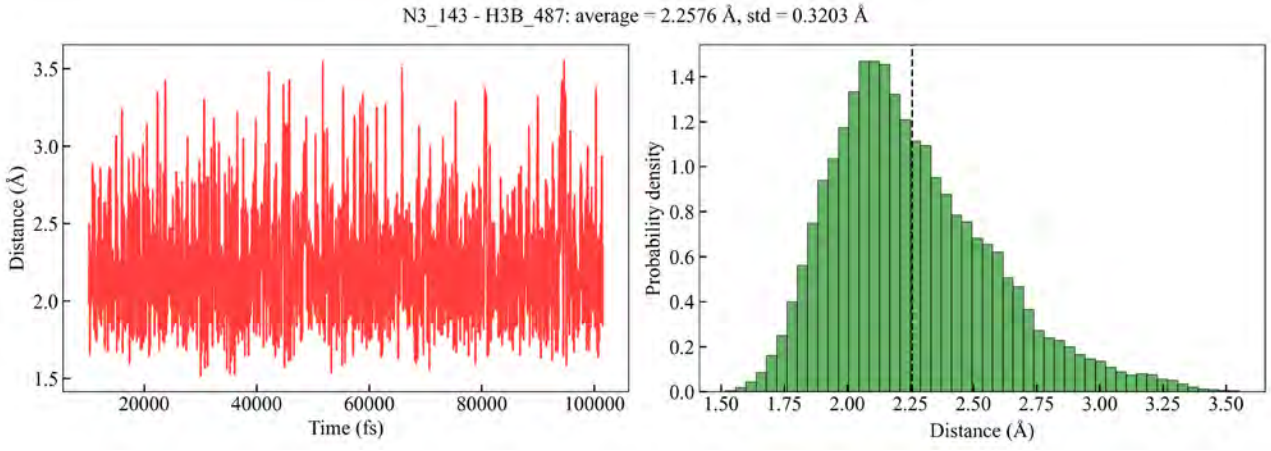
O2_133 - H8B_211	1.6553	0.1457	91387
O2_134 - H8B_210	1.6598	0.1487	91387
O2_134 - H8B_212	1.6610	0.1565	91387
O2_257 - H8B_333	1.6595	0.1444	91387
O2_257 - H8B_335	1.6613	0.1443	91387
O2_258 - H8B_334	1.6621	0.1486	91387
O2_258 - H8B_336	1.6599	0.1460	91387
O2_381 - H8B_457	1.6553	0.1455	91387
O2_381 - H8B_459	1.6580	0.1483	91387
O2_382 - H8B_458	1.6549	0.1397	91387
O2_382 - H8B_460	1.6559	0.1427	91387
O2_505 - H8B_581	1.6619	0.1492	91387
O2_505 - H8B_583	1.6533	0.1389	91387
O2_506 - H8B_582	1.6643	0.1498	91387
O2_506 - H8B_584	1.6578	0.1443	91387
O2_629 - H8B_705	1.6578	0.1467	91387
O2_629 - H8B_707	1.6569	0.1471	91387
O2_630 - H8B_706	1.6615	0.1486	91387
O2_630 - H8B_708	1.6631	0.1488	91387
O2_753 - H8B_829	1.6605	0.1497	91387
O2_753 - H8B_831	1.6600	0.1505	91387
O2_754 - H8B_830	1.6663	0.1527	91387
O2_754 - H8B_832	1.6619	0.1486	91387
O2_877 - H8B_953	1.6569	0.1398	91387
O2_877 - H8B_955	1.6567	0.1451	91387
O2_878 - H8B_954	1.6559	0.1384	91387
O2_878 - H8B_956	1.6547	0.1413	91387
O2_9 - H8B_85	1.6628	0.1538	91387
O2_9 - H8B_87	1.6575	0.1481	91387

Bond Distance Plots

N3 - H3B

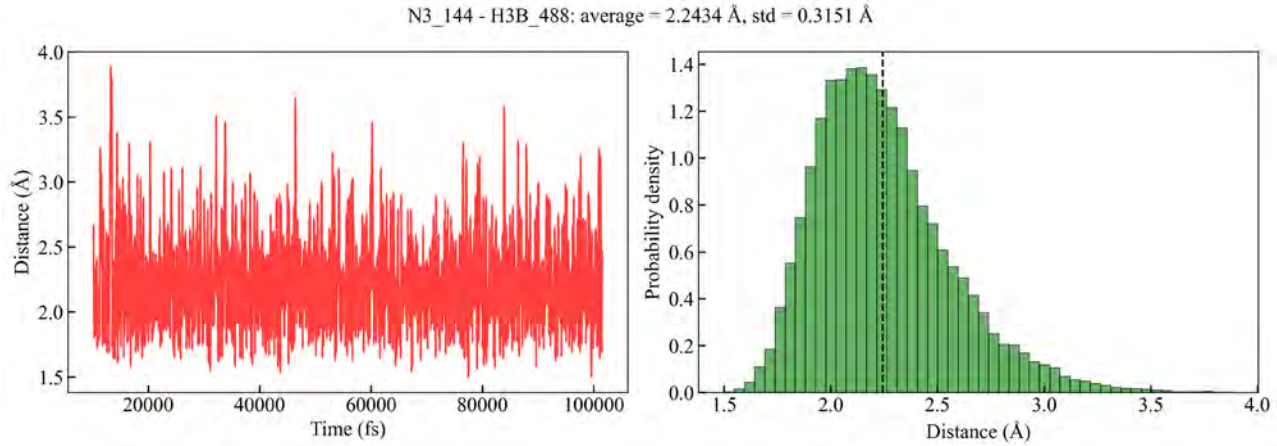
N3_143 - H3B_487

Average distance = 2.2576 Å; standard deviation = 0.3203 Å; number of points = 91387



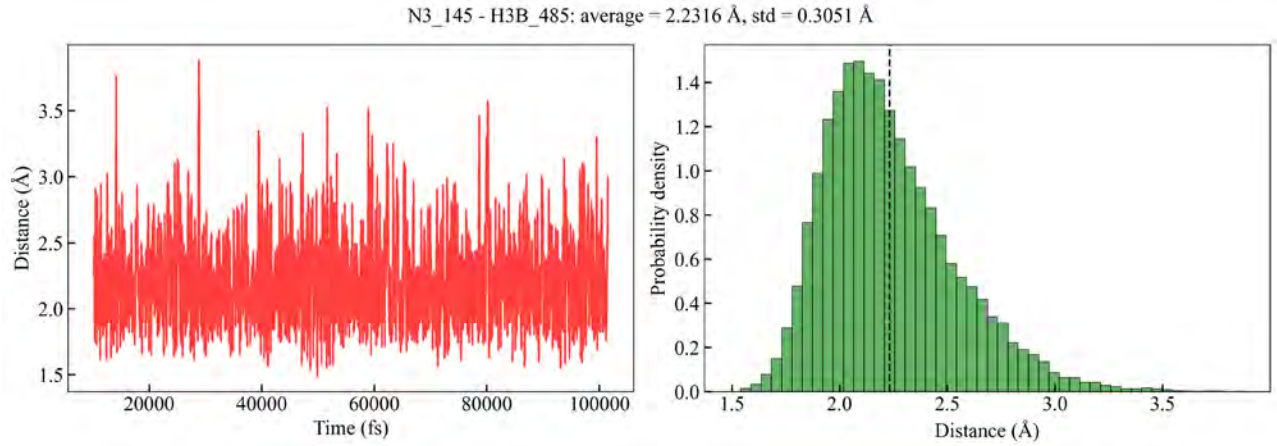
N3_144 - H3B_488

Average distance = 2.2434 Å; standard deviation = 0.3151 Å; number of points = 91387



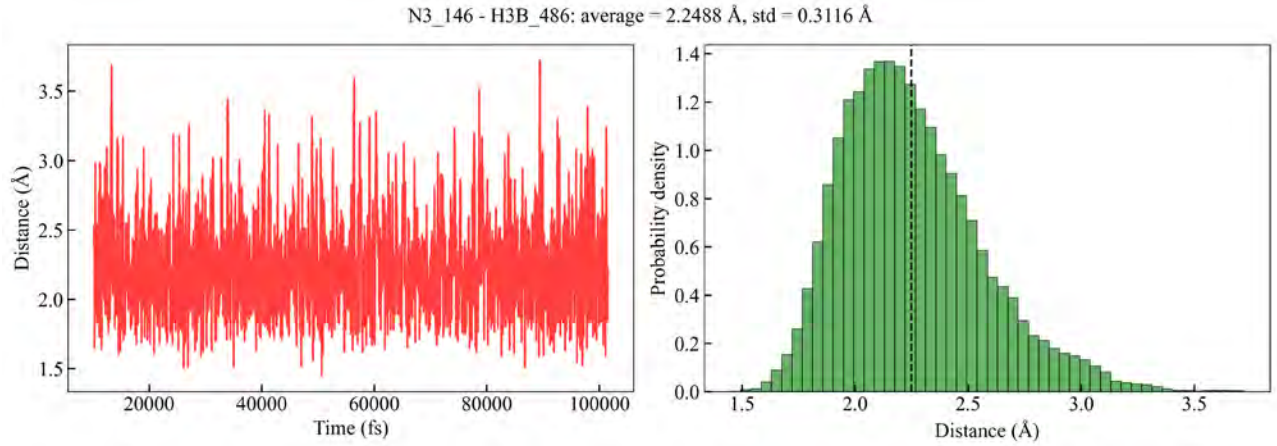
N3_145 - H3B_485

Average distance = 2.2316 Å; standard deviation = 0.3051 Å; number of points = 91387



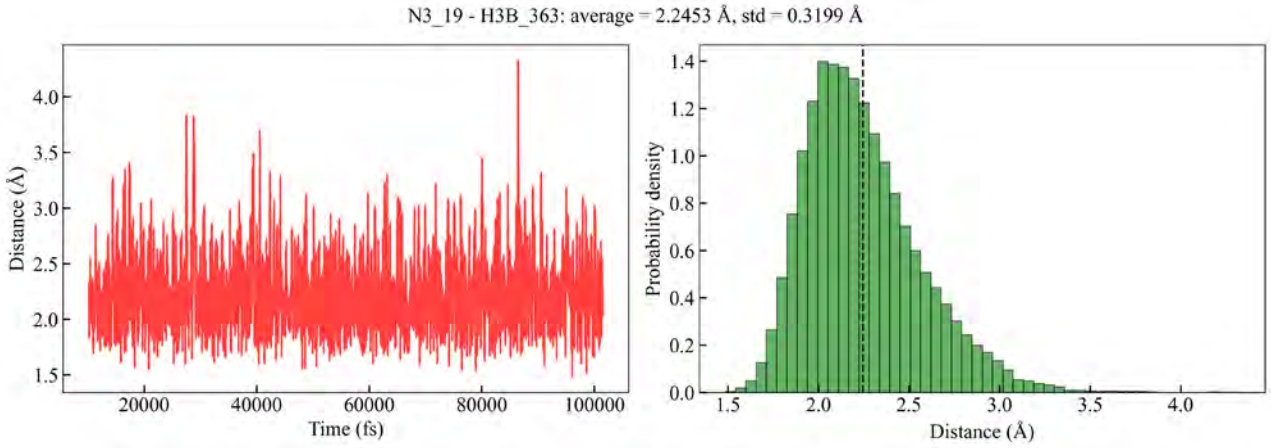
N3_146 - H3B_486

Average distance = 2.2488 Å; standard deviation = 0.3116 Å; number of points = 91387



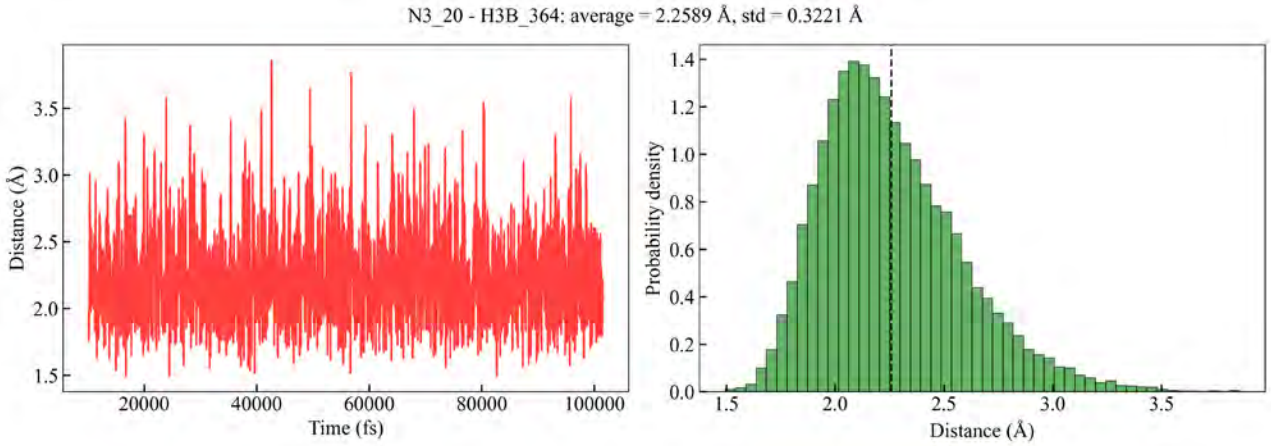
N3_19 - H3B_363

Average distance = 2.2453 Å; standard deviation = 0.3199 Å; number of points = 91387



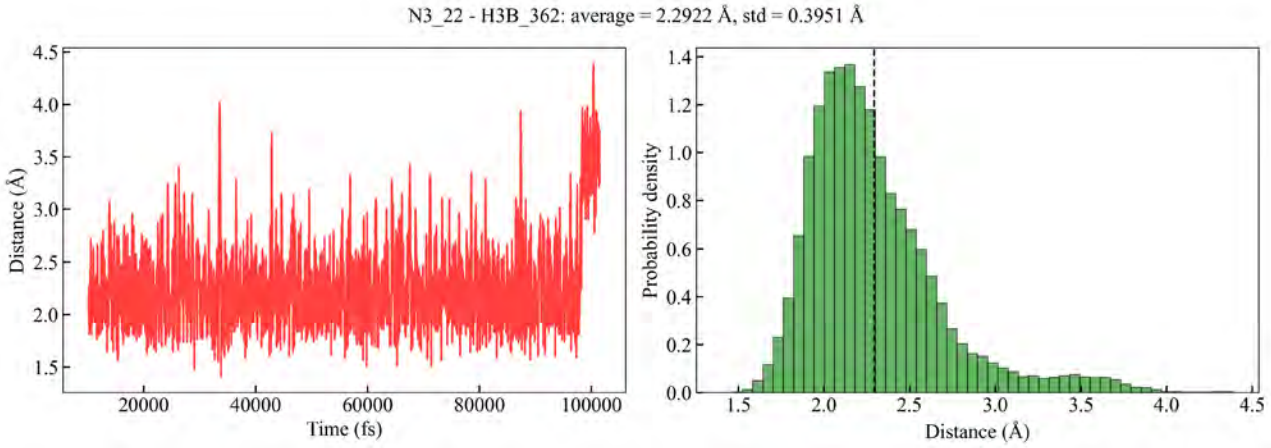
N3_20 - H3B_364

Average distance = 2.2589 Å; standard deviation = 0.3221 Å; number of points = 91387



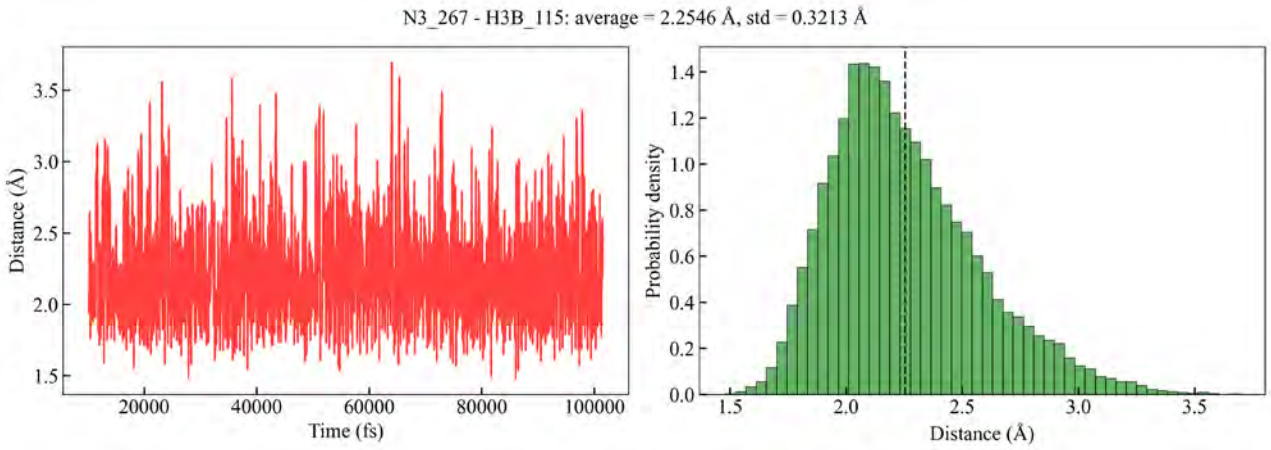
N3_22 - H3B_362

Average distance = 2.2922 Å; standard deviation = 0.3951 Å; number of points = 91387



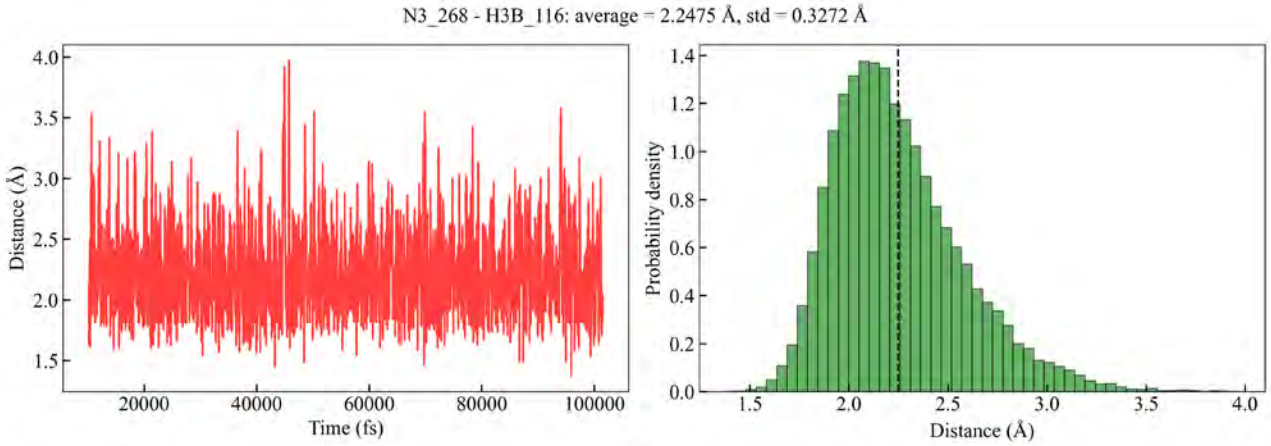
N3_267 - H3B_115

Average distance = 2.2546 Å; standard deviation = 0.3213 Å; number of points = 91387



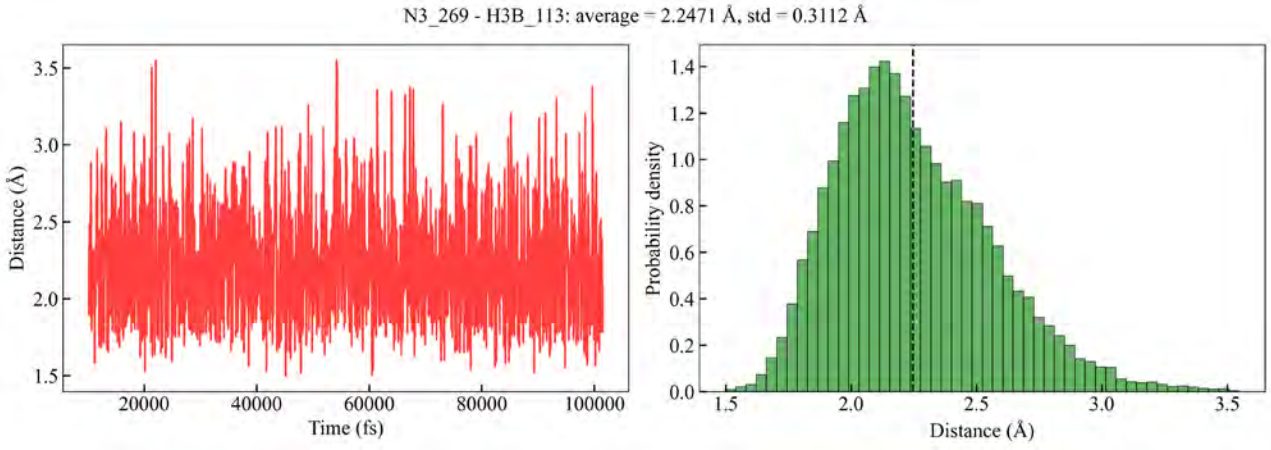
N3_268 - H3B_116

Average distance = 2.2475 Å; standard deviation = 0.3272 Å; number of points = 91387



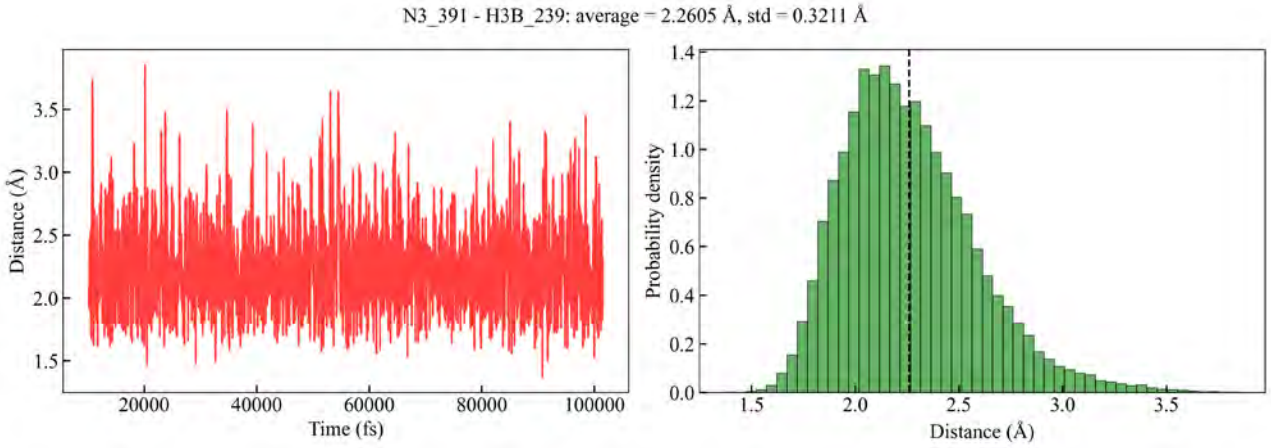
N3_269 - H3B_113

Average distance = 2.2471 Å; standard deviation = 0.3112 Å; number of points = 91387



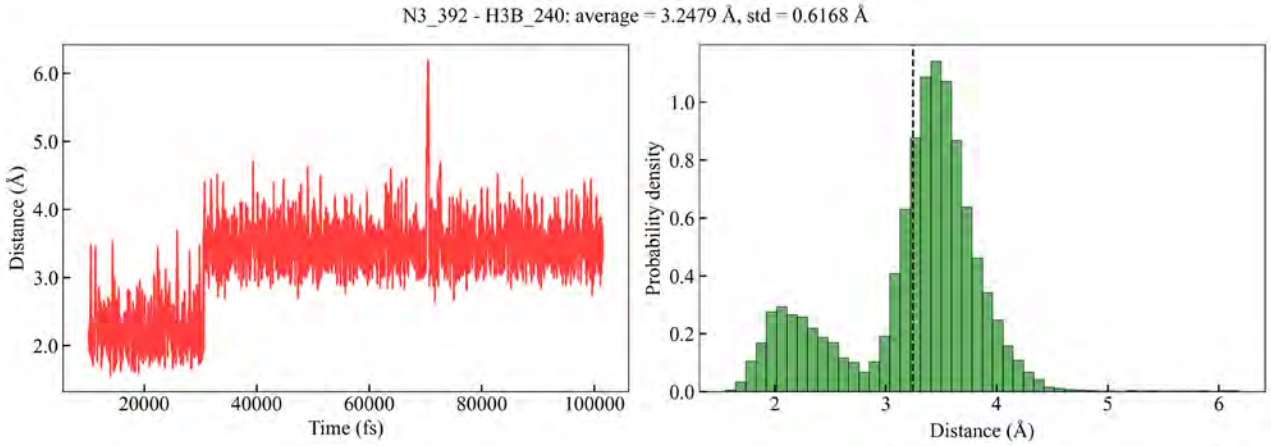
N3_391 - H3B_239

Average distance = 2.2605 Å; standard deviation = 0.3211 Å; number of points = 91387



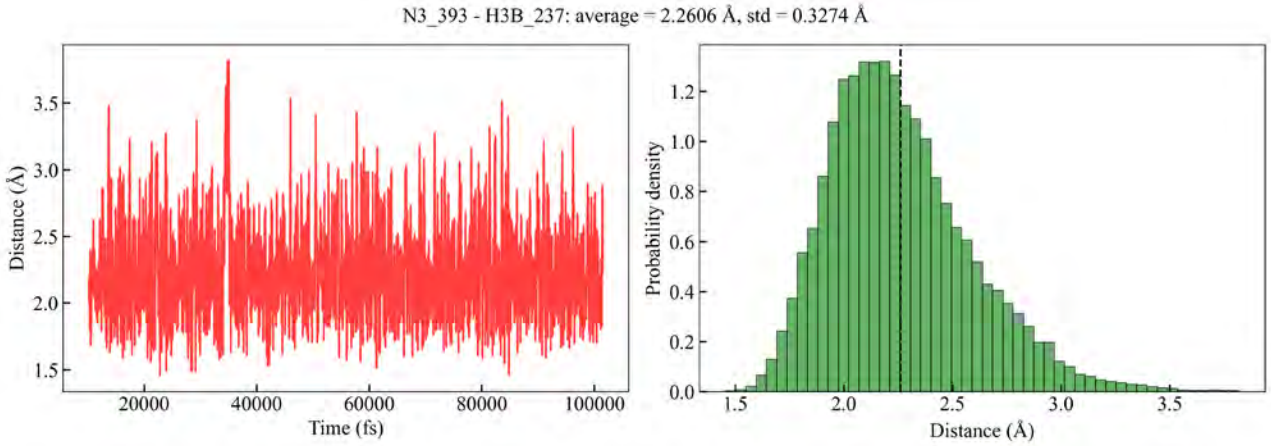
N3_392 - H3B_240

Average distance = 3.2479 Å; standard deviation = 0.6168 Å; number of points = 91387



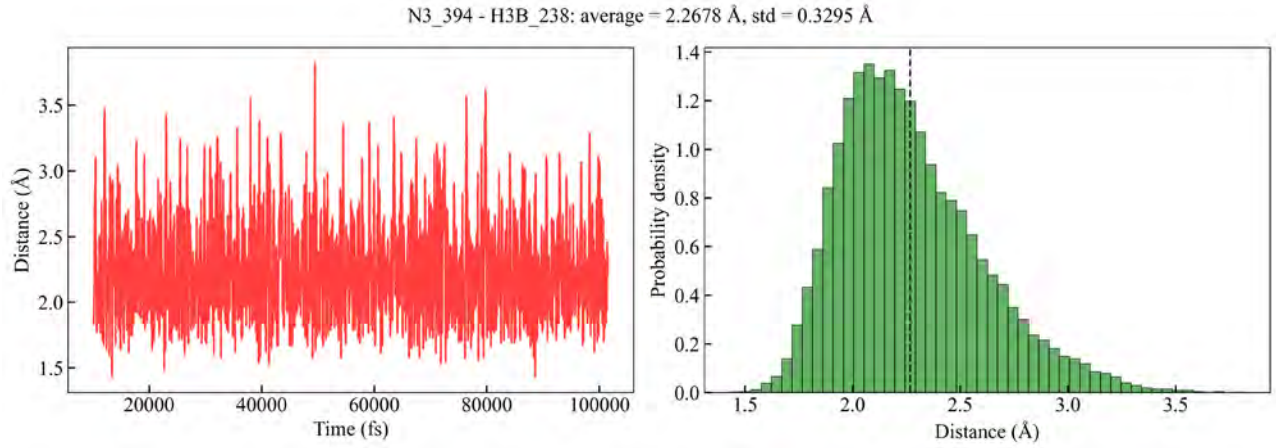
N3_393 - H3B_237

Average distance = 2.2606 Å; standard deviation = 0.3274 Å; number of points = 91387



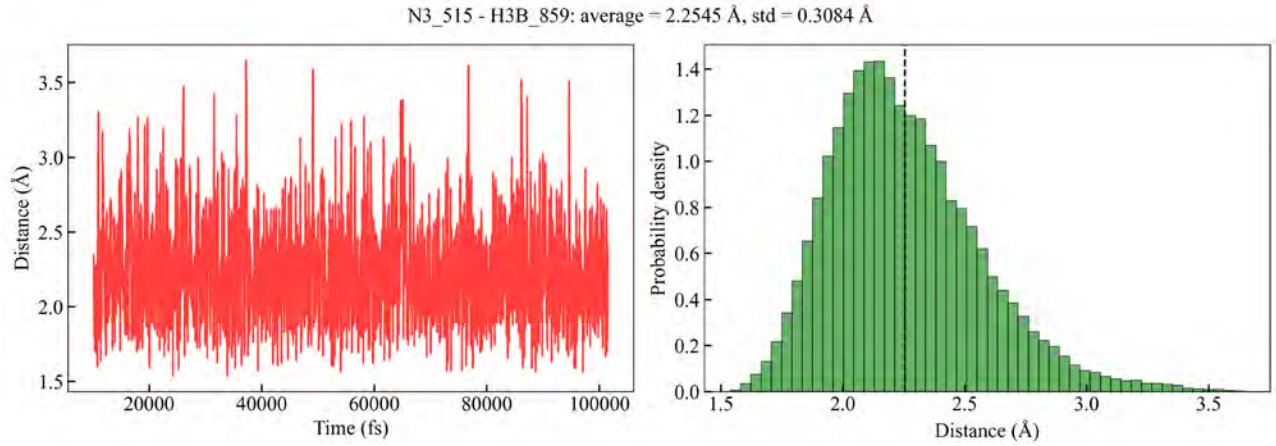
N3_394 - H3B_238

Average distance = 2.2678 Å; standard deviation = 0.3295 Å; number of points = 91387



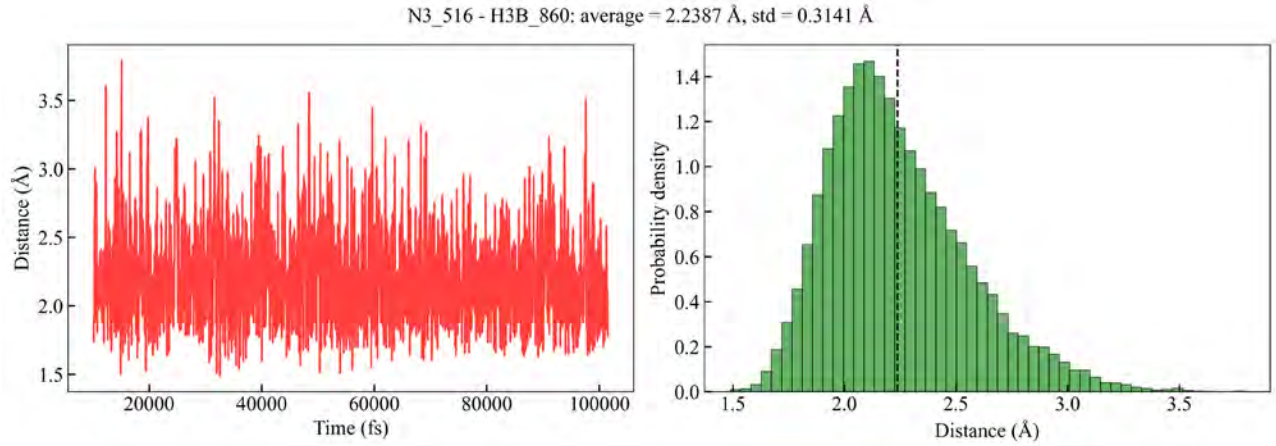
N3_515 - H3B_859

Average distance = 2.2545 Å; standard deviation = 0.3084 Å; number of points = 91387



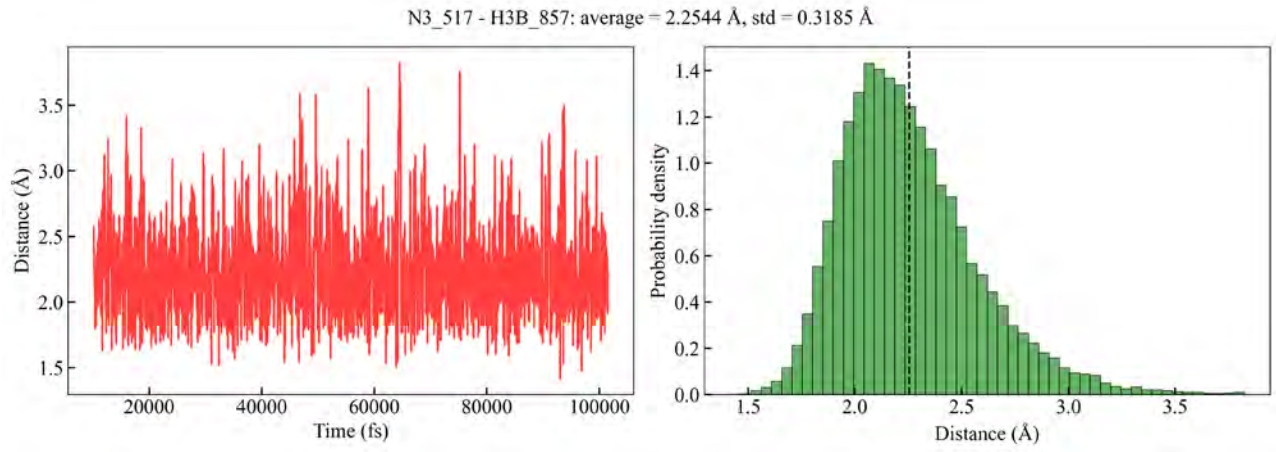
N3_516 - H3B_860

Average distance = 2.2387 Å; standard deviation = 0.3141 Å; number of points = 91387



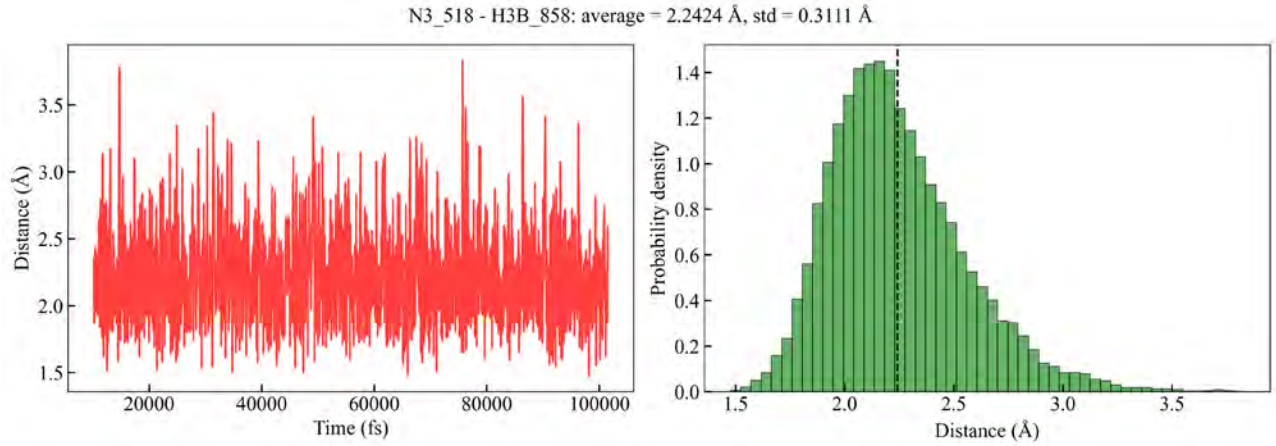
N3_517 - H3B_857

Average distance = 2.2544 Å; standard deviation = 0.3185 Å; number of points = 91387



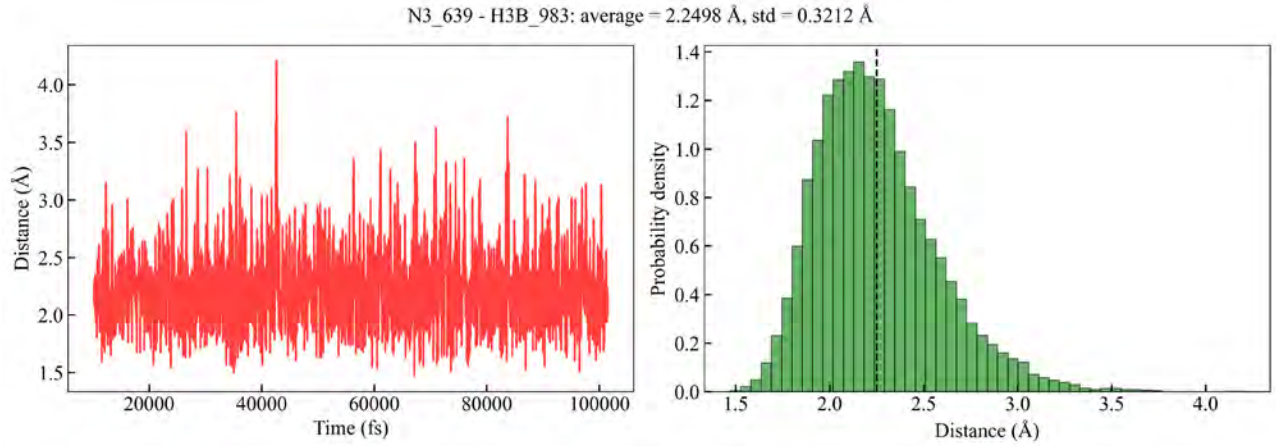
N3_518 - H3B_858

Average distance = 2.2424 Å; standard deviation = 0.3111 Å; number of points = 91387



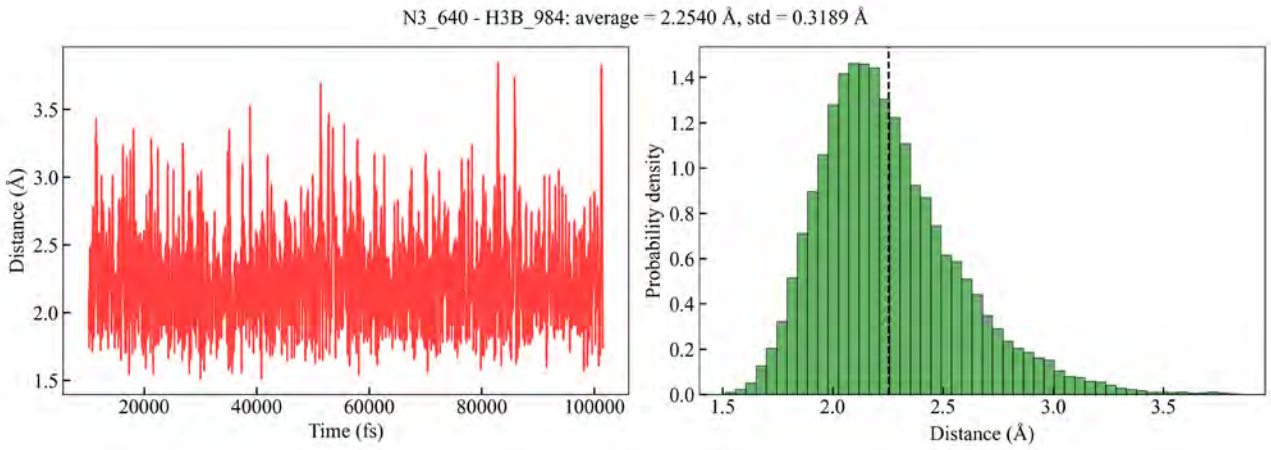
N3_639 - H3B_983

Average distance = 2.2498 Å; standard deviation = 0.3212 Å; number of points = 91387



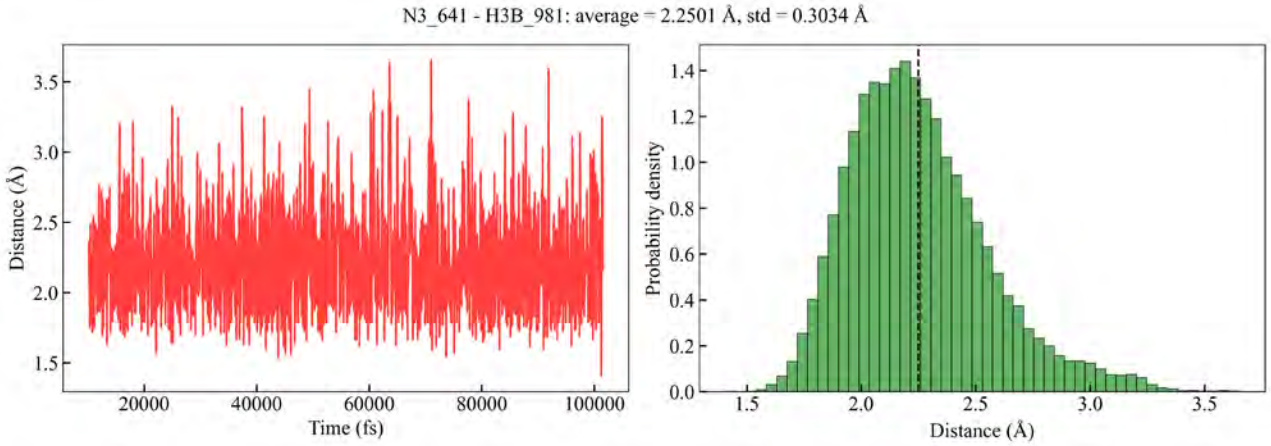
N3_640 - H3B_984

Average distance = 2.2540 Å; standard deviation = 0.3189 Å; number of points = 91387



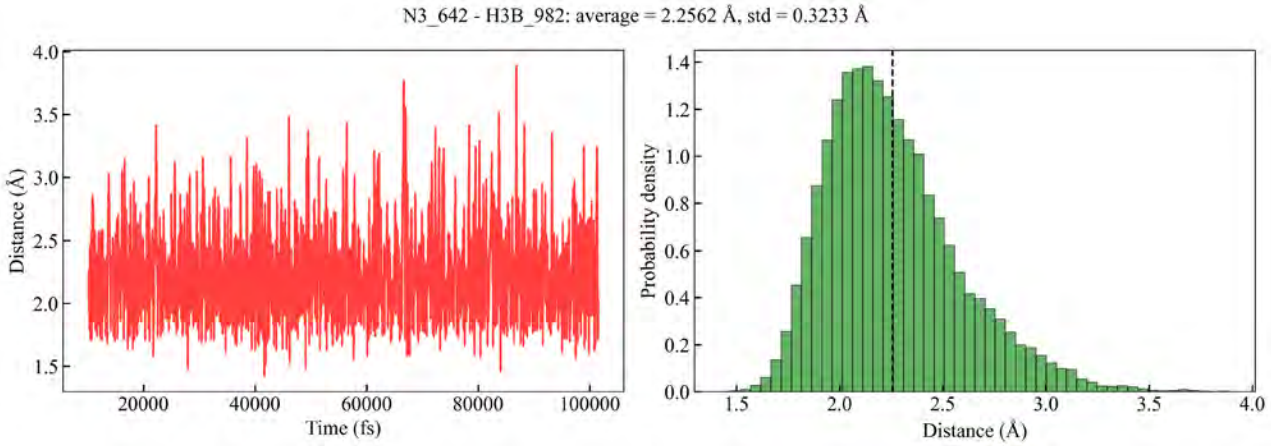
N3_641 - H3B_981

Average distance = 2.2501 Å; standard deviation = 0.3034 Å; number of points = 91387



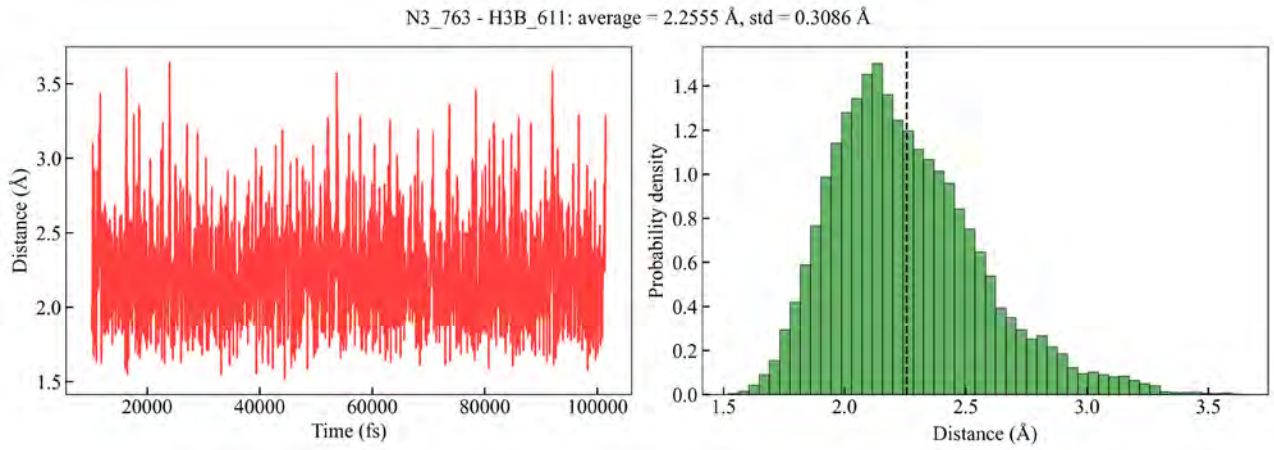
N3_642 - H3B_982

Average distance = 2.2562 Å; standard deviation = 0.3233 Å; number of points = 91387



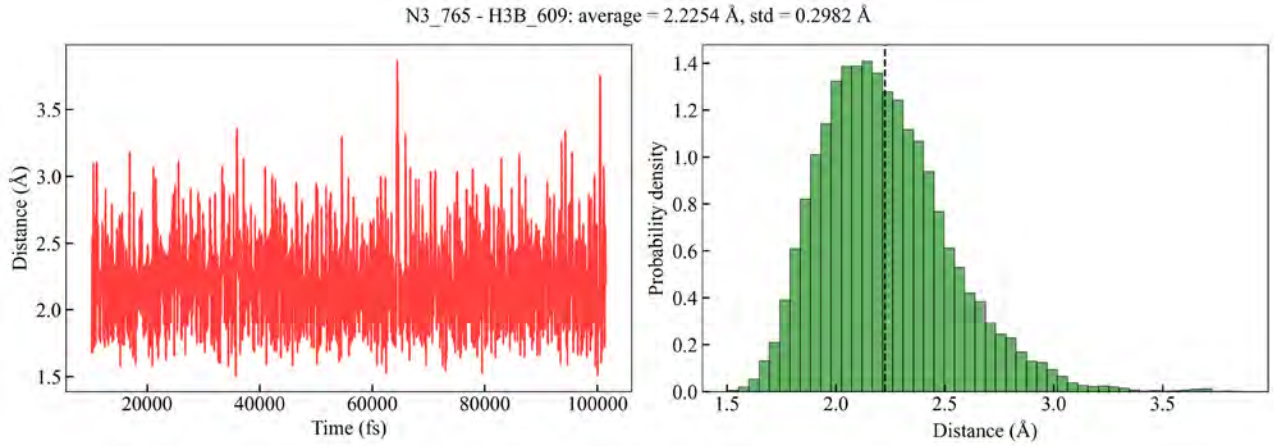
N3_763 - H3B_611

Average distance = 2.2555 Å; standard deviation = 0.3086 Å; number of points = 91387



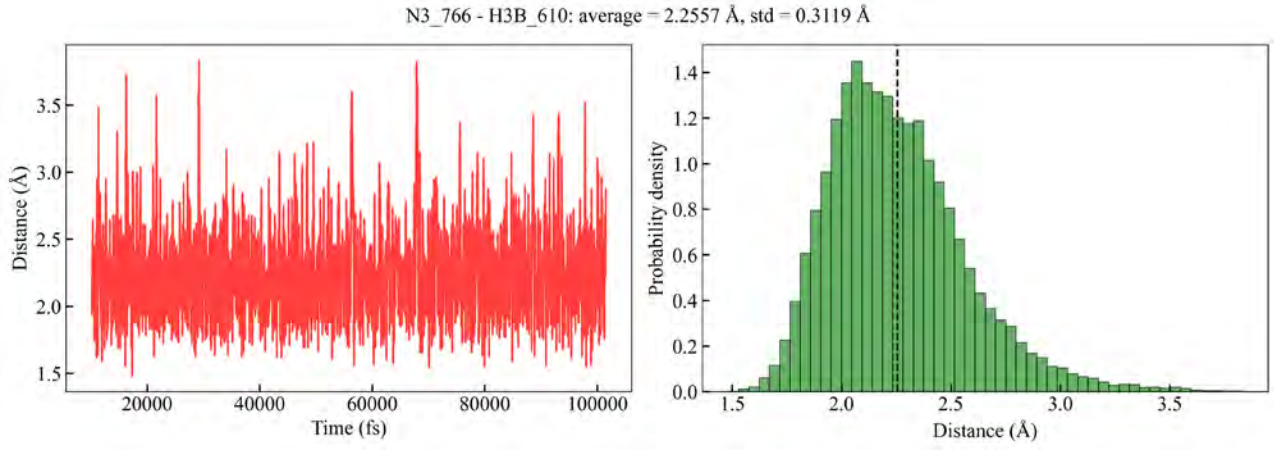
N3_765 - H3B_609

Average distance = 2.2254 Å; standard deviation = 0.2982 Å; number of points = 91387



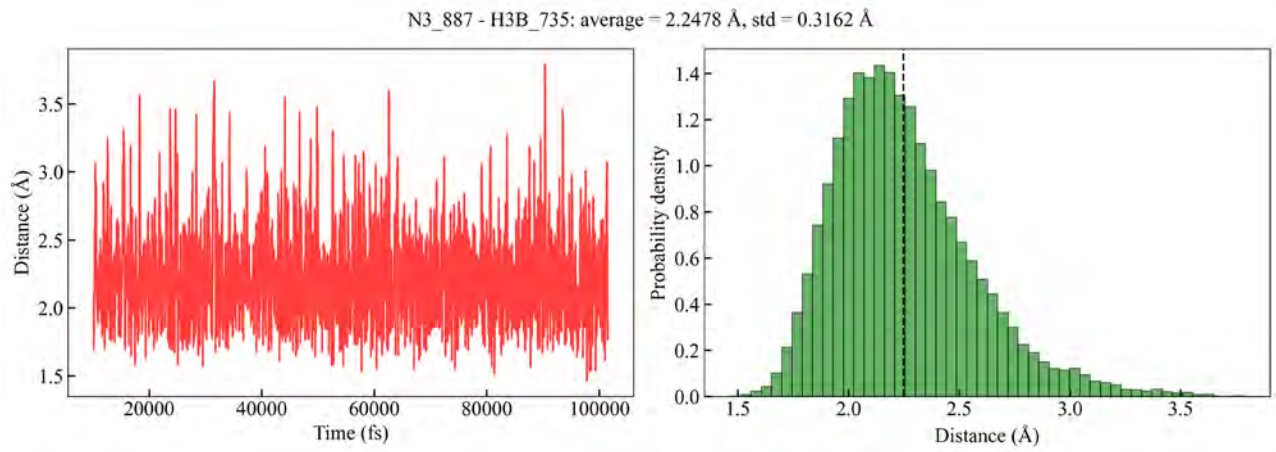
N3_766 - H3B_610

Average distance = 2.2557 Å; standard deviation = 0.3119 Å; number of points = 91387



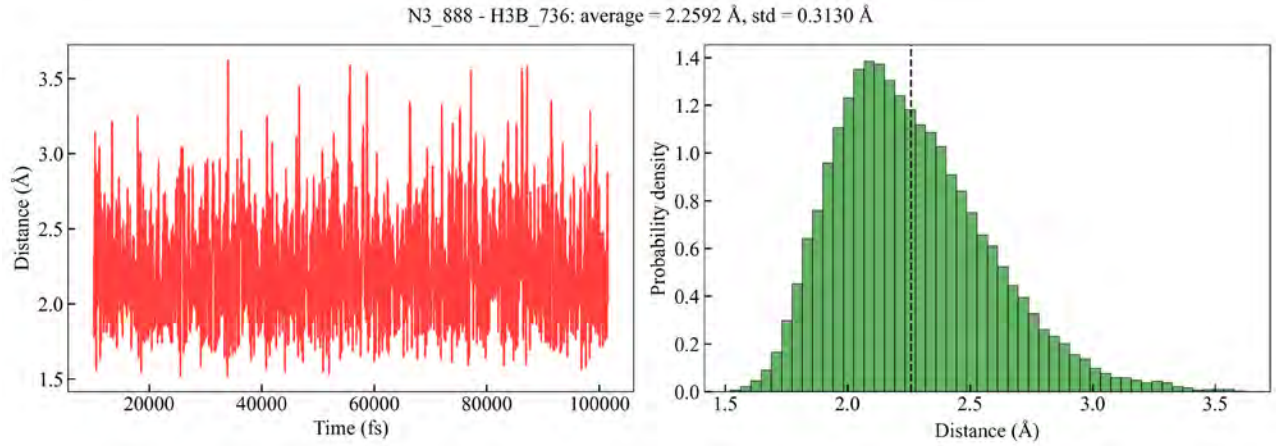
N3_887 - H3B_735

Average distance = 2.2478 Å; standard deviation = 0.3162 Å; number of points = 91387



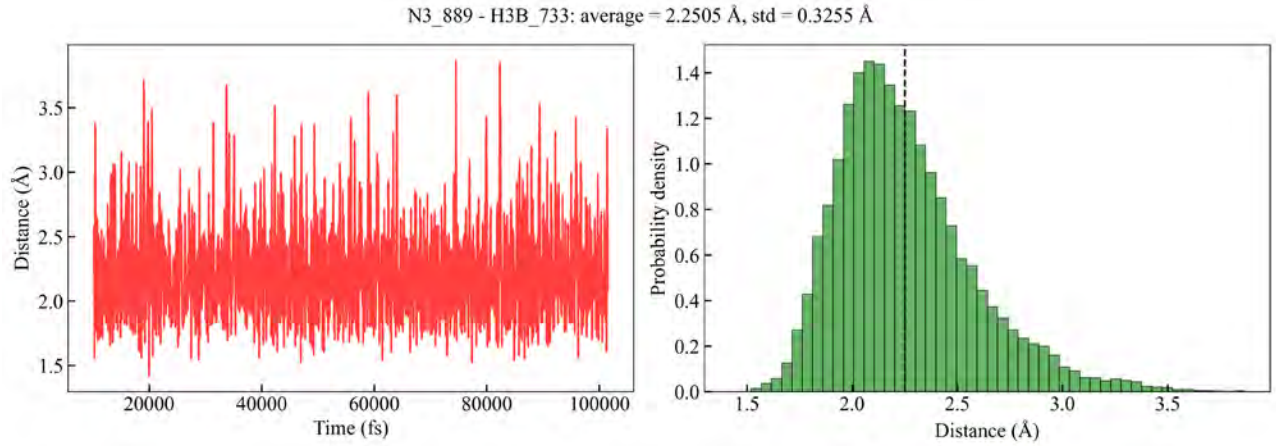
N3_888 - H3B_736

Average distance = 2.2592 Å; standard deviation = 0.3130 Å; number of points = 91387



N3_889 - H3B_733

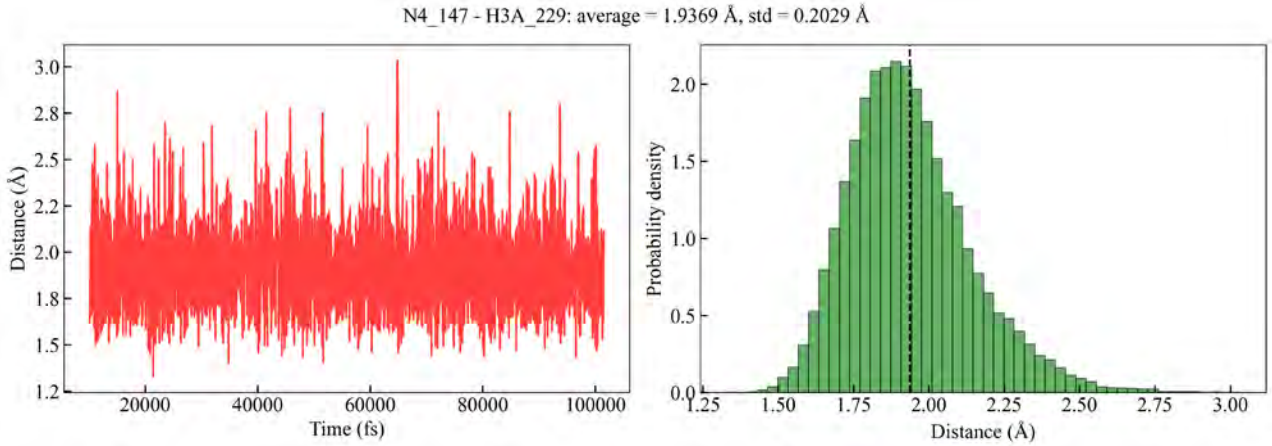
Average distance = 2.2505 Å; standard deviation = 0.3255 Å; number of points = 91387



N4 - H3A

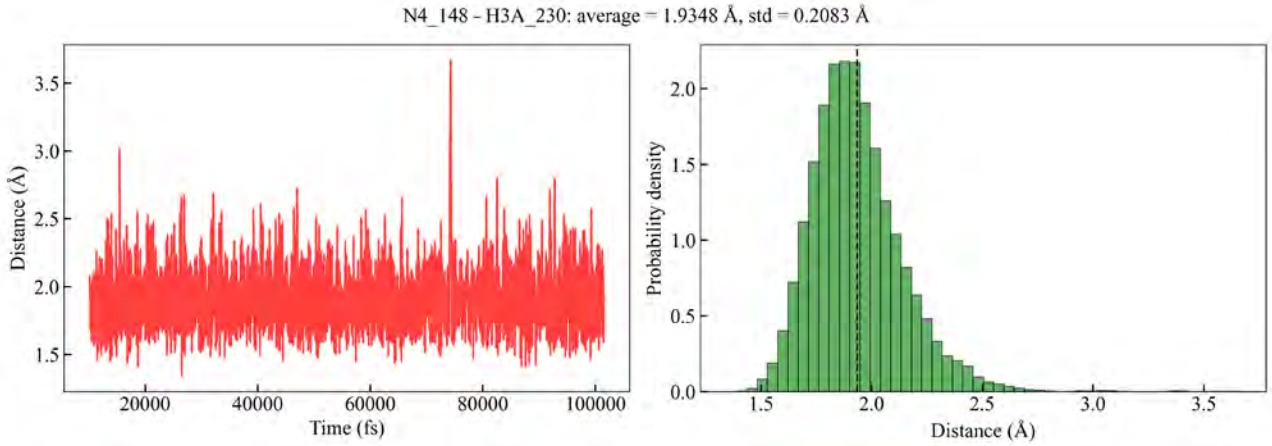
N4_147 - H3A_229

Average distance = 1.9369 Å; standard deviation = 0.2029 Å; number of points = 91387



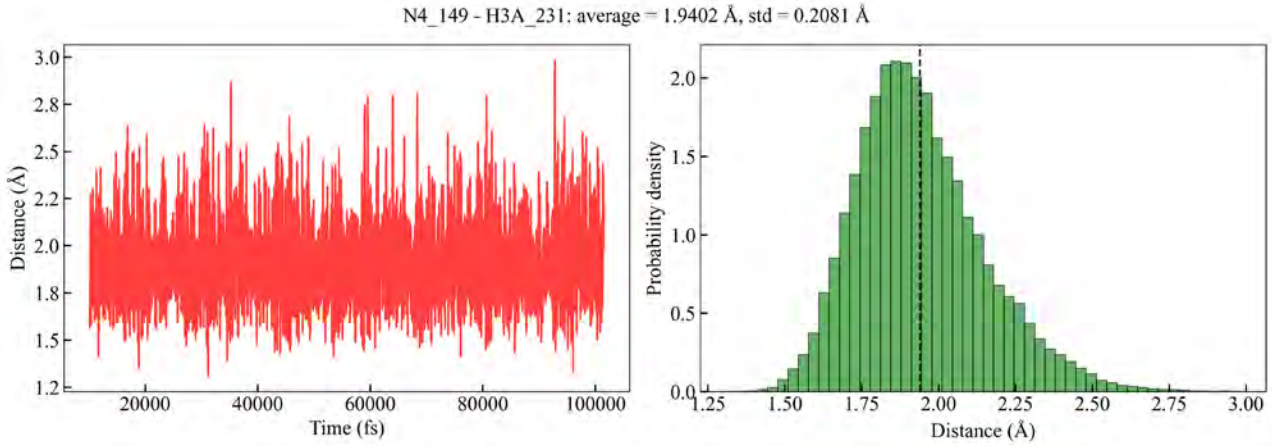
N4_148 - H3A_230

Average distance = 1.9348 Å; standard deviation = 0.2083 Å; number of points = 91387



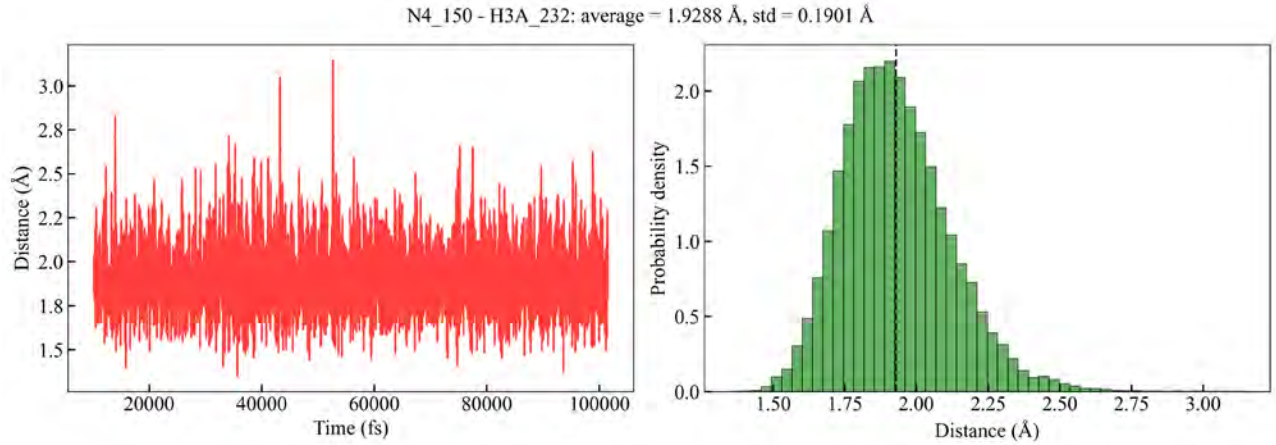
N4_149 - H3A_231

Average distance = 1.9402 Å; standard deviation = 0.2081 Å; number of points = 91387



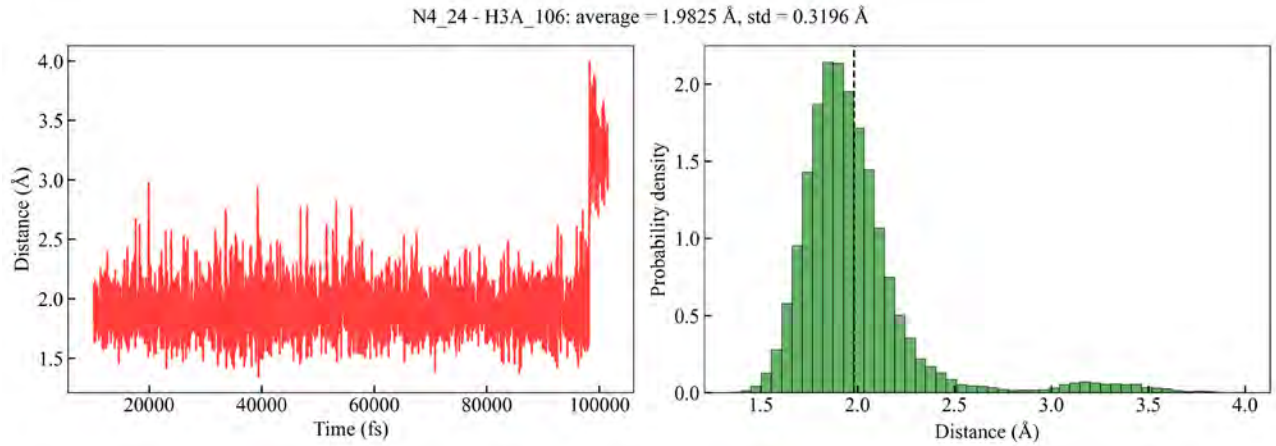
N4_150 - H3A_232

Average distance = 1.9288 Å; standard deviation = 0.1901 Å; number of points = 91387



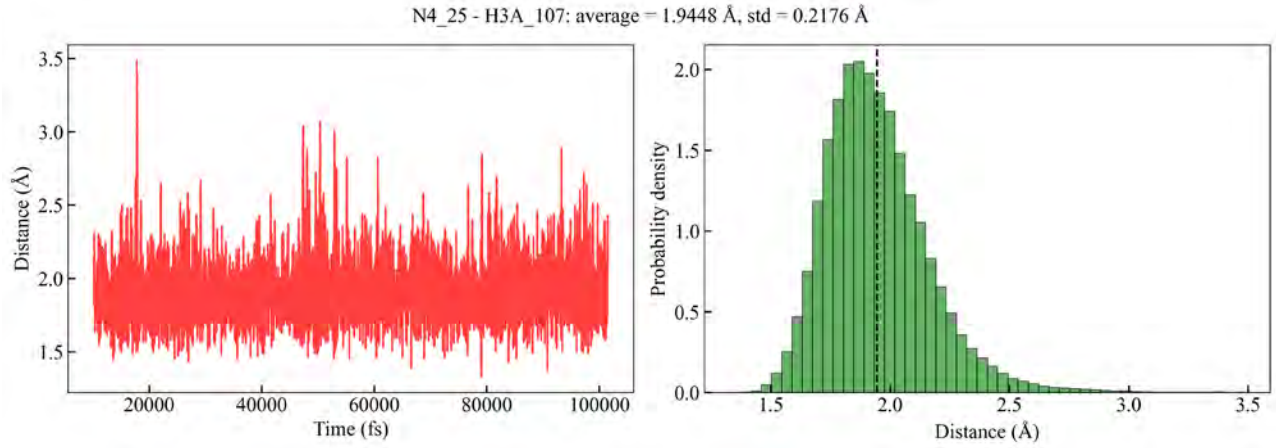
N4_24 - H3A_106

Average distance = 1.9825 Å; standard deviation = 0.3196 Å; number of points = 91387



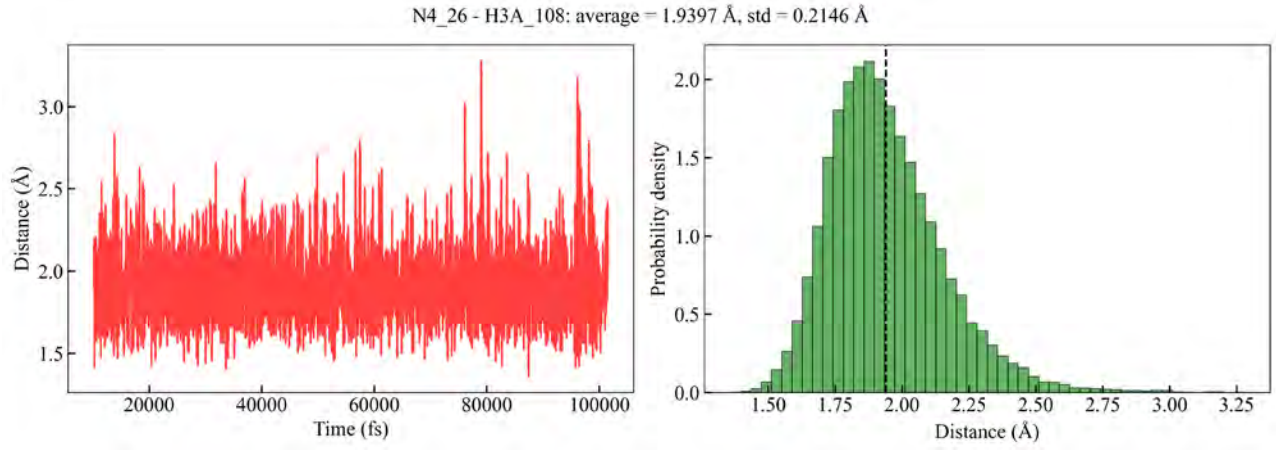
N4_25 - H3A_107

Average distance = 1.9448 Å; standard deviation = 0.2176 Å; number of points = 91387



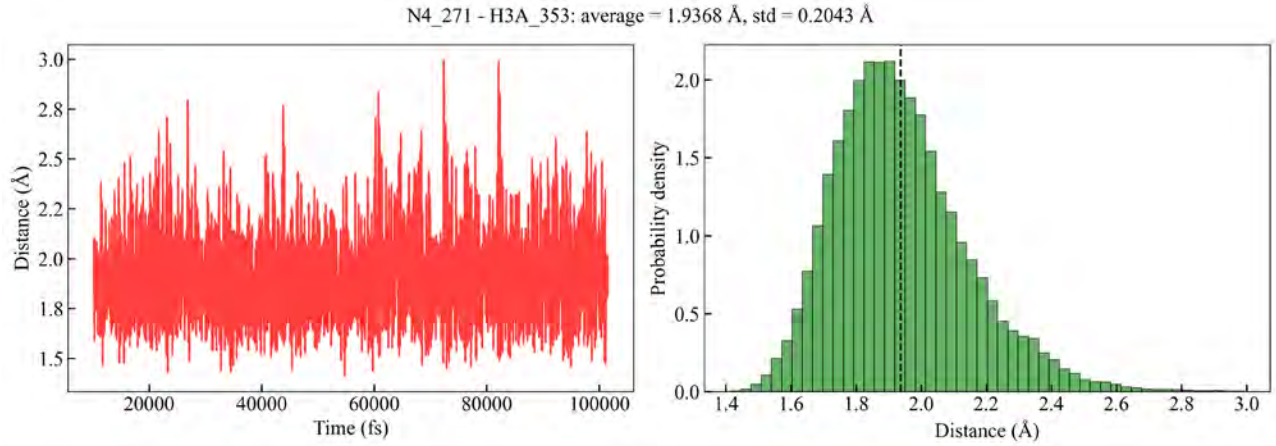
N4_26 - H3A_108

Average distance = 1.9397 Å; standard deviation = 0.2146 Å; number of points = 91387



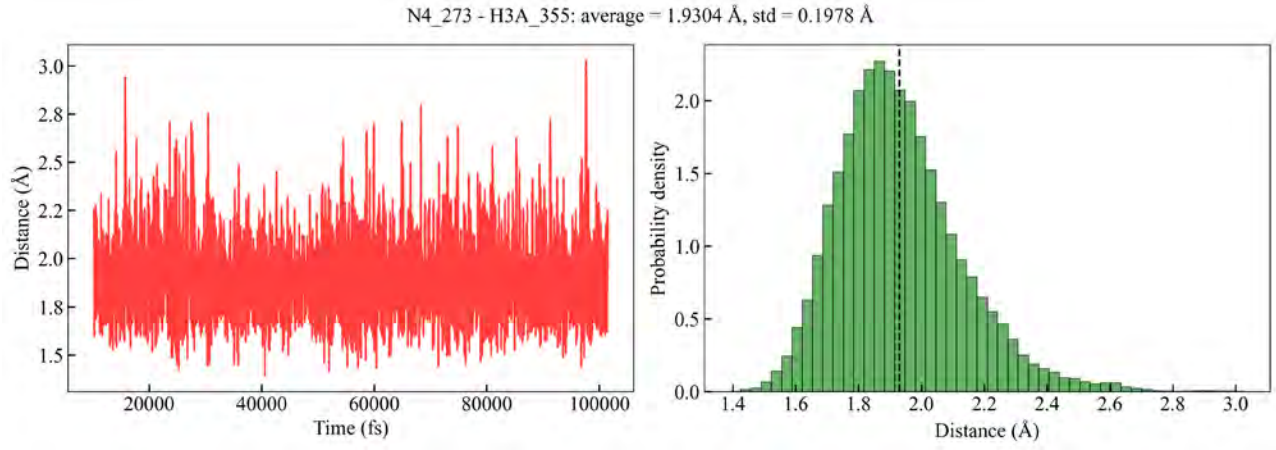
N4_271 - H3A_353

Average distance = 1.9368 Å; standard deviation = 0.2043 Å; number of points = 91387



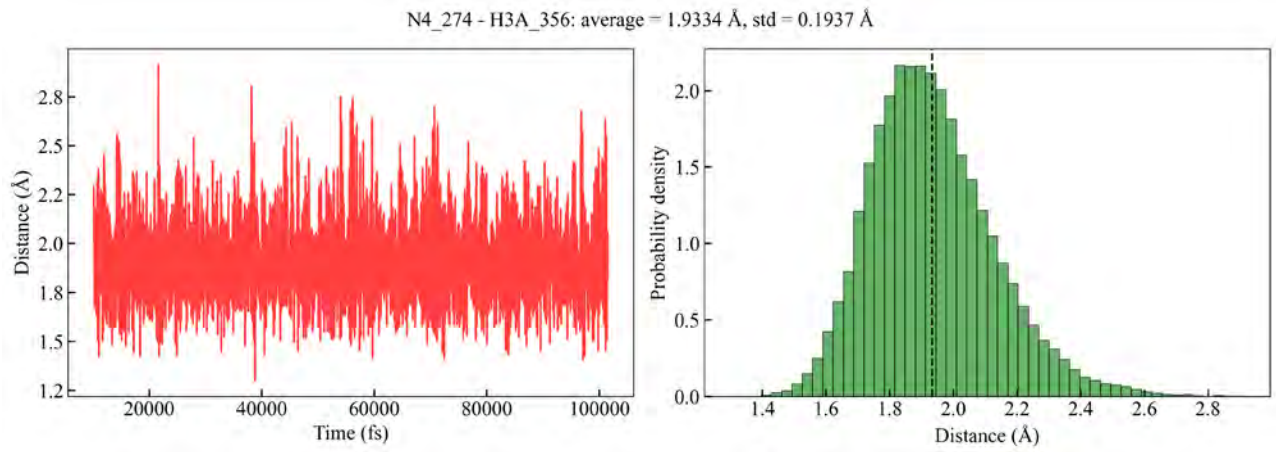
N4_273 - H3A_355

Average distance = 1.9304 Å; standard deviation = 0.1978 Å; number of points = 91387



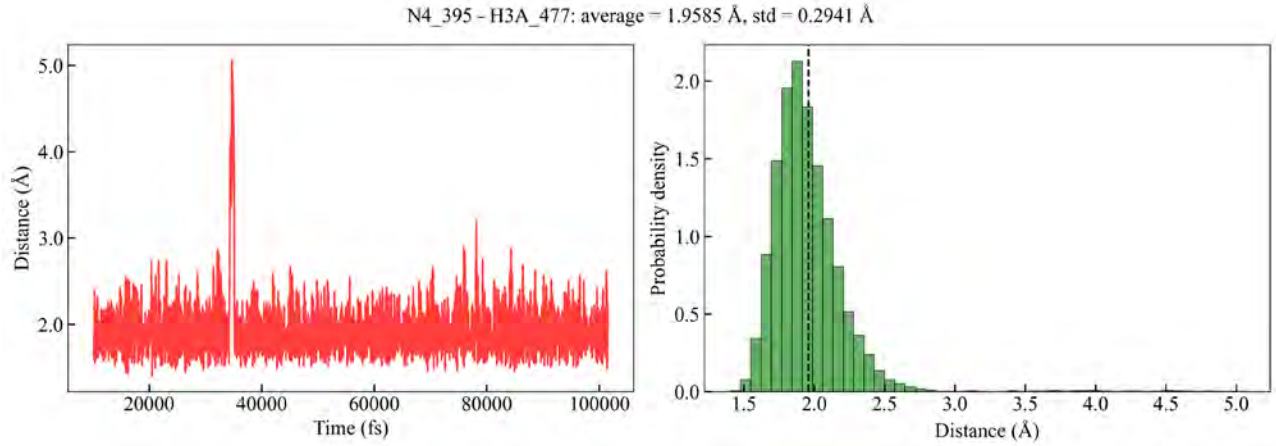
N4_274 - H3A_356

Average distance = 1.9334 Å; standard deviation = 0.1937 Å; number of points = 91387



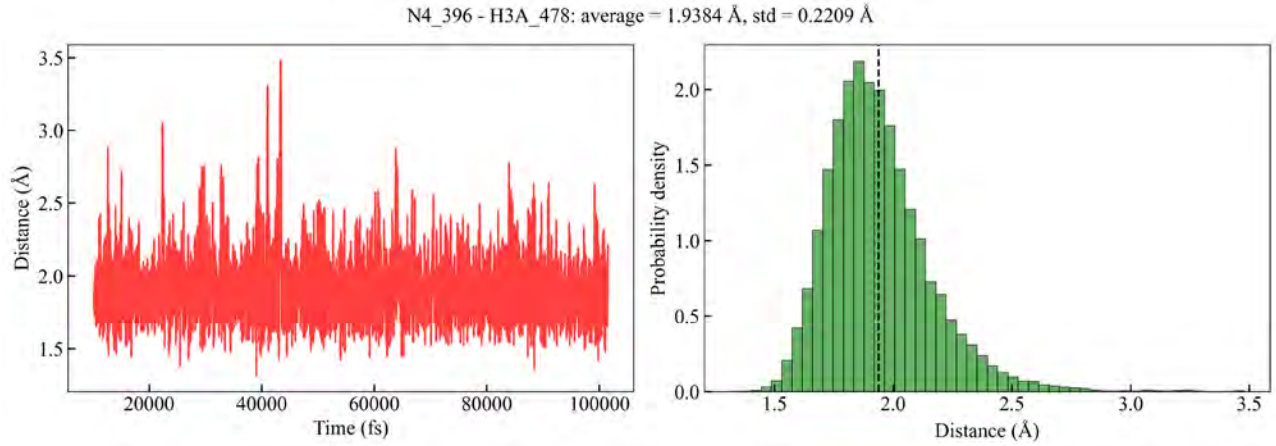
N4_395 - H3A_477

Average distance = 1.9585 Å; standard deviation = 0.2941 Å; number of points = 91387



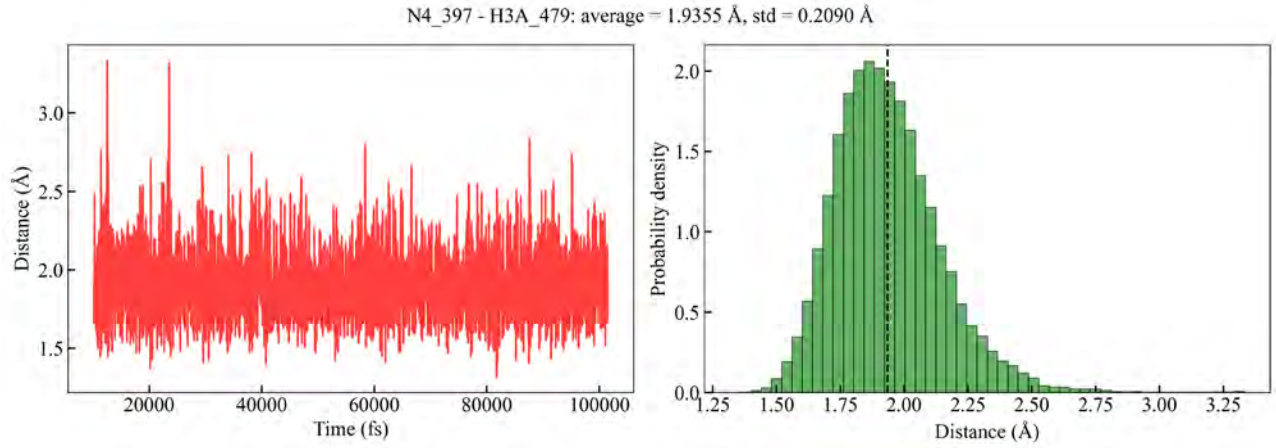
N4_396 - H3A_478

Average distance = 1.9384 Å; standard deviation = 0.2209 Å; number of points = 91387



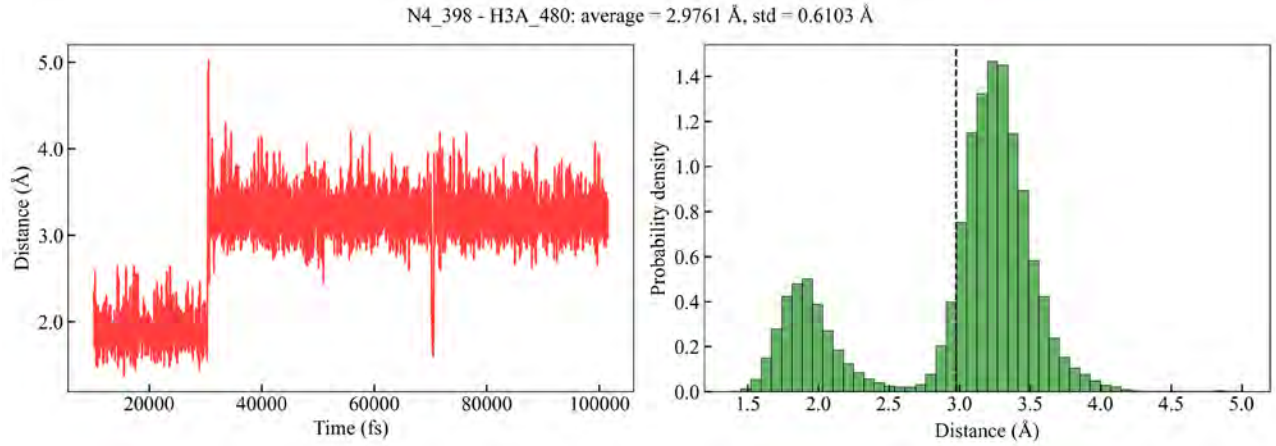
N4_397 - H3A_479

Average distance = 1.9355 Å; standard deviation = 0.2090 Å; number of points = 91387



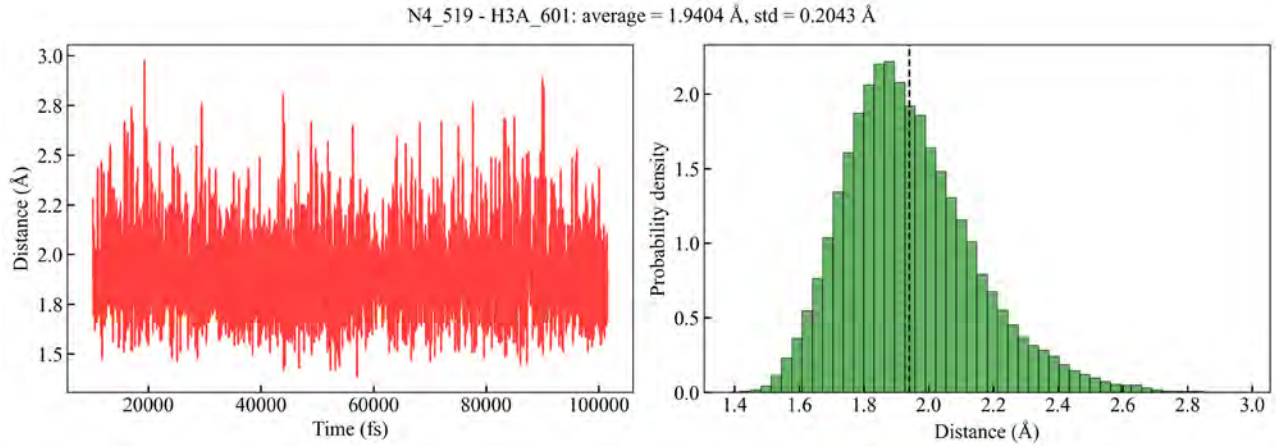
N4_398 - H3A_480

Average distance = 2.9761 Å; standard deviation = 0.6103 Å; number of points = 91387



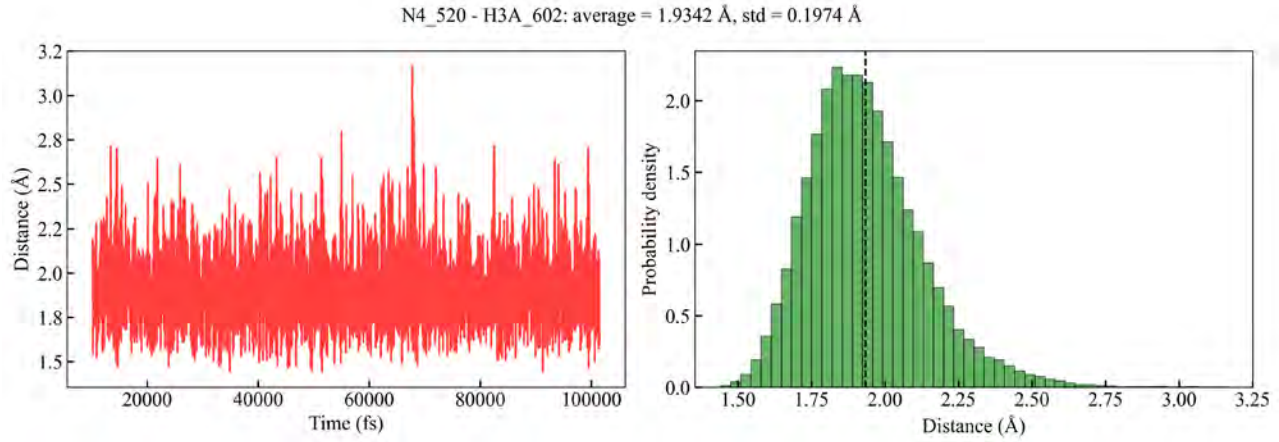
N4_519 - H3A_601

Average distance = 1.9404 Å; standard deviation = 0.2043 Å; number of points = 91387



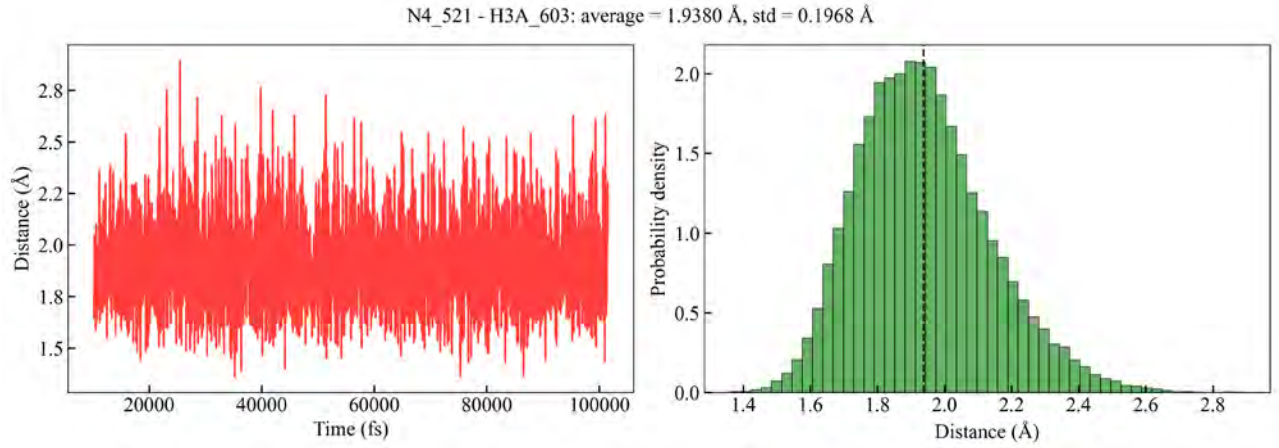
N4_520 - H3A_602

Average distance = 1.9342 Å; standard deviation = 0.1974 Å; number of points = 91387



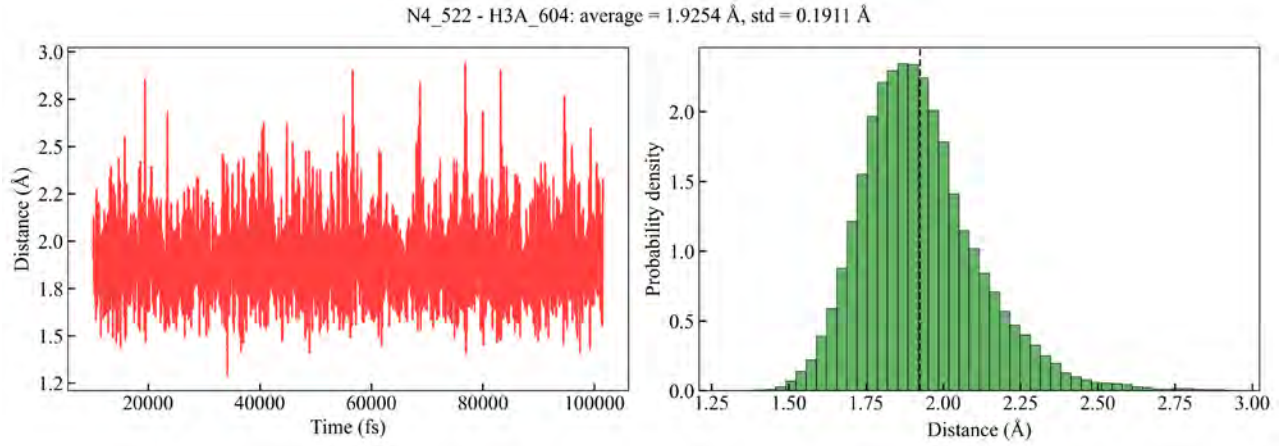
N4_521 - H3A_603

Average distance = 1.9380 Å; standard deviation = 0.1968 Å; number of points = 91387



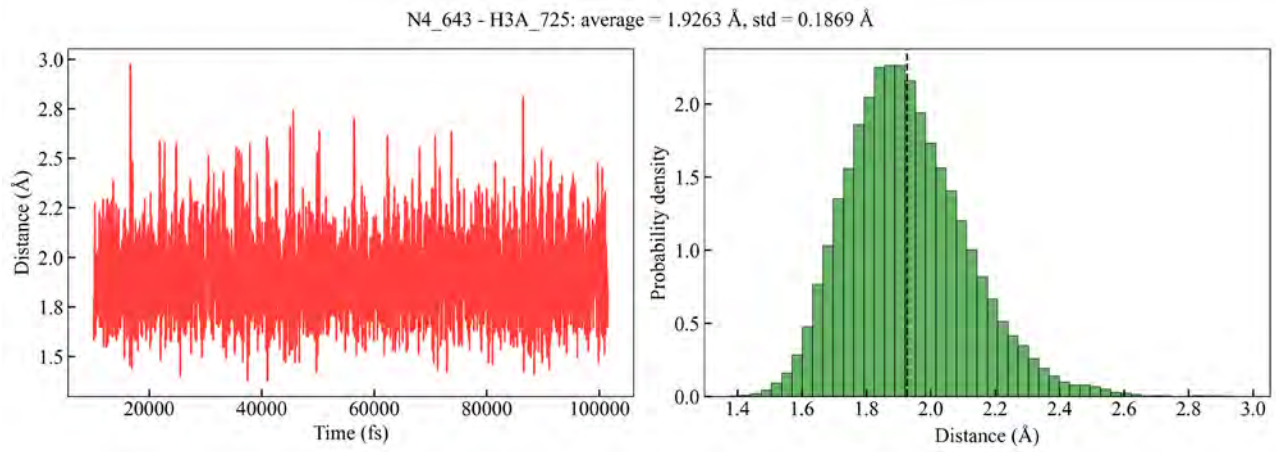
N4_522 - H3A_604

Average distance = 1.9254 Å; standard deviation = 0.1911 Å; number of points = 91387



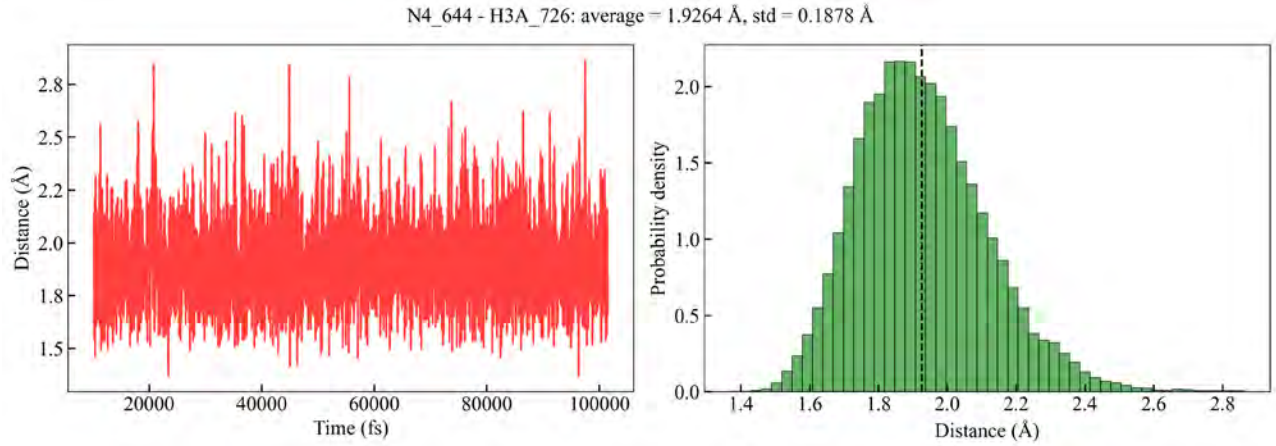
N4_643 - H3A_725

Average distance = 1.9263 Å; standard deviation = 0.1869 Å; number of points = 91387



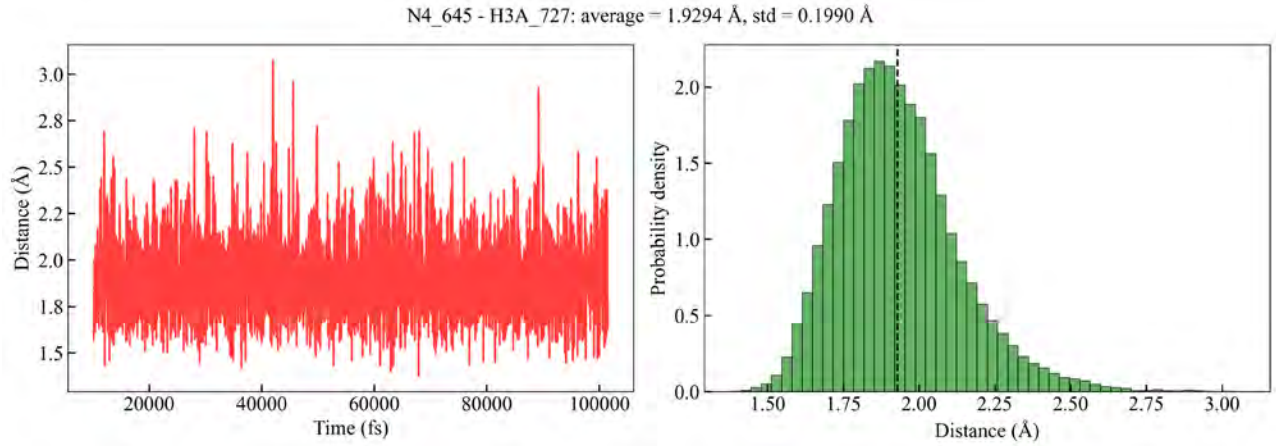
N4_644 - H3A_726

Average distance = 1.9264 Å; standard deviation = 0.1878 Å; number of points = 91387



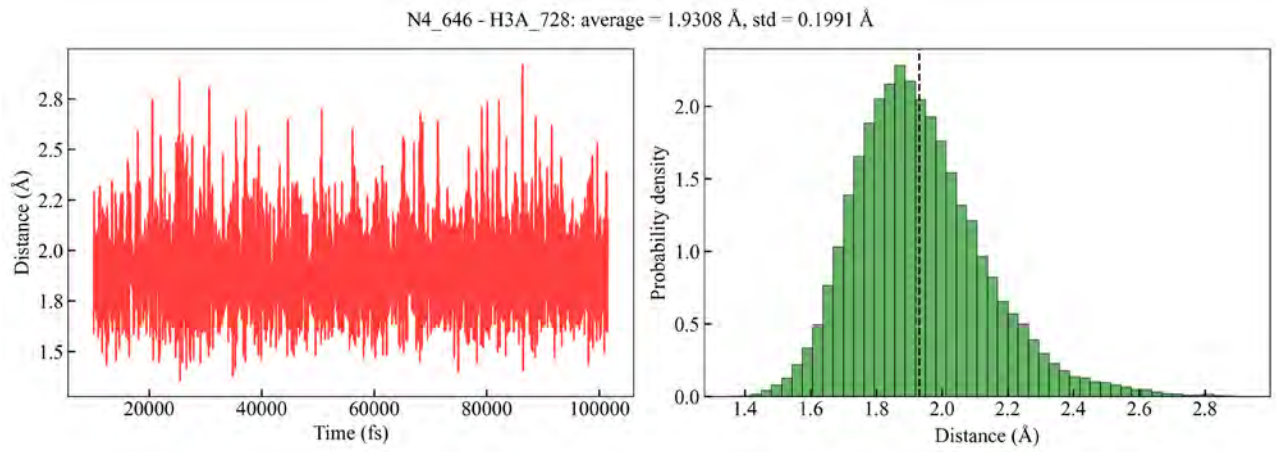
N4_645 - H3A_727

Average distance = 1.9294 Å; standard deviation = 0.1990 Å; number of points = 91387



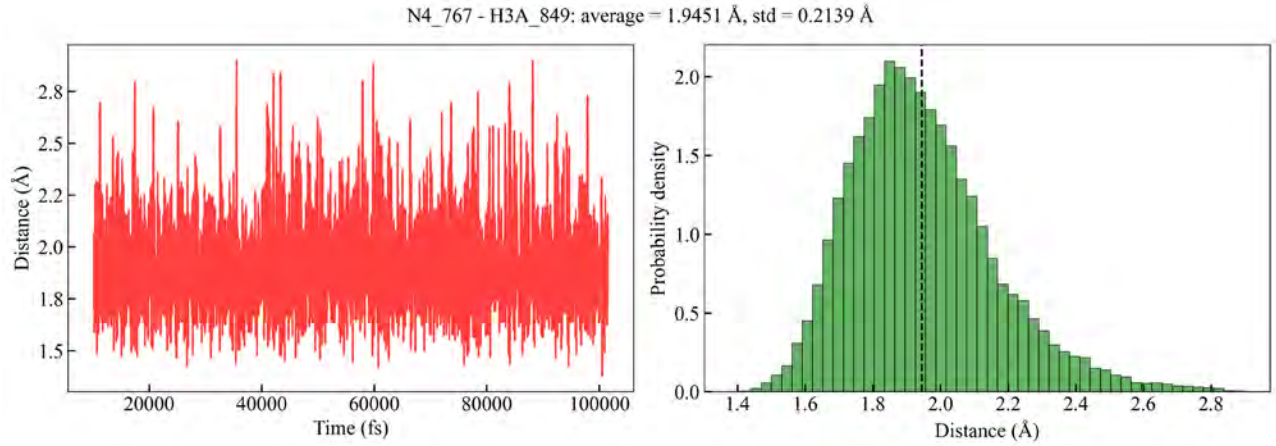
N4_646 - H3A_728

Average distance = 1.9308 Å; standard deviation = 0.1991 Å; number of points = 91387



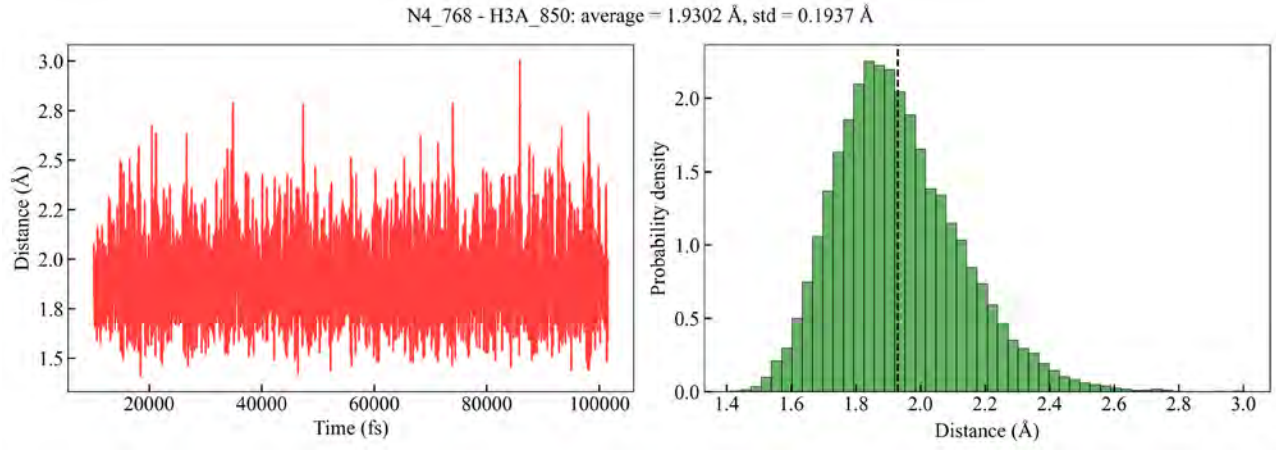
N4_767 - H3A_849

Average distance = 1.9451 Å; standard deviation = 0.2139 Å; number of points = 91387



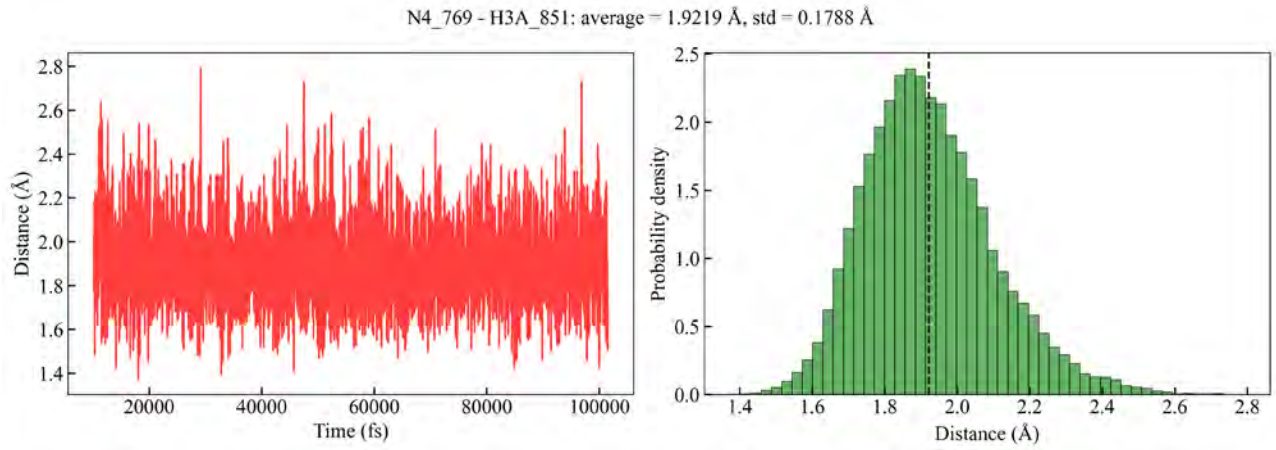
N4_768 - H3A_850

Average distance = 1.9302 Å; standard deviation = 0.1937 Å; number of points = 91387



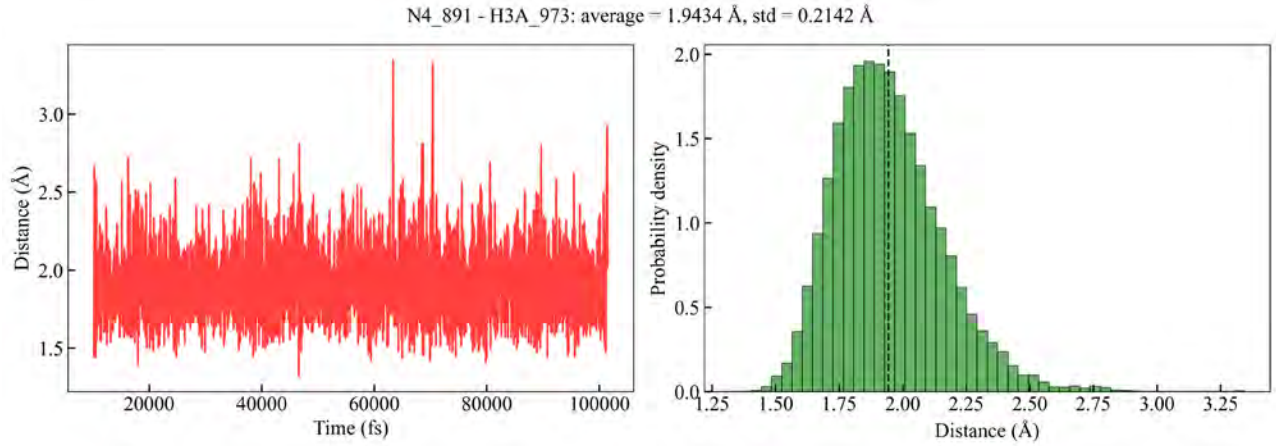
N4_769 - H3A_851

Average distance = 1.9219 Å; standard deviation = 0.1788 Å; number of points = 91387



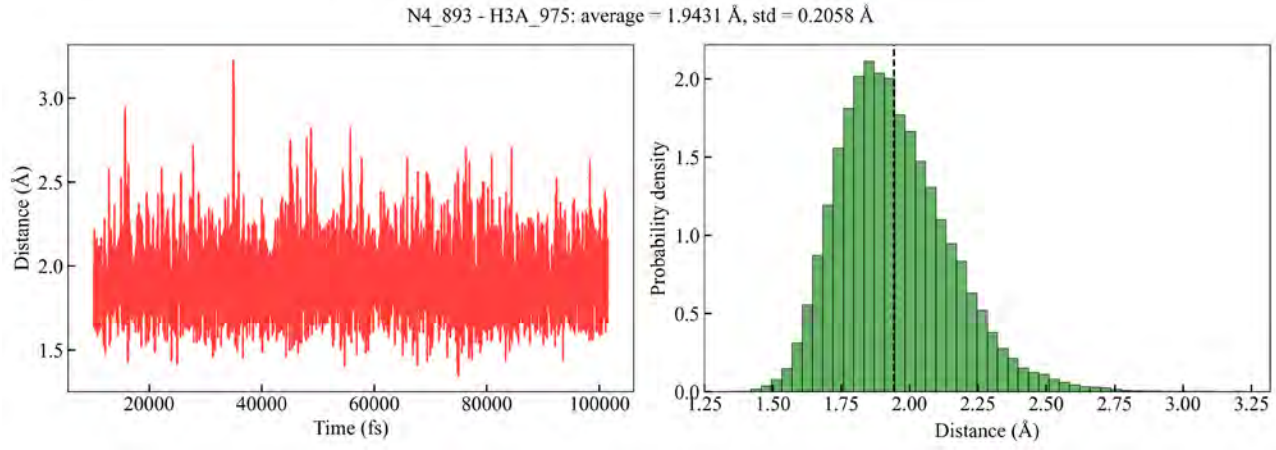
N4_891 - H3A_973

Average distance = 1.9434 Å; standard deviation = 0.2142 Å; number of points = 91387



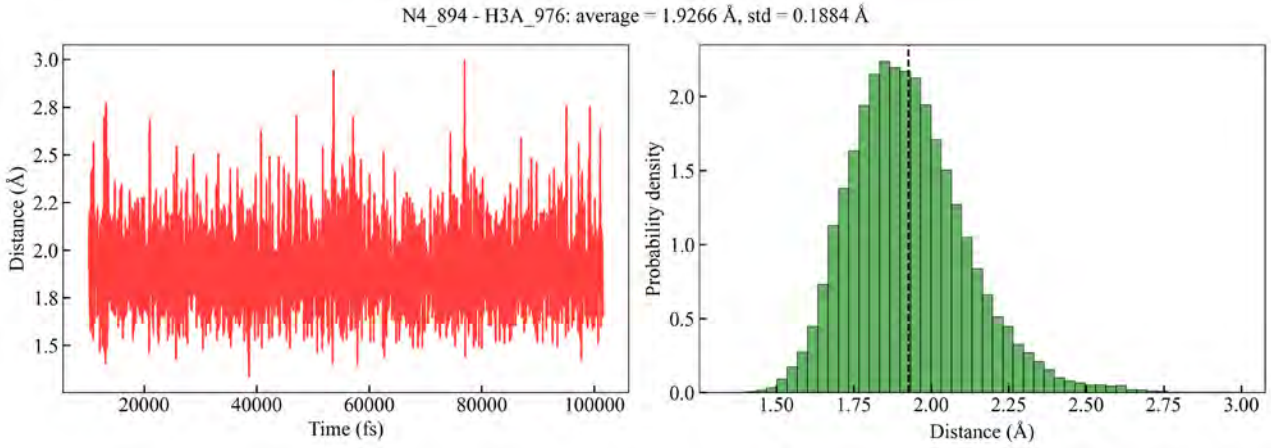
N4_893 - H3A_975

Average distance = 1.9431 Å; standard deviation = 0.2058 Å; number of points = 91387



N4_894 - H3A_976

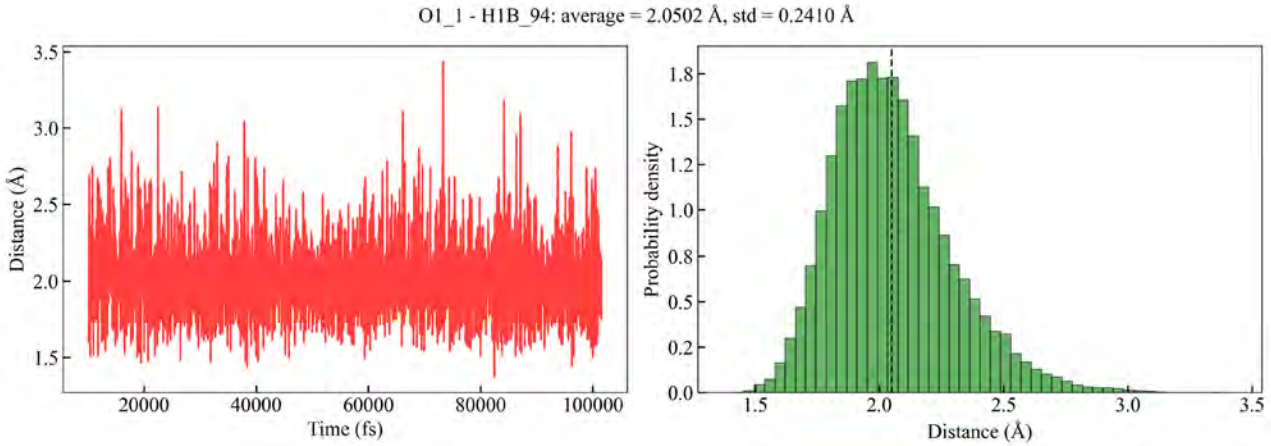
Average distance = 1.9266 Å; standard deviation = 0.1884 Å; number of points = 91387


N4_894 - H3A_976: average = 1.9266 Å, std = 0.1884 Å
Distance (Å)
Time (fs)
Probability density
Distance (Å)

O1 - H1B

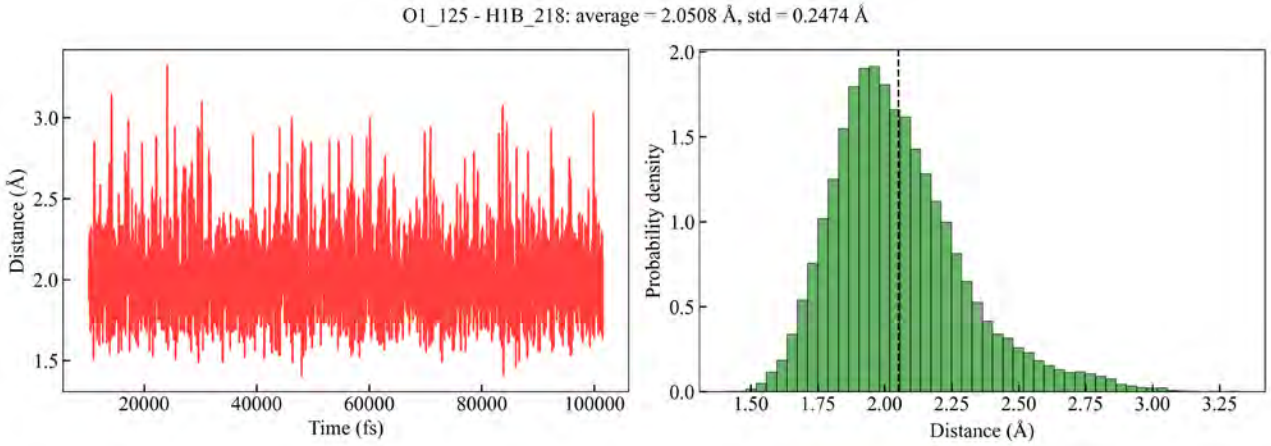
O1_1 - H1B_94

Average distance = 2.0502 Å; standard deviation = 0.2410 Å; number of points = 91387



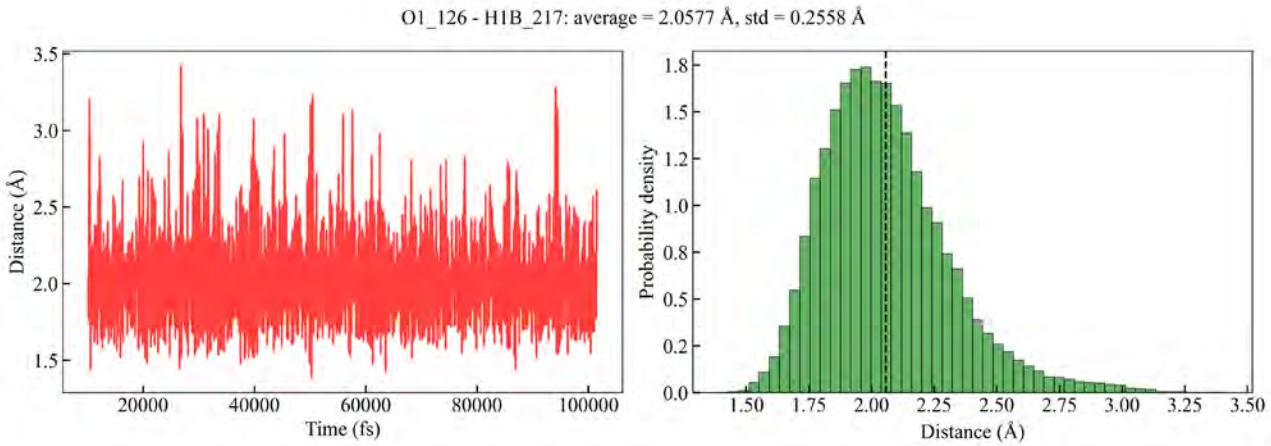
O1_125 - H1B_218

Average distance = 2.0508 Å; standard deviation = 0.2474 Å; number of points = 91387



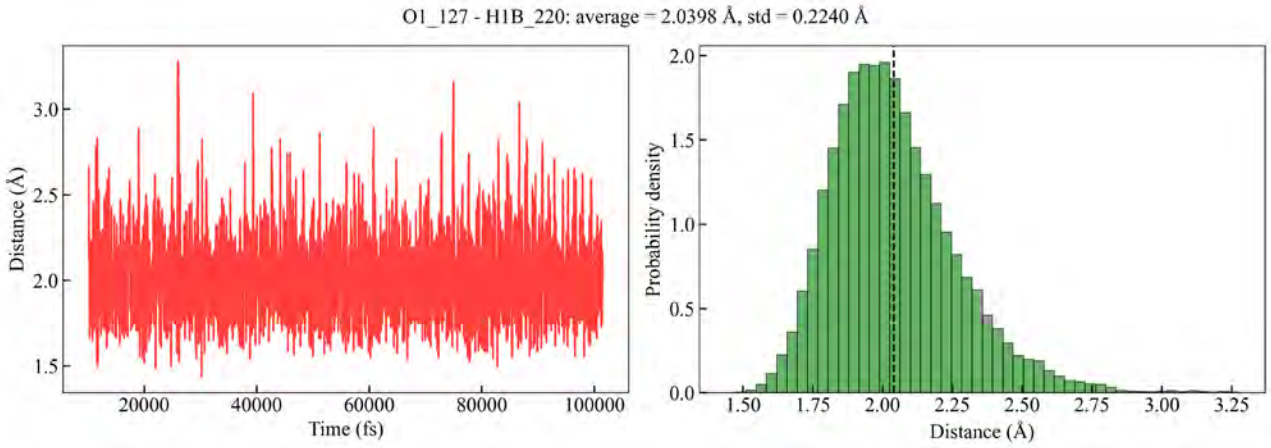
O1_126 - H1B_217

Average distance = 2.0577 Å; standard deviation = 0.2558 Å; number of points = 91387



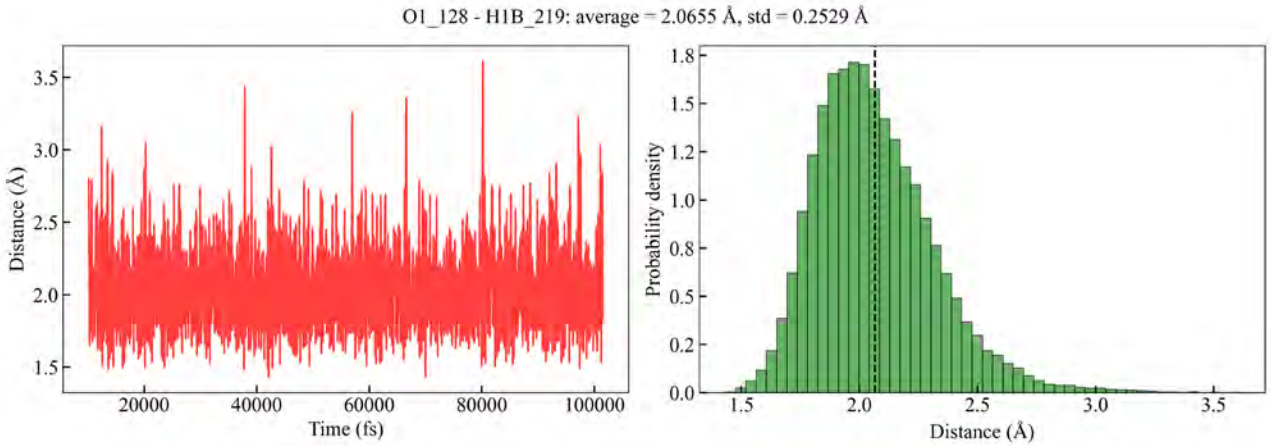
O1_127 - H1B_220

Average distance = 2.0398 Å; standard deviation = 0.2240 Å; number of points = 91387



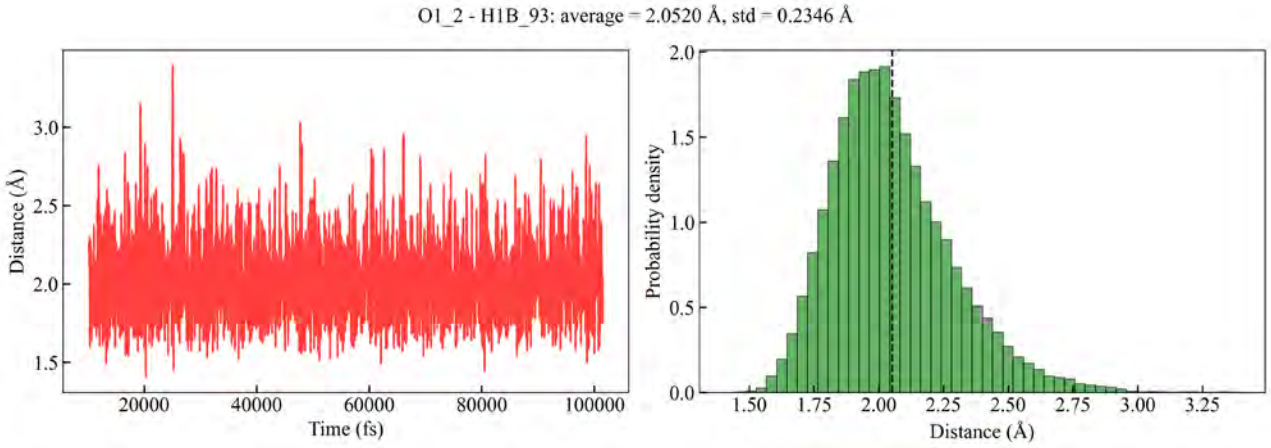
O1_128 - H1B_219

Average distance = 2.0655 Å; standard deviation = 0.2529 Å; number of points = 91387



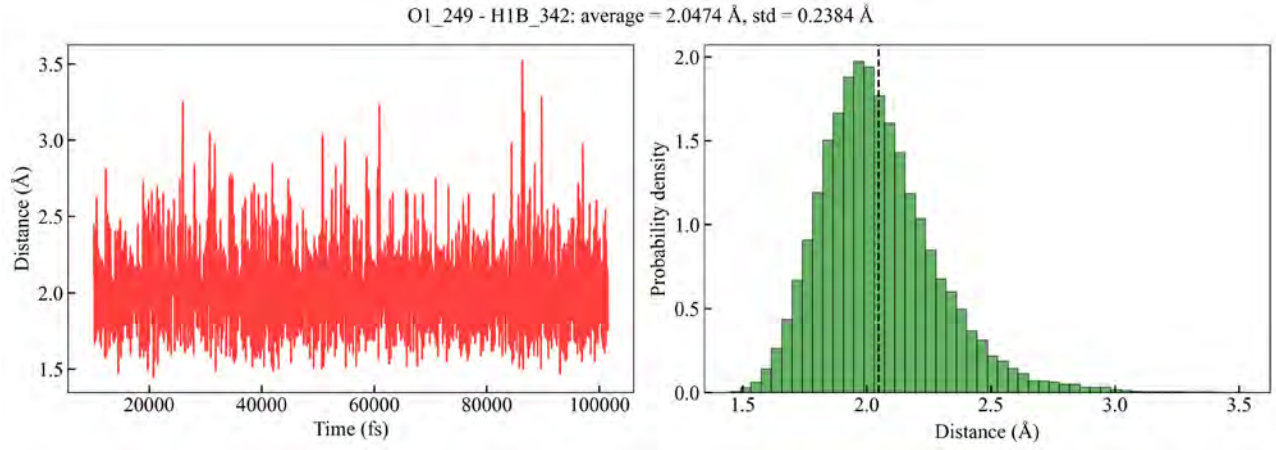
O1_2 - H1B_93

Average distance = 2.0520 Å; standard deviation = 0.2346 Å; number of points = 91387



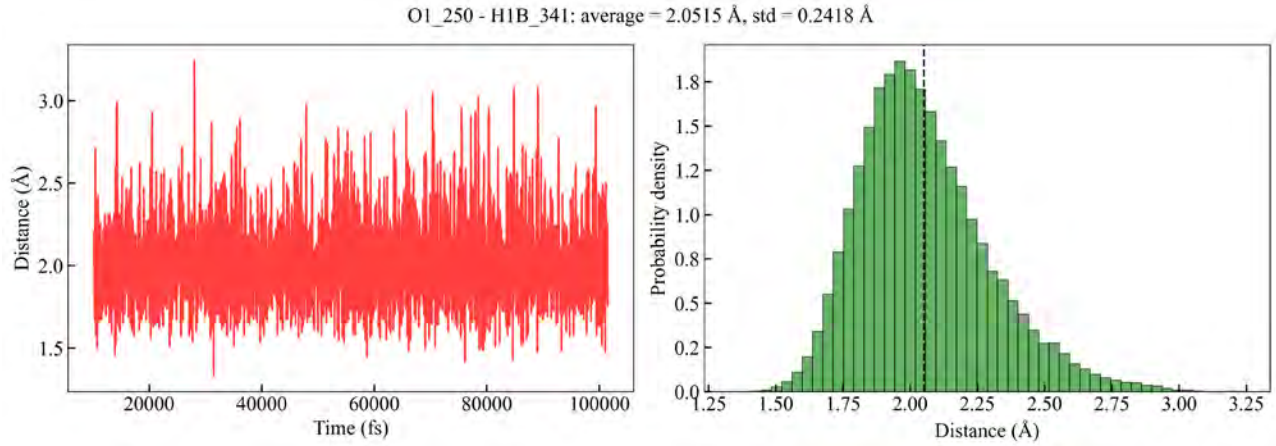
O1_249 - H1B_342

Average distance = 2.0474 Å; standard deviation = 0.2384 Å; number of points = 91387



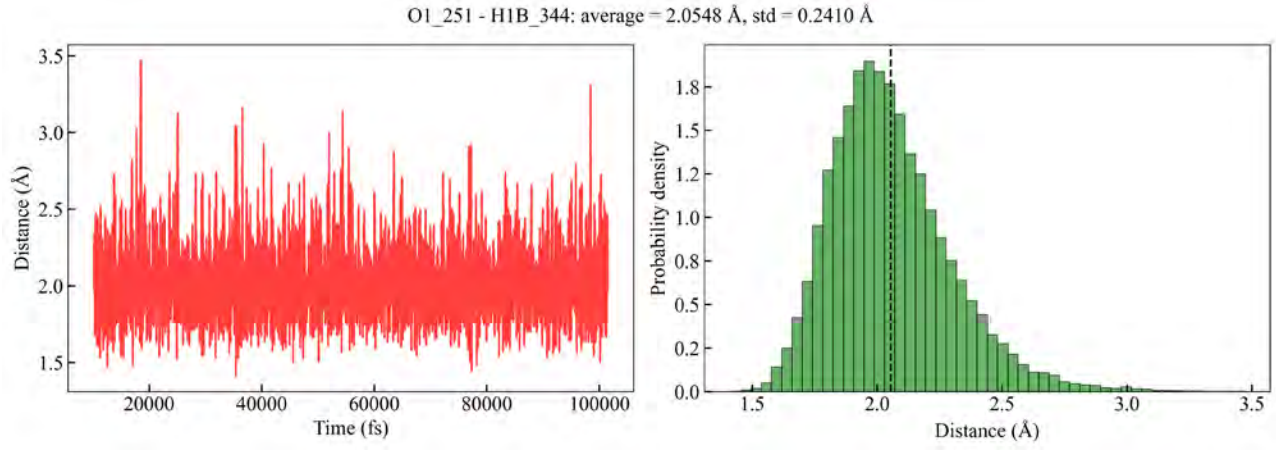
O1_250 - H1B_341

Average distance = 2.0515 Å; standard deviation = 0.2418 Å; number of points = 91387



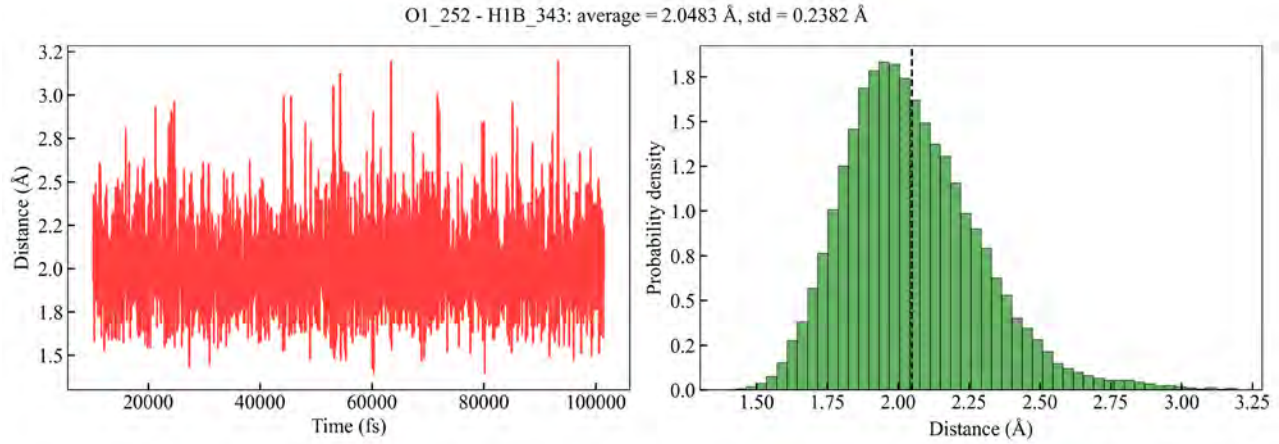
O1_251 - H1B_344

Average distance = 2.0548 Å; standard deviation = 0.2410 Å; number of points = 91387



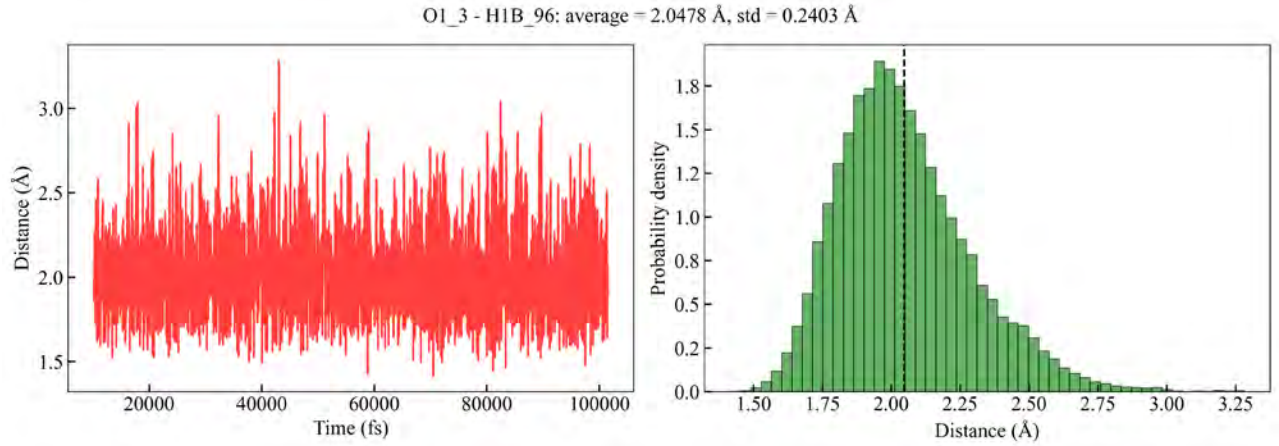
O1_252 - H1B_343

Average distance = 2.0483 Å; standard deviation = 0.2382 Å; number of points = 91387



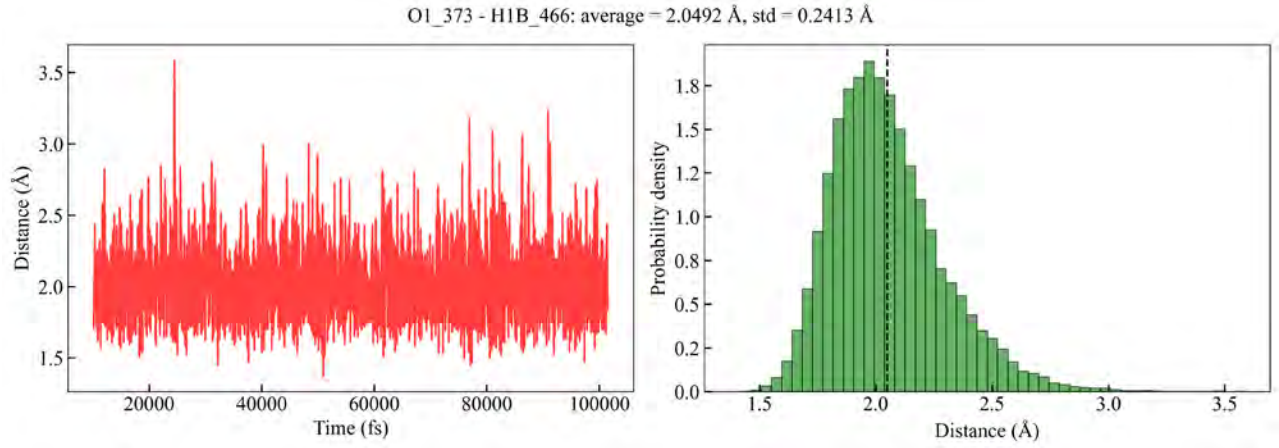
O1_3 - H1B_96

Average distance = 2.0478 Å; standard deviation = 0.2403 Å; number of points = 91387



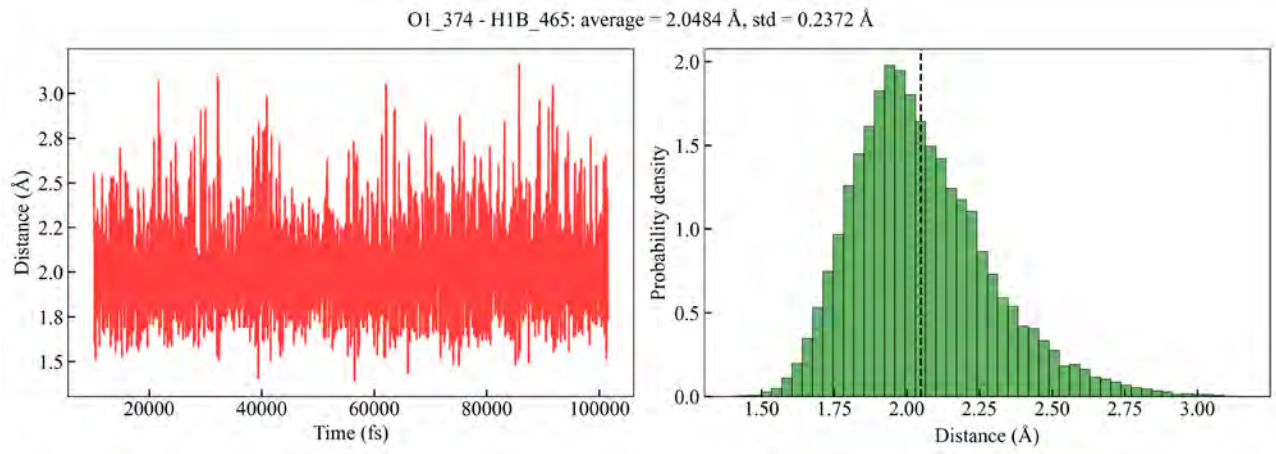
O1_373 - H1B_466

Average distance = 2.0492 Å; standard deviation = 0.2413 Å; number of points = 91387



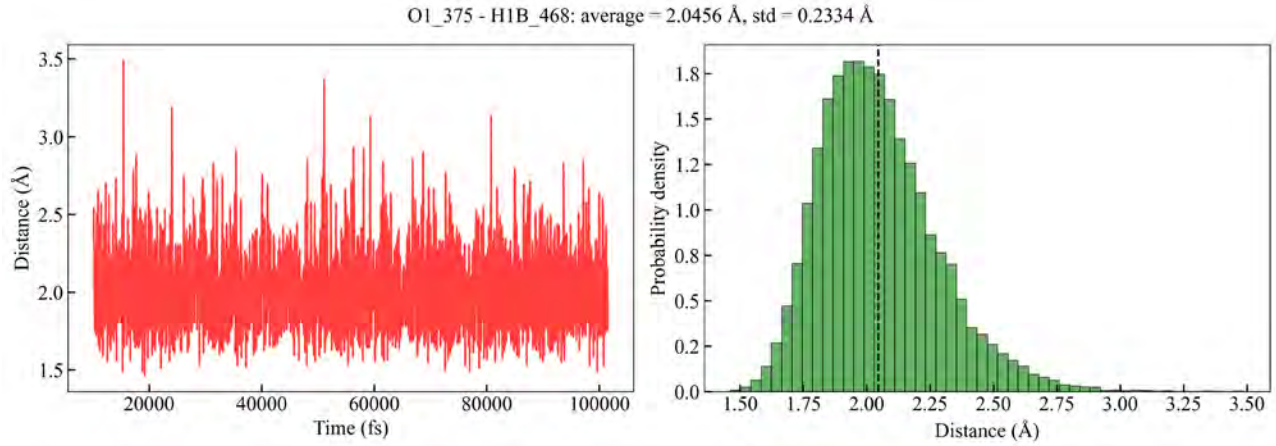
O1_374 - H1B_465

Average distance = 2.0484 Å; standard deviation = 0.2372 Å; number of points = 91387



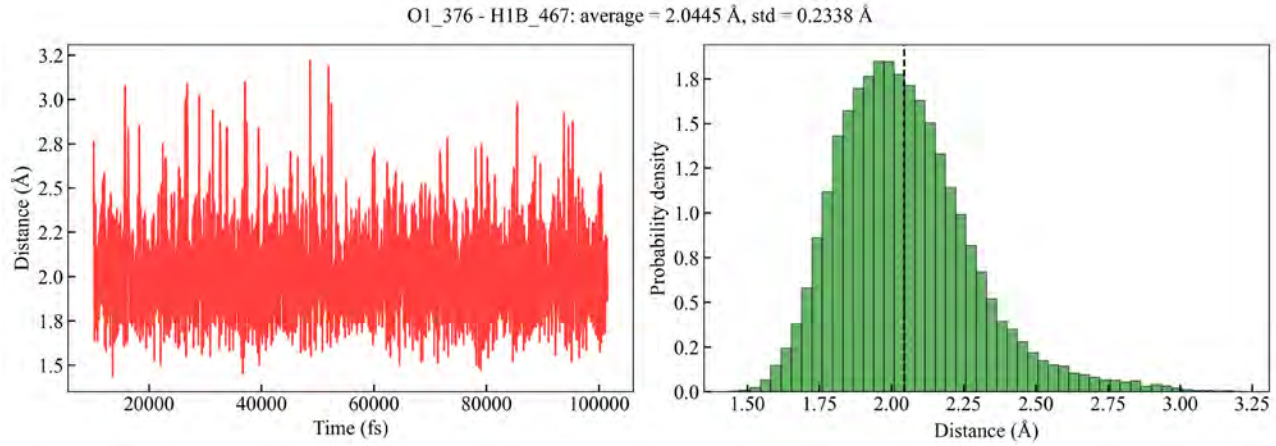
O1_375 - H1B_468

Average distance = 2.0456 Å; standard deviation = 0.2334 Å; number of points = 91387



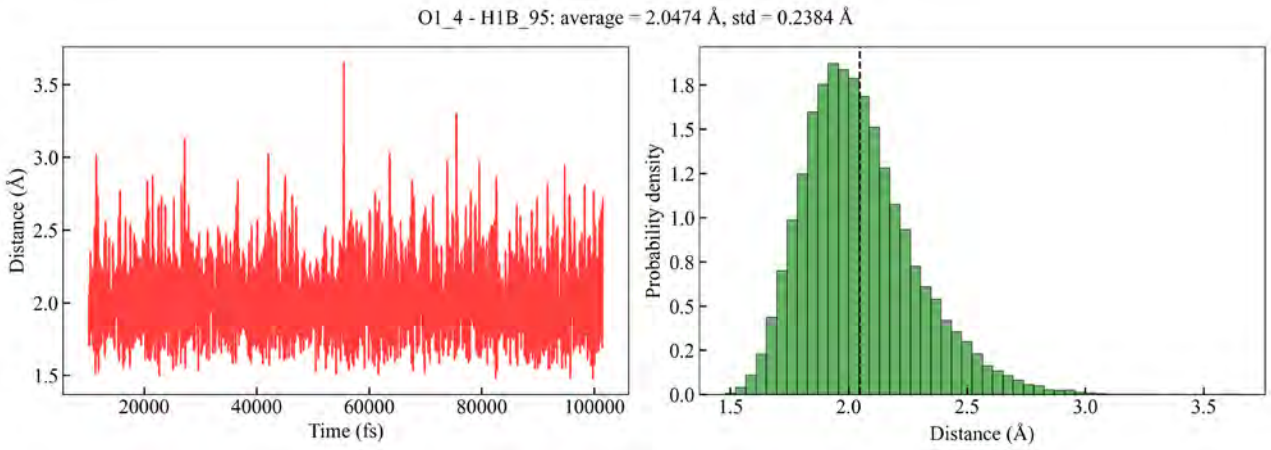
O1_376 - H1B_467

Average distance = 2.0445 Å; standard deviation = 0.2338 Å; number of points = 91387



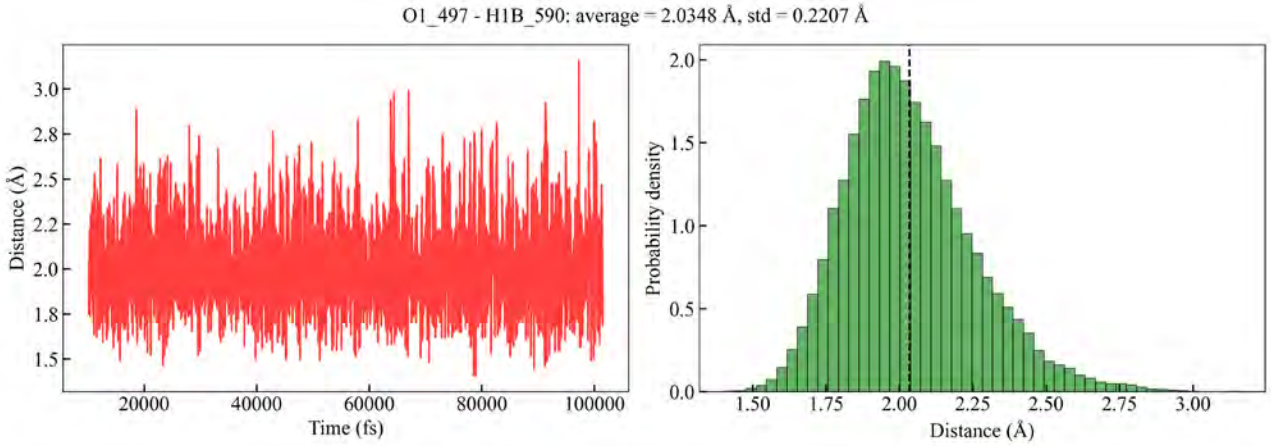
O1_4 - H1B_95

Average distance = 2.0474 Å; standard deviation = 0.2384 Å; number of points = 91387



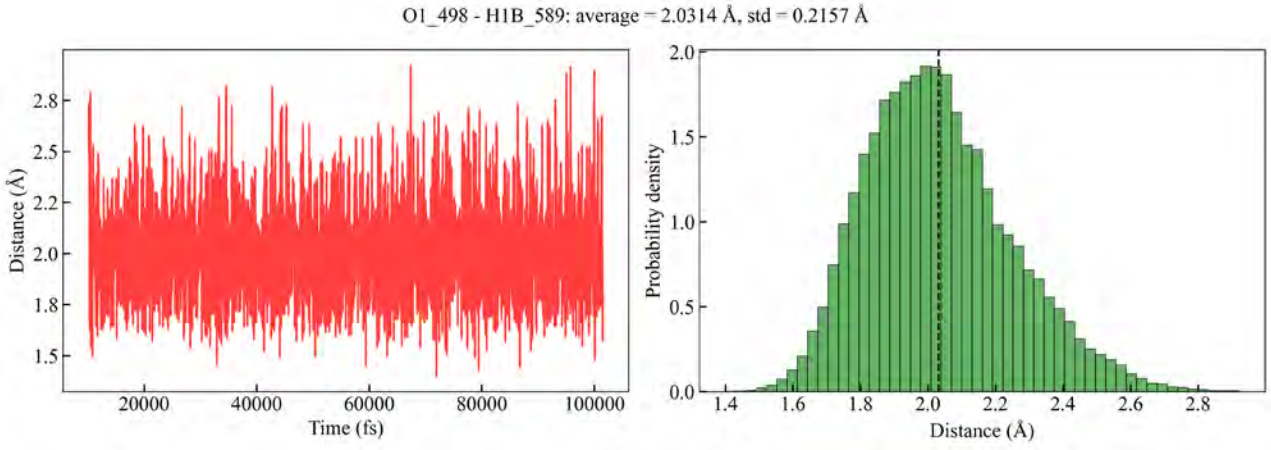
O1_497 - H1B_590

Average distance = 2.0348 Å; standard deviation = 0.2207 Å; number of points = 91387



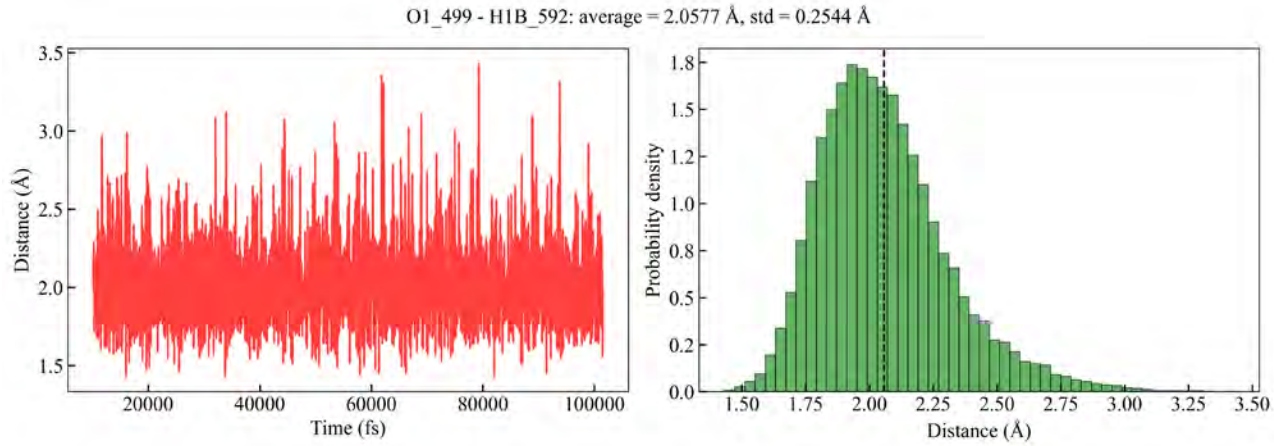
O1_498 - H1B_589

Average distance = 2.0314 Å; standard deviation = 0.2157 Å; number of points = 91387



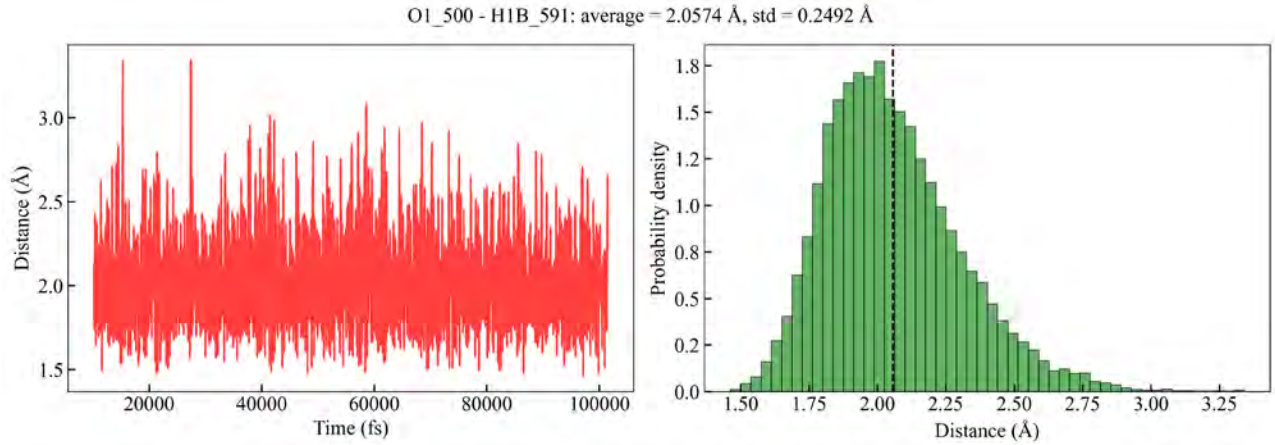
O1_499 - H1B_592

Average distance = 2.0577 Å; standard deviation = 0.2544 Å; number of points = 91387



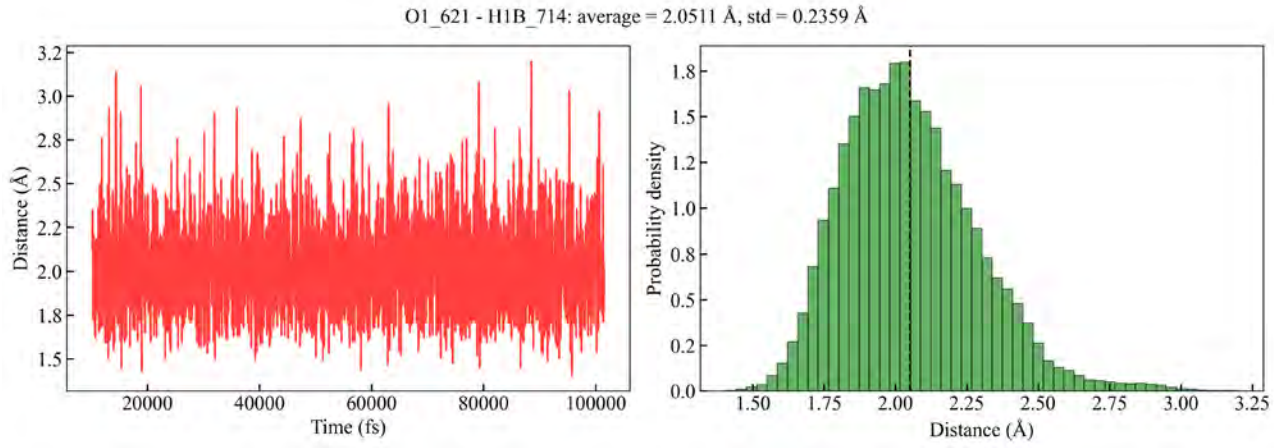
O1_500 - H1B_591

Average distance = 2.0574 Å; standard deviation = 0.2492 Å; number of points = 91387



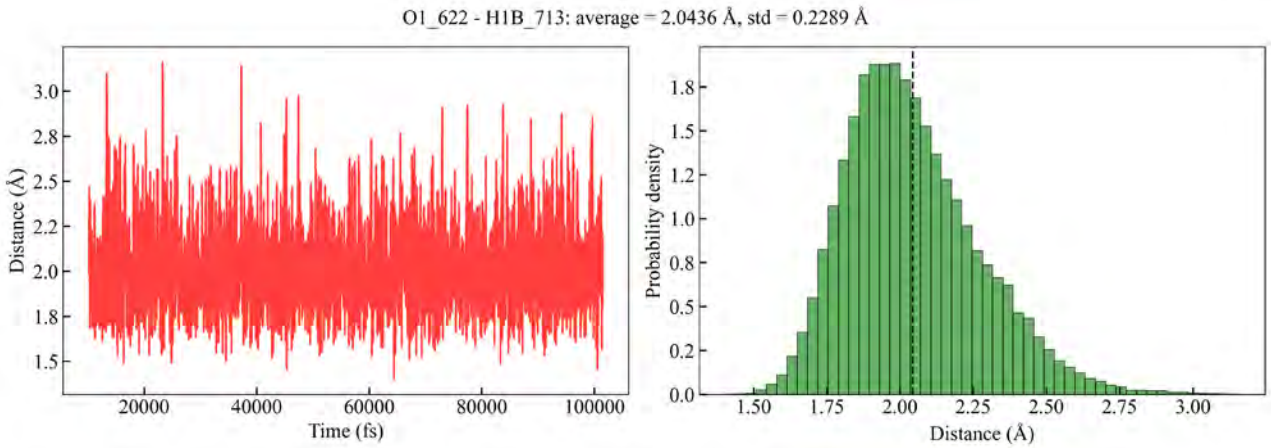
O1_621 - H1B_714

Average distance = 2.0511 Å; standard deviation = 0.2359 Å; number of points = 91387



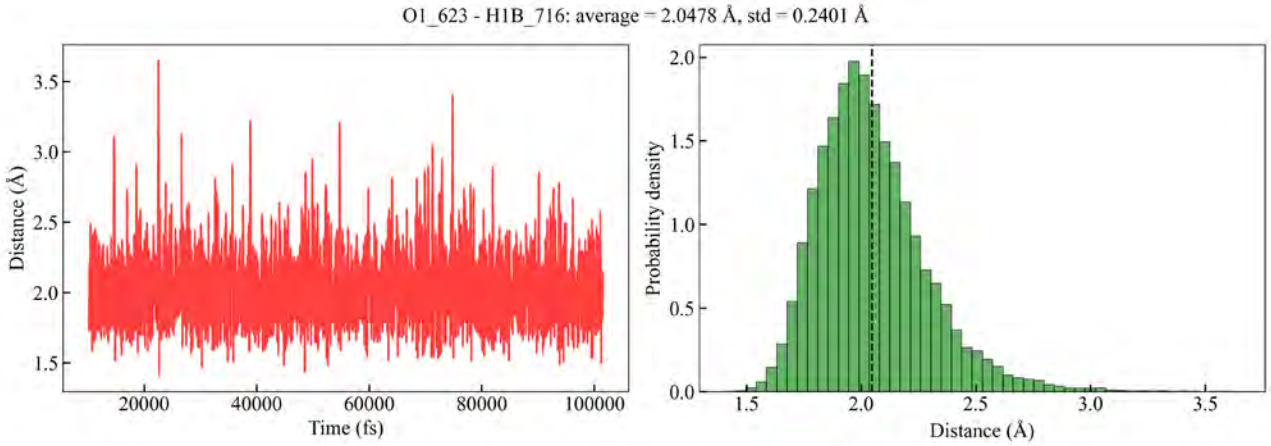
O1_622 - H1B_713

Average distance = 2.0436 Å; standard deviation = 0.2289 Å; number of points = 91387



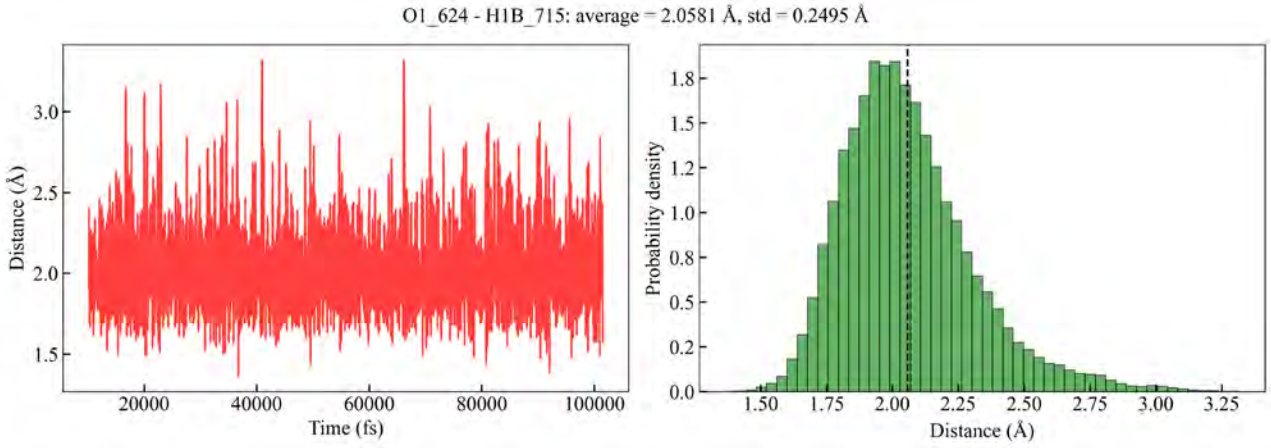
O1_623 - H1B_716

Average distance = 2.0478 Å; standard deviation = 0.2401 Å; number of points = 91387



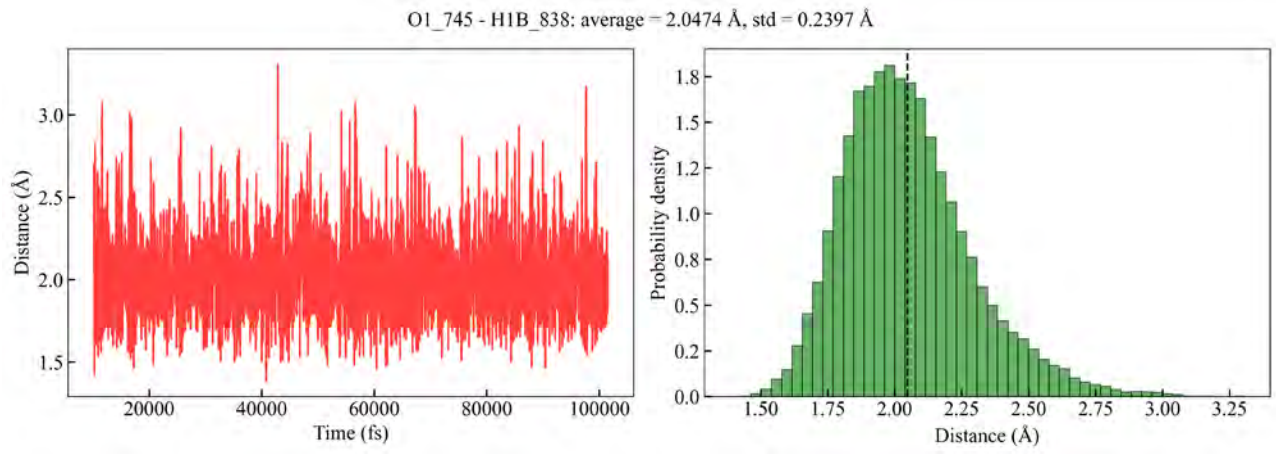
O1_624 - H1B_715

Average distance = 2.0581 Å; standard deviation = 0.2495 Å; number of points = 91387



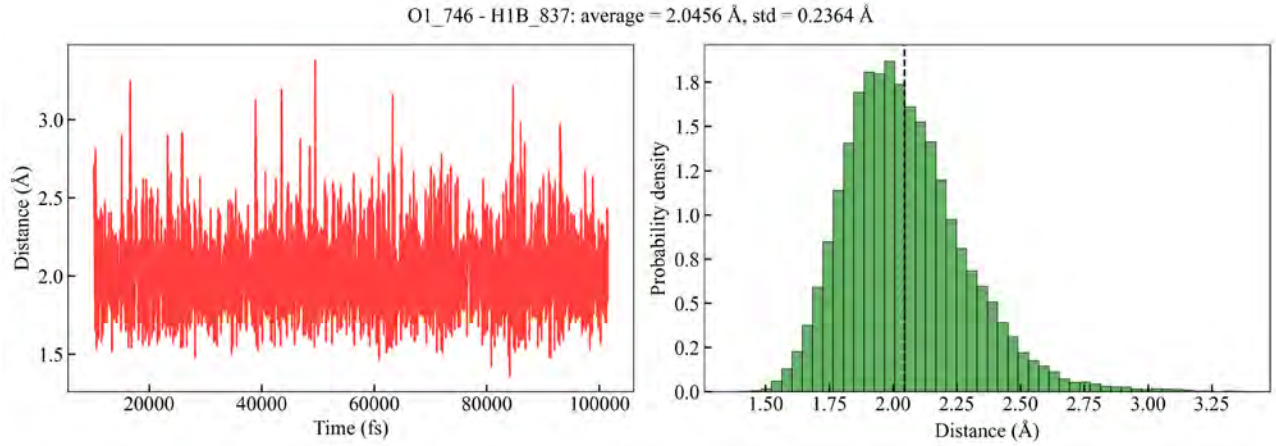
O1_745 - H1B_838

Average distance = 2.0474 Å; standard deviation = 0.2397 Å; number of points = 91387



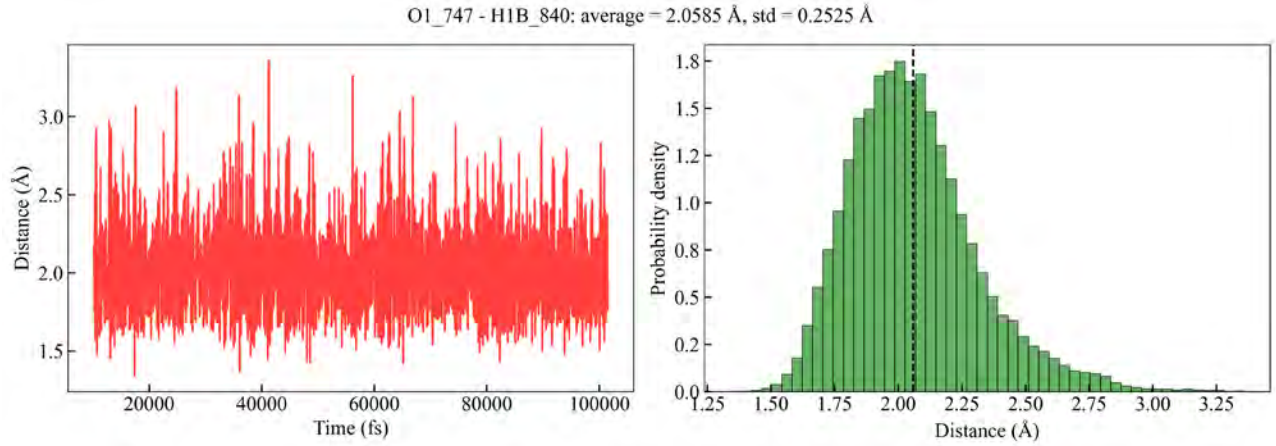
O1_746 - H1B_837

Average distance = 2.0456 Å; standard deviation = 0.2364 Å; number of points = 91387



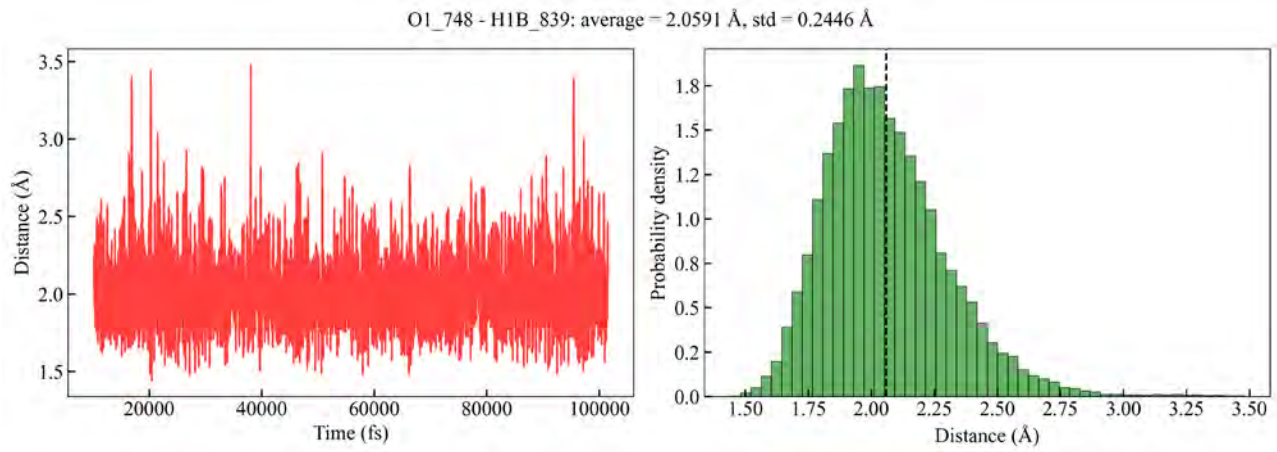
O1_747 - H1B_840

Average distance = 2.0585 Å; standard deviation = 0.2525 Å; number of points = 91387



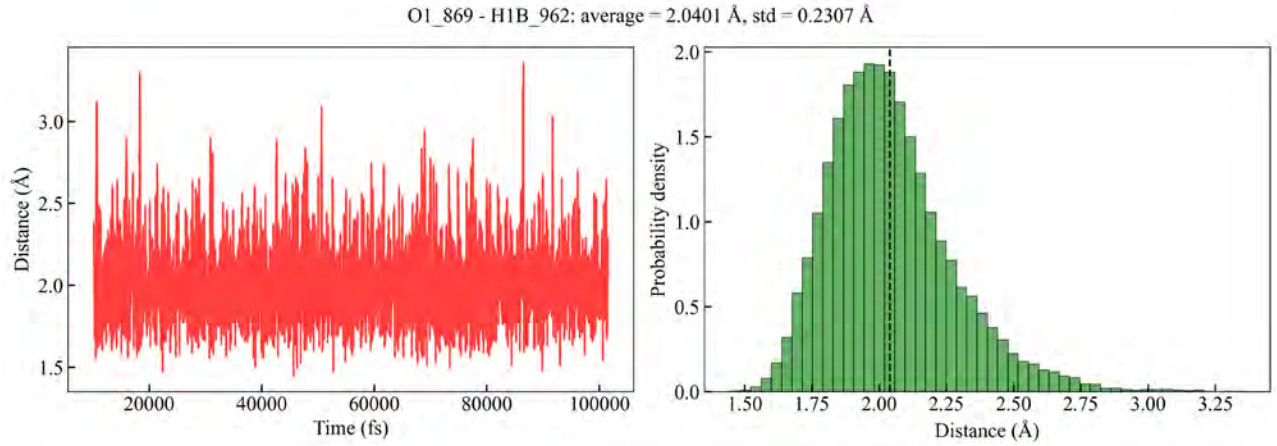
O1_748 - H1B_839

Average distance = 2.0591 Å; standard deviation = 0.2446 Å; number of points = 91387



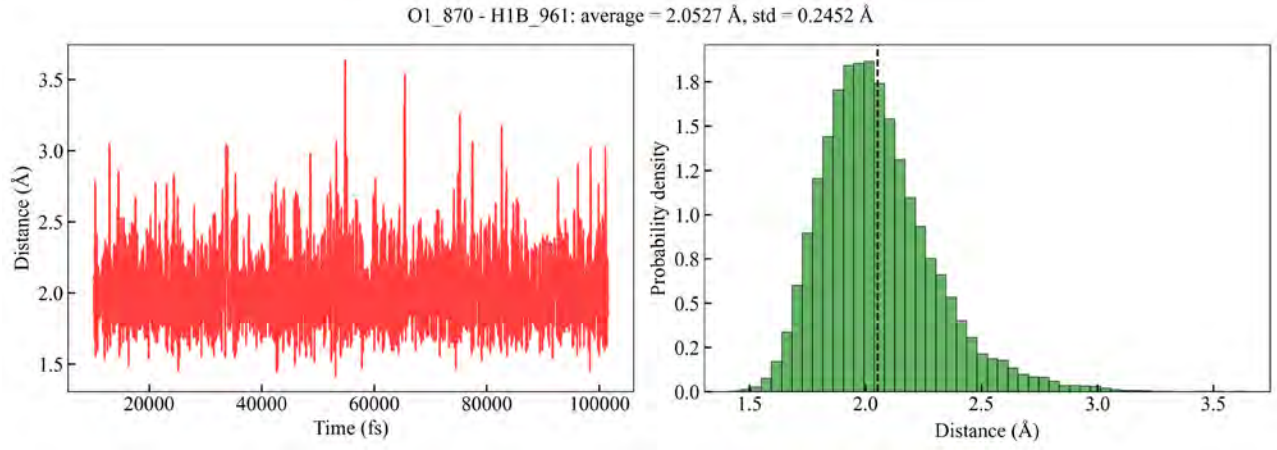
O1_869 - H1B_962

Average distance = 2.0401 Å; standard deviation = 0.2307 Å; number of points = 91387



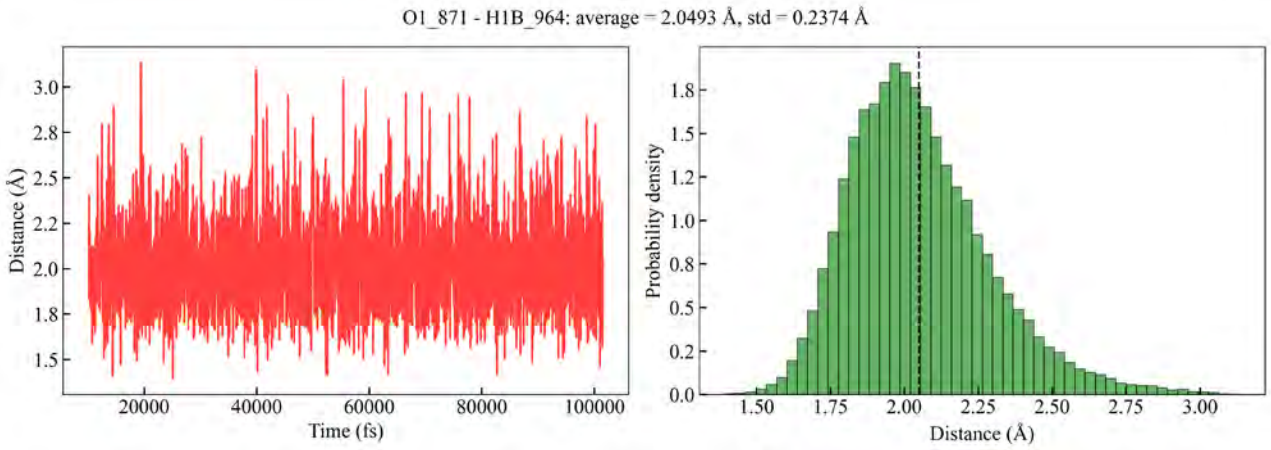
O1_870 - H1B_961

Average distance = 2.0527 Å; standard deviation = 0.2452 Å; number of points = 91387



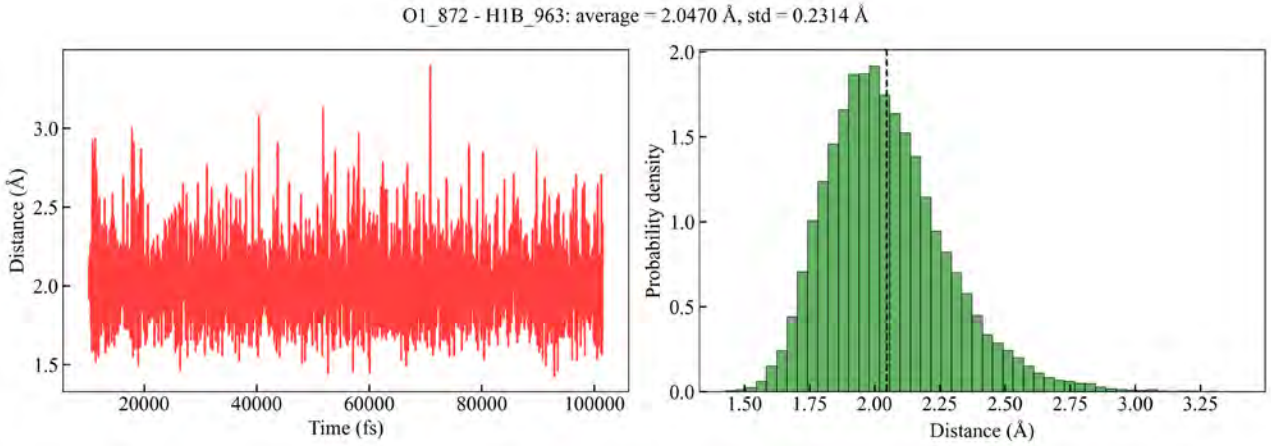
O1_871 - H1B_964

Average distance = 2.0493 Å; standard deviation = 0.2374 Å; number of points = 91387



O1_872 - H1B_963

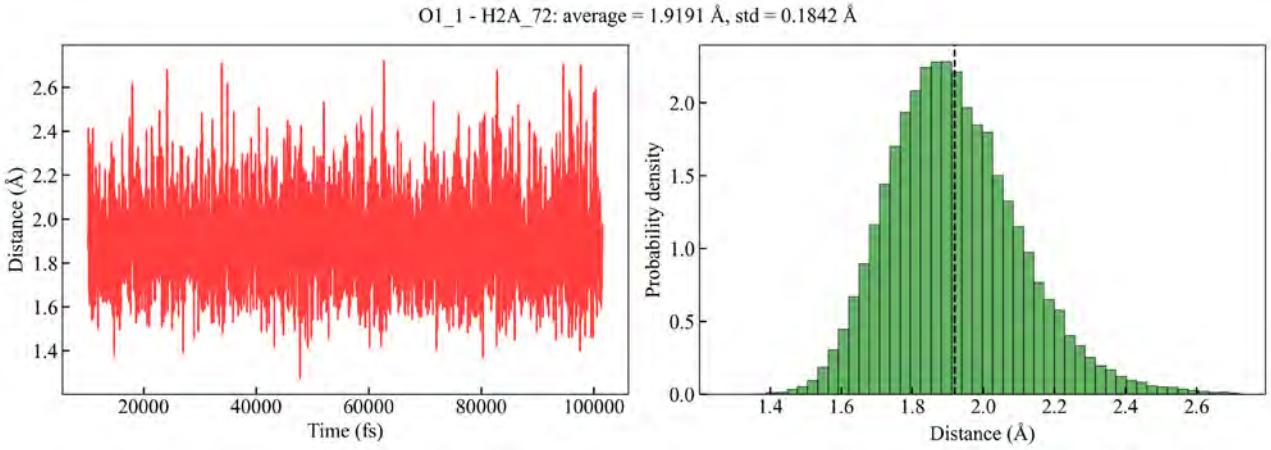
Average distance = 2.0470 Å; standard deviation = 0.2314 Å; number of points = 91387



O1 - H2A

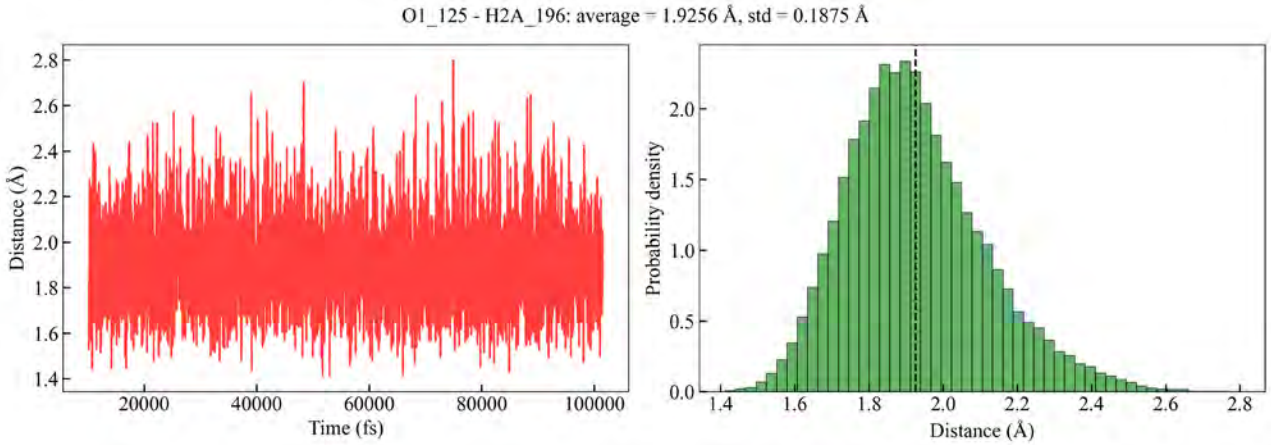
O1_1 - H2A_72

Average distance = 1.9191 Å; standard deviation = 0.1842 Å; number of points = 91387



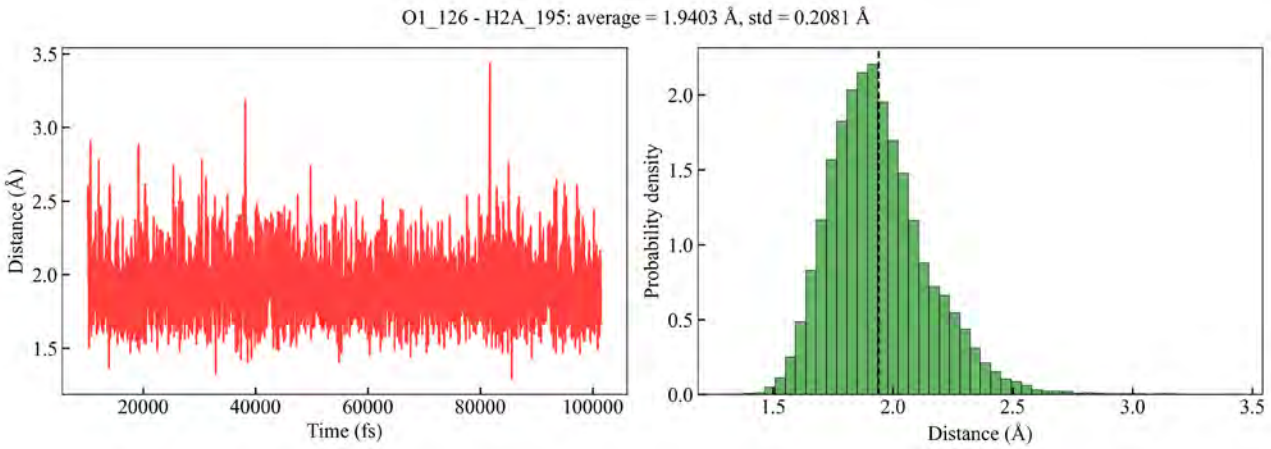
O1_125 - H2A_196

Average distance = 1.9256 Å; standard deviation = 0.1875 Å; number of points = 91387



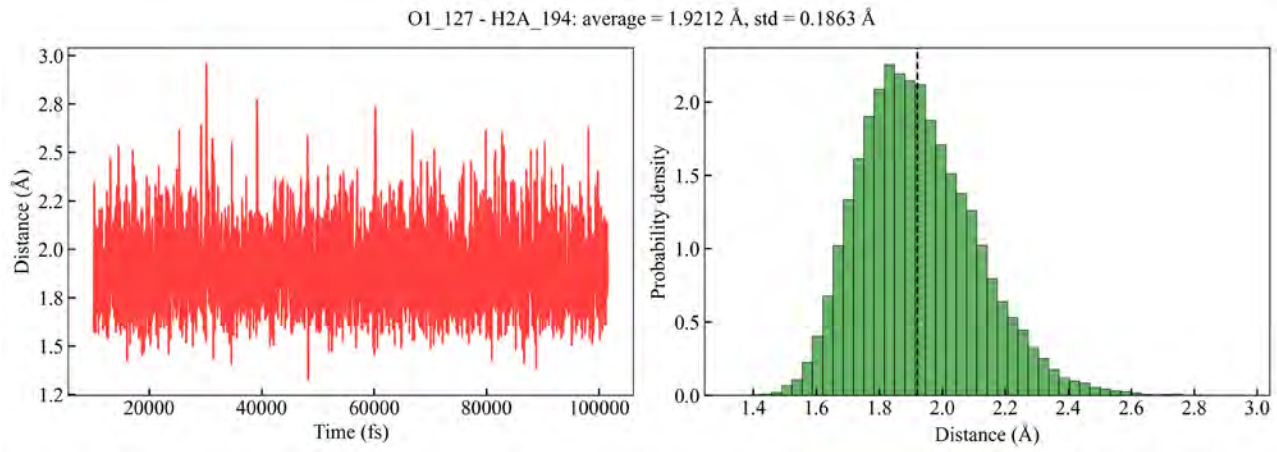
O1_126 - H2A_195

Average distance = 1.9403 Å; standard deviation = 0.2081 Å; number of points = 91387



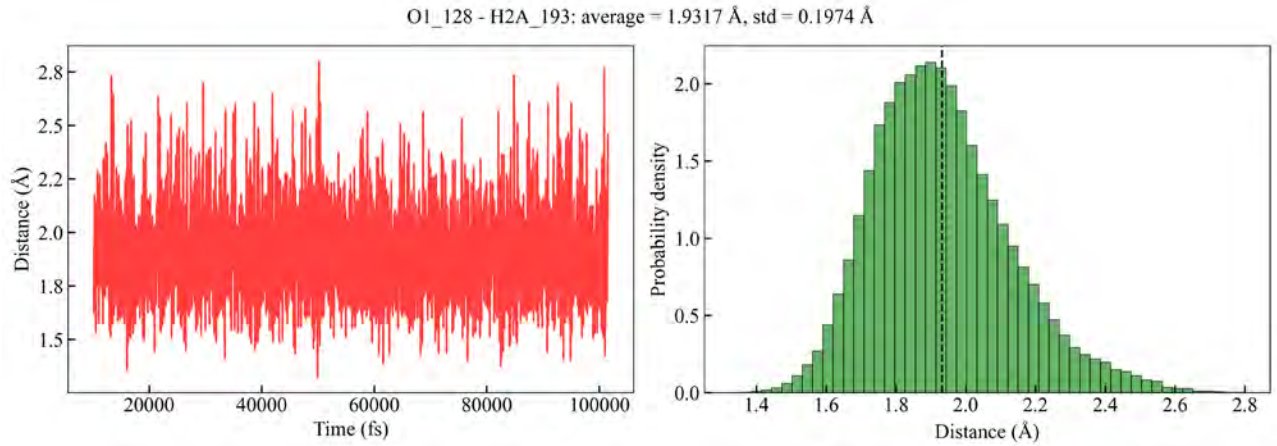
O1_127 - H2A_194

Average distance = 1.9212 Å; standard deviation = 0.1863 Å; number of points = 91387



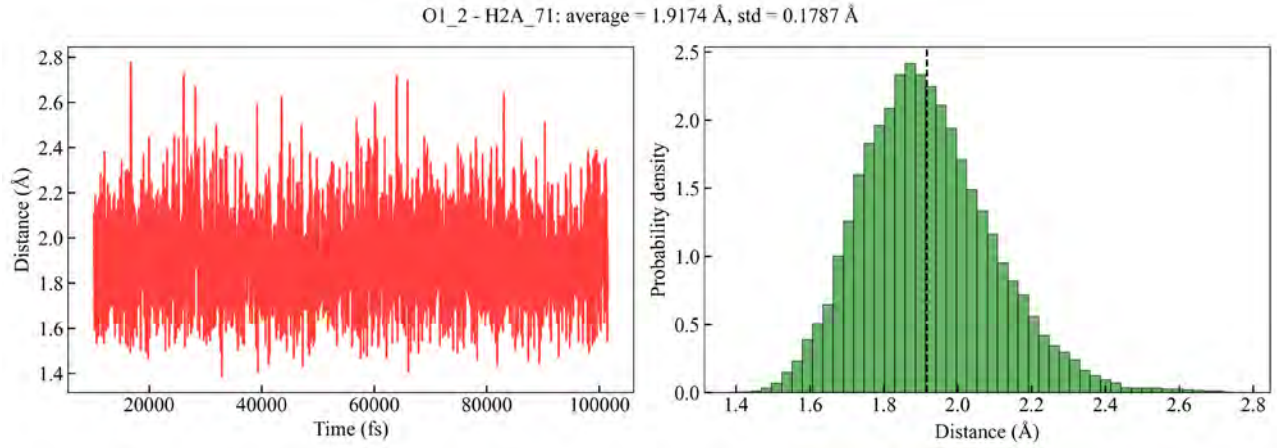
O1_128 - H2A_193

Average distance = 1.9317 Å; standard deviation = 0.1974 Å; number of points = 91387



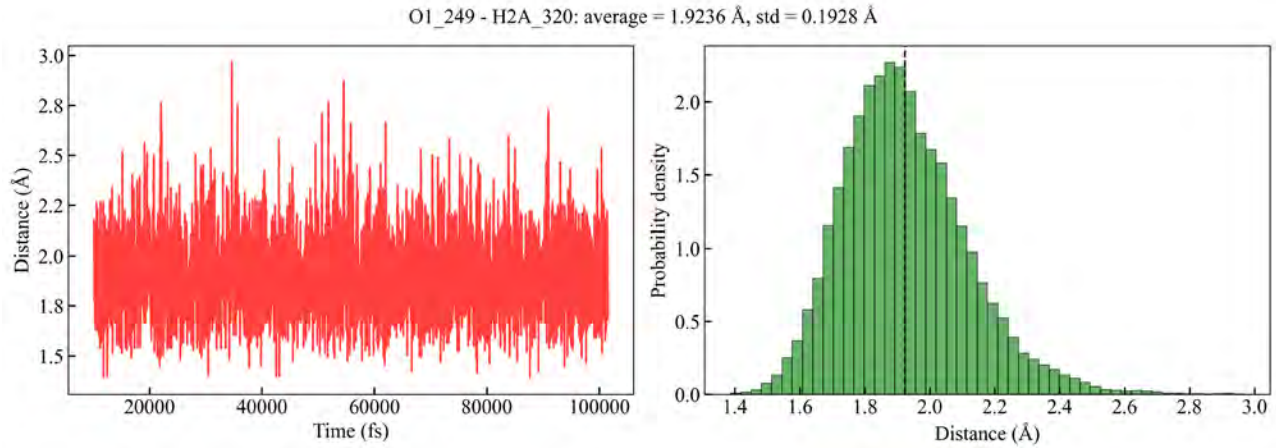
O1_2 - H2A_71

Average distance = 1.9174 Å; standard deviation = 0.1787 Å; number of points = 91387



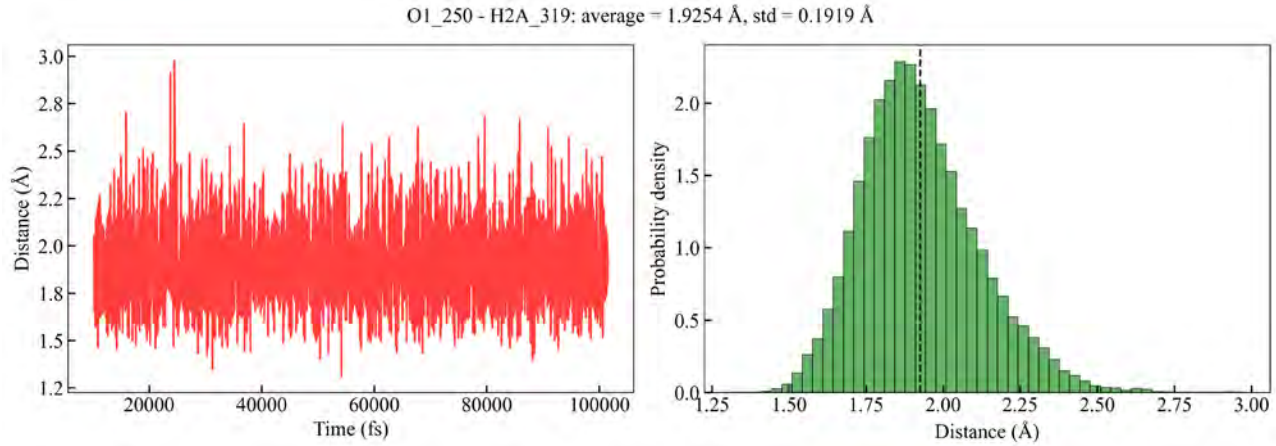
O1_249 - H2A_320

Average distance = 1.9236 Å; standard deviation = 0.1928 Å; number of points = 91387



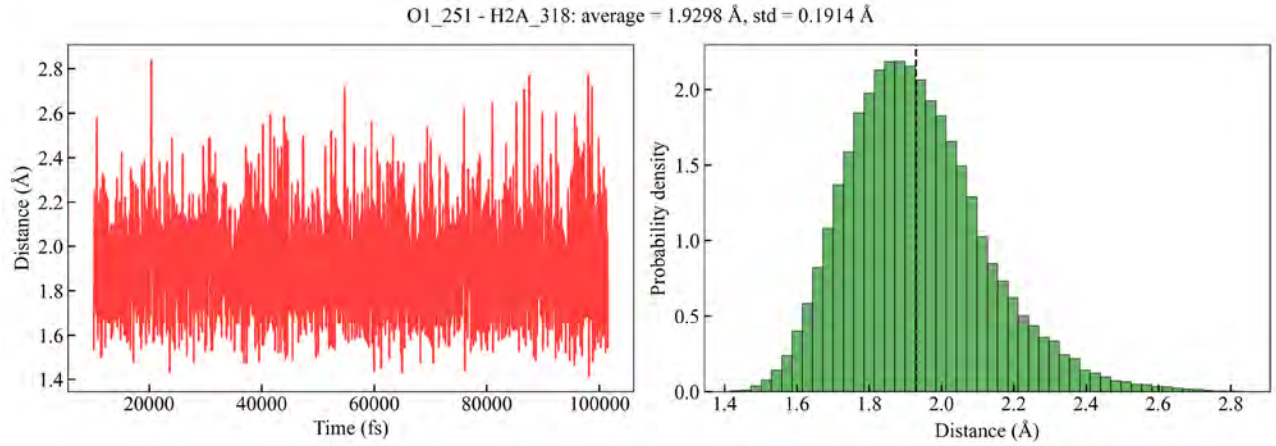
O1_250 - H2A_319

Average distance = 1.9254 Å; standard deviation = 0.1919 Å; number of points = 91387



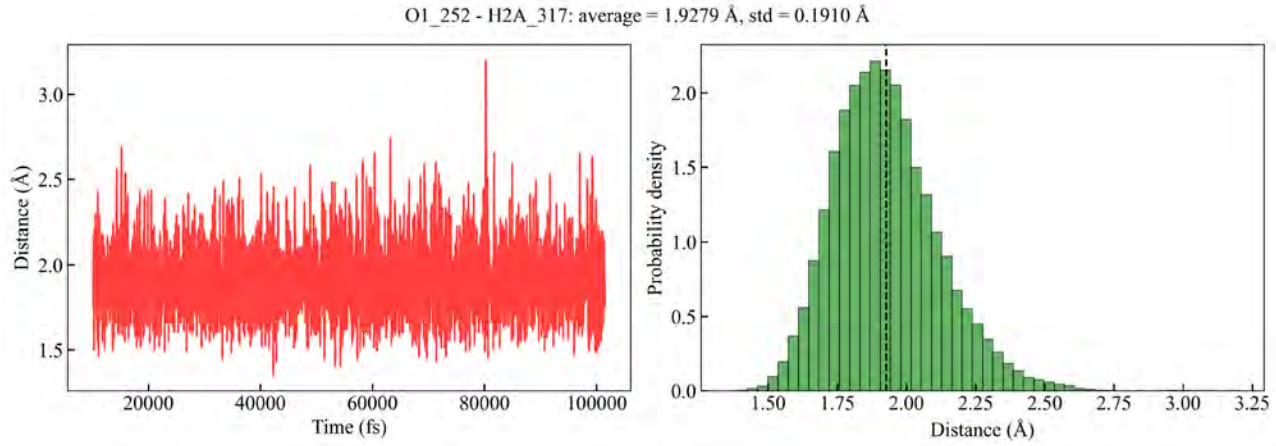
O1_251 - H2A_318

Average distance = 1.9298 Å; standard deviation = 0.1914 Å; number of points = 91387



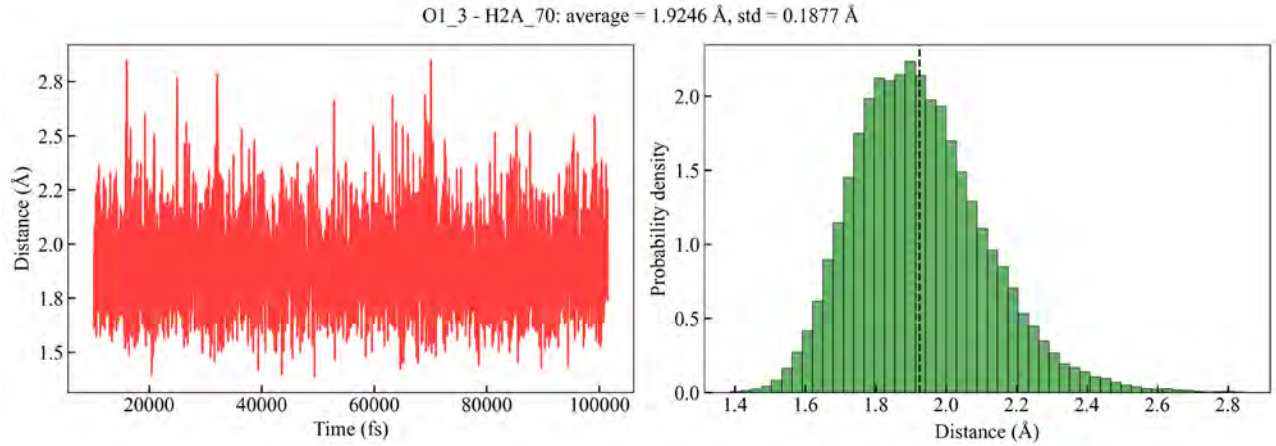
O1_252 - H2A_317

Average distance = 1.9279 Å; standard deviation = 0.1910 Å; number of points = 91387



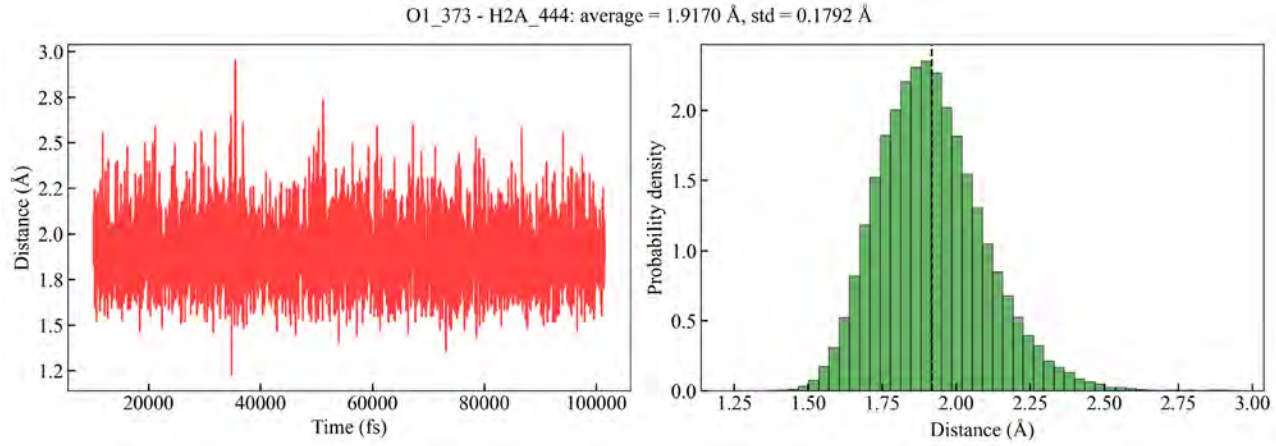
O1_3 - H2A_70

Average distance = 1.9246 Å; standard deviation = 0.1877 Å; number of points = 91387



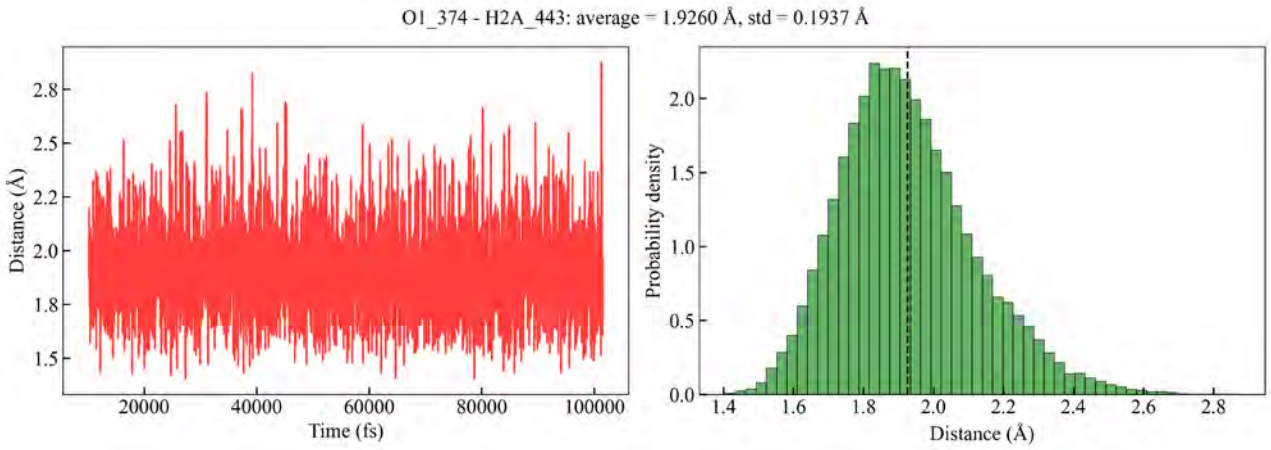
O1_373 - H2A_444

Average distance = 1.9170 Å; standard deviation = 0.1792 Å; number of points = 91387



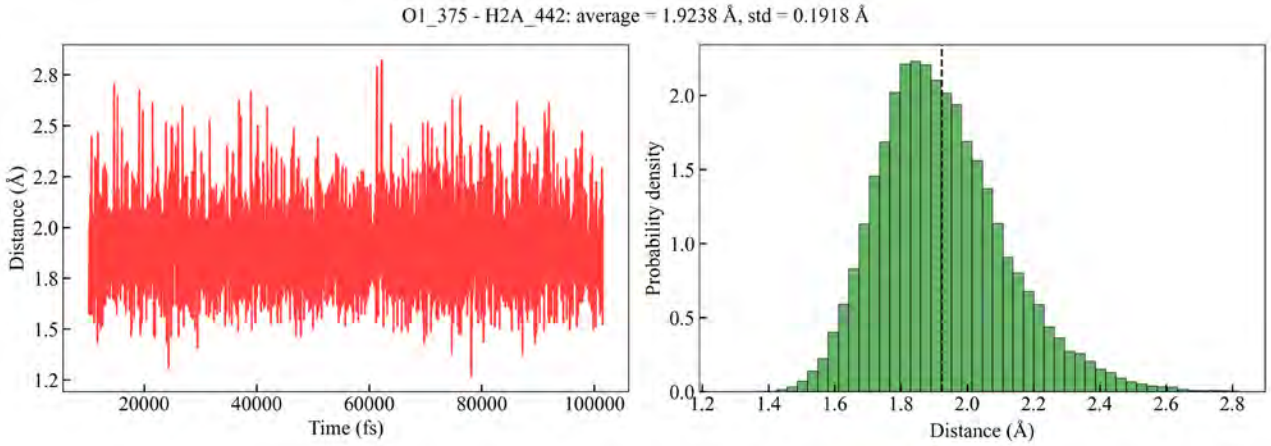
O1_374 - H2A_443

Average distance = 1.9260 Å; standard deviation = 0.1937 Å; number of points = 91387



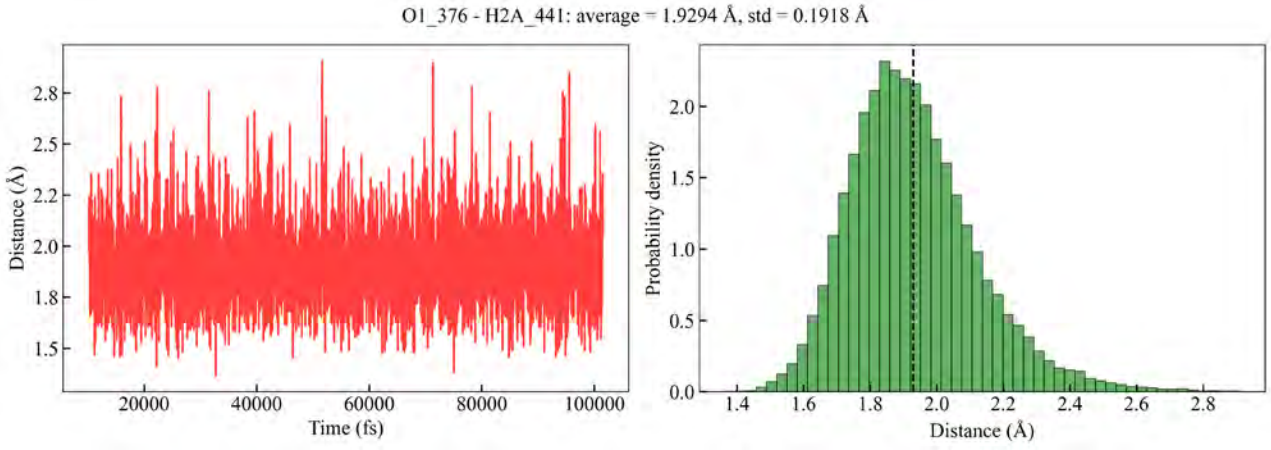
O1_375 - H2A_442

Average distance = 1.9238 Å; standard deviation = 0.1918 Å; number of points = 91387



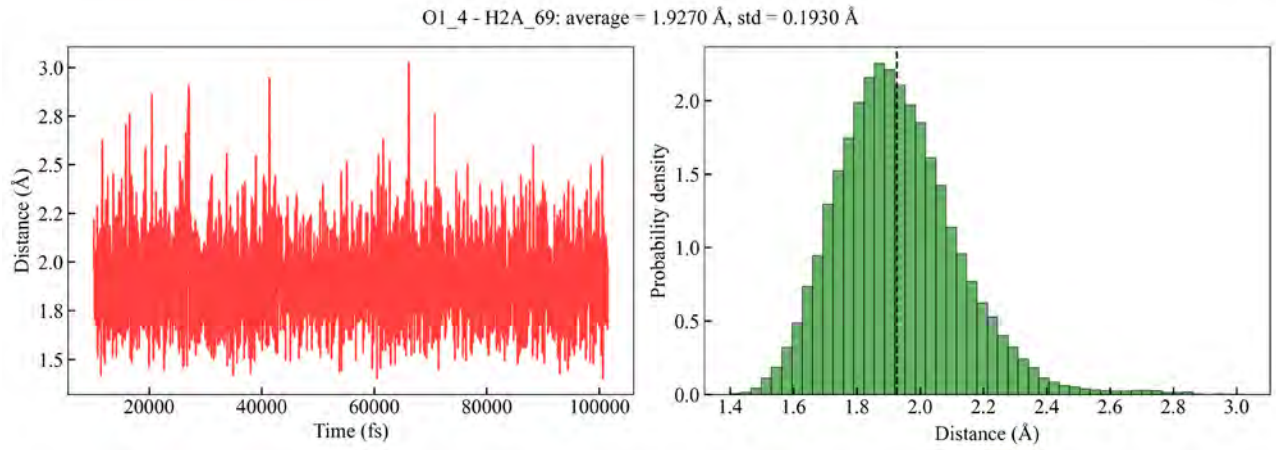
O1_376 - H2A_441

Average distance = 1.9294 Å; standard deviation = 0.1918 Å; number of points = 91387



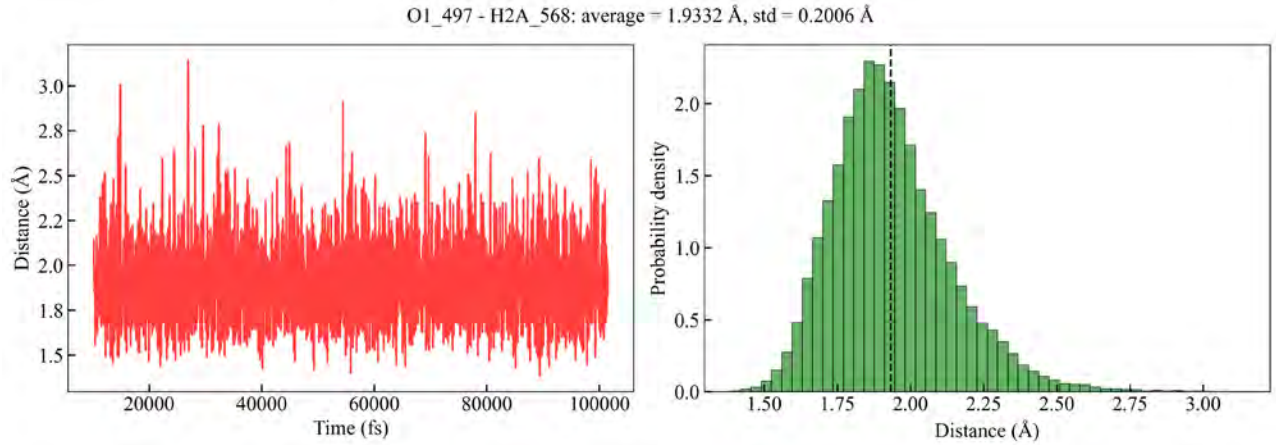
O1_4 - H2A_69

Average distance = 1.9270 Å; standard deviation = 0.1930 Å; number of points = 91387



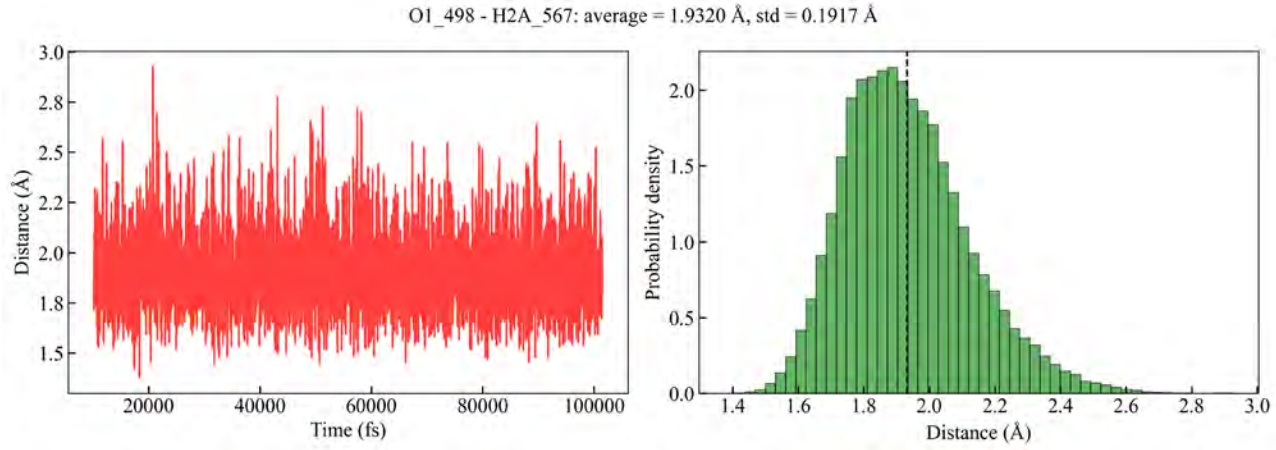
O1_497 - H2A_568

Average distance = 1.9332 Å; standard deviation = 0.2006 Å; number of points = 91387



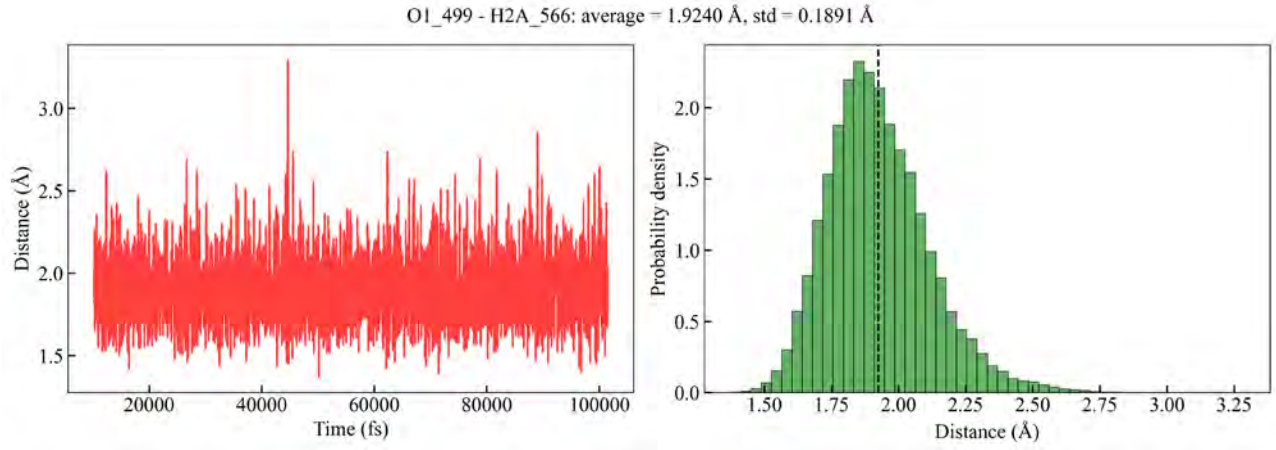
O1_498 - H2A_567

Average distance = 1.9320 Å; standard deviation = 0.1917 Å; number of points = 91387



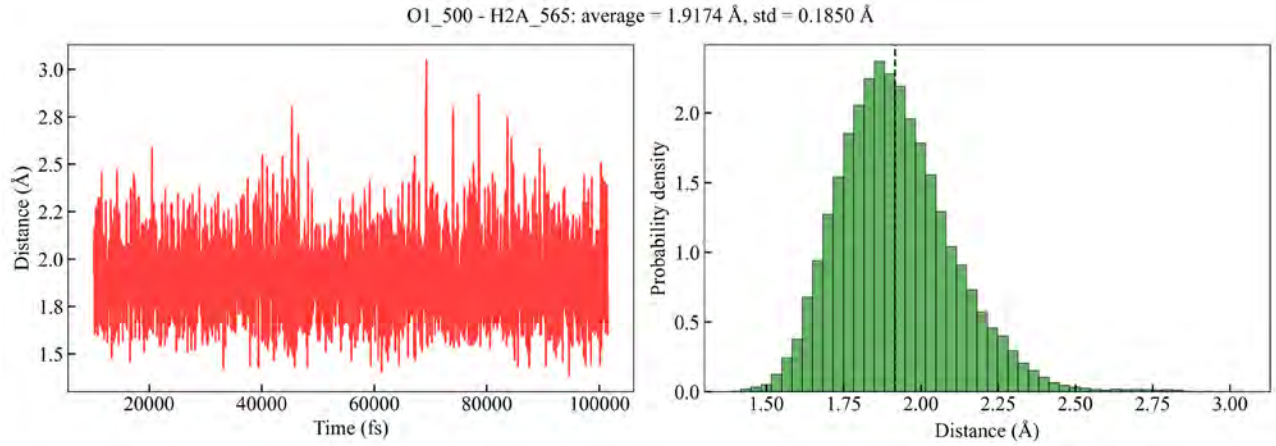
O1_499 - H2A_566

Average distance = 1.9240 Å; standard deviation = 0.1891 Å; number of points = 91387



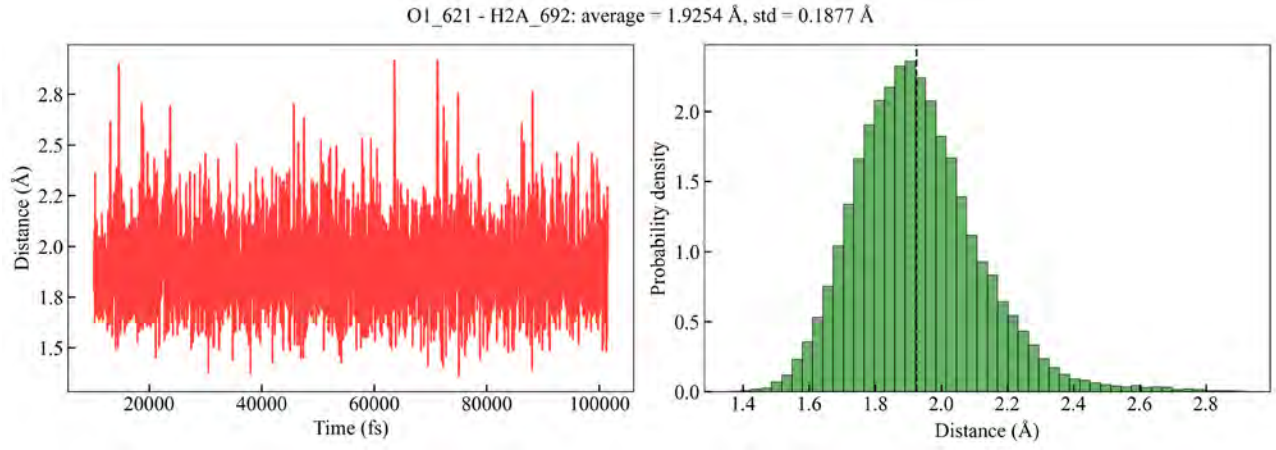
O1_500 - H2A_565

Average distance = 1.9174 Å; standard deviation = 0.1850 Å; number of points = 91387



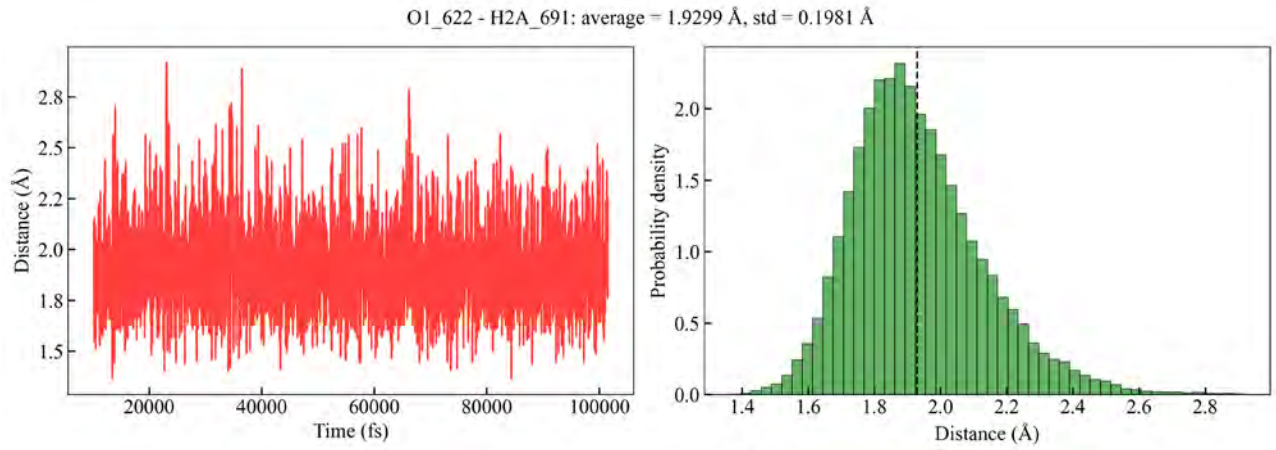
O1_621 - H2A_692

Average distance = 1.9254 Å; standard deviation = 0.1877 Å; number of points = 91387



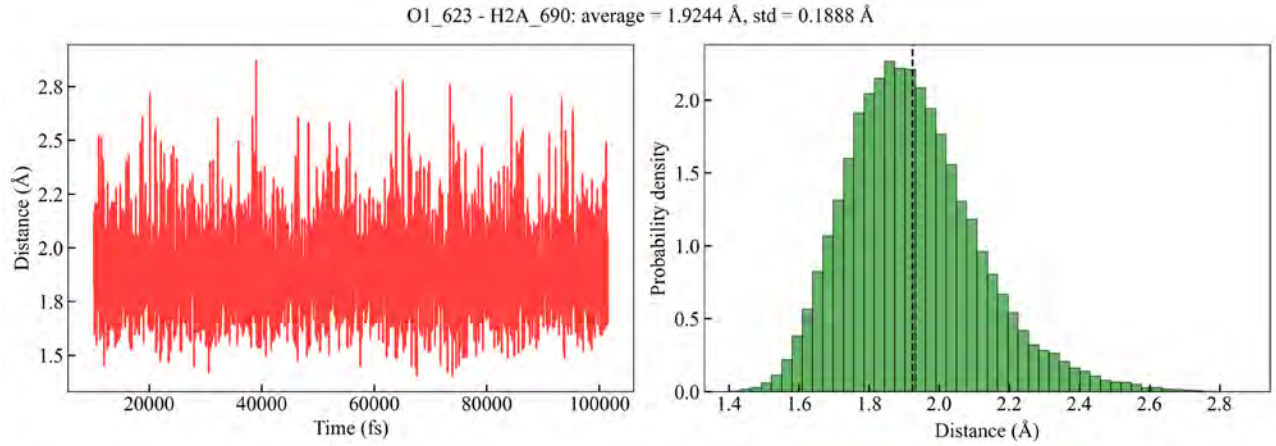
O1_622 - H2A_691

Average distance = 1.9299 Å; standard deviation = 0.1981 Å; number of points = 91387



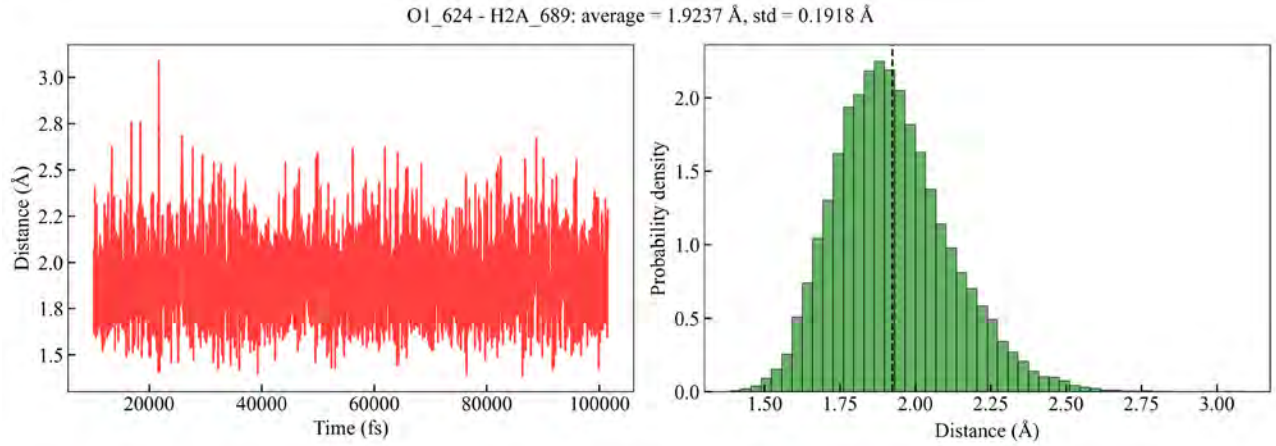
O1_623 - H2A_690

Average distance = 1.9244 Å; standard deviation = 0.1888 Å; number of points = 91387



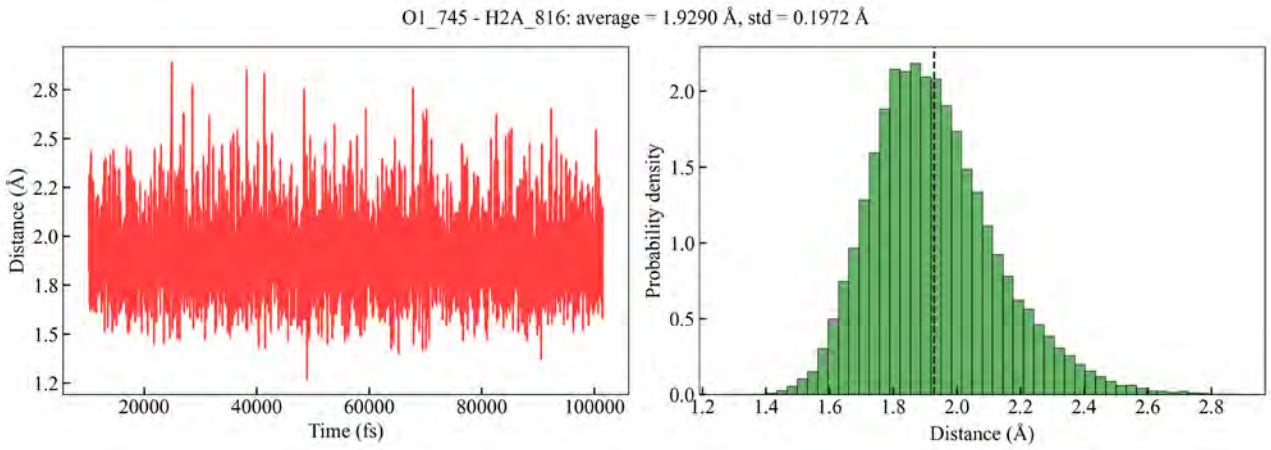
O1_624 - H2A_689

Average distance = 1.9237 Å; standard deviation = 0.1918 Å; number of points = 91387



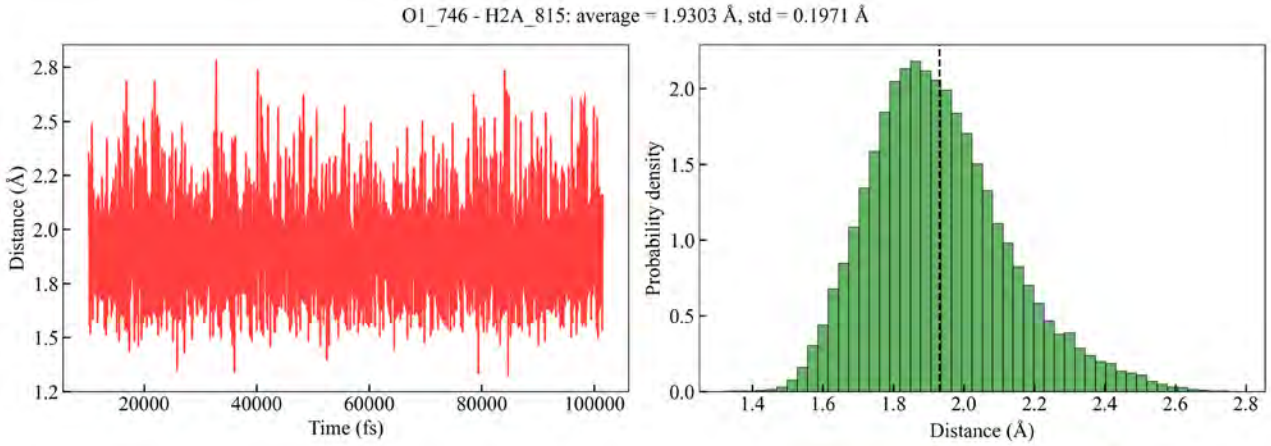
O1_745 - H2A_816

Average distance = 1.9290 Å; standard deviation = 0.1972 Å; number of points = 91387



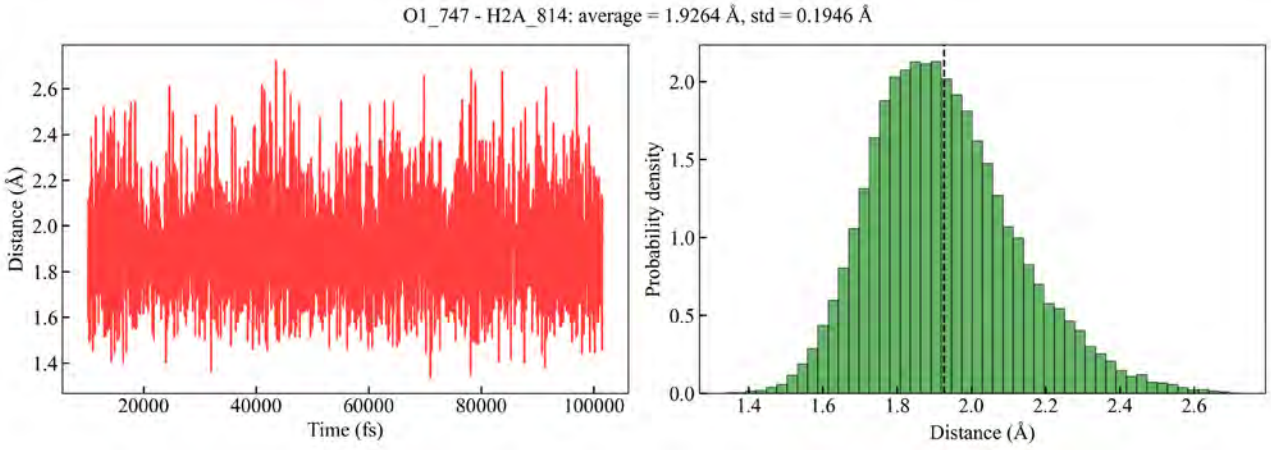
O1_746 - H2A_815

Average distance = 1.9303 Å; standard deviation = 0.1971 Å; number of points = 91387



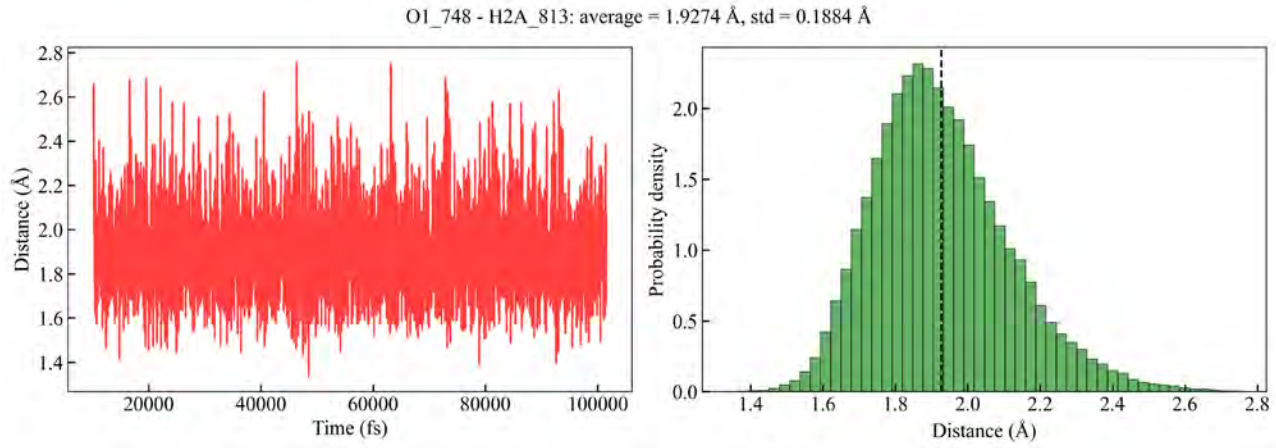
O1_747 - H2A_814

Average distance = 1.9264 Å; standard deviation = 0.1946 Å; number of points = 91387



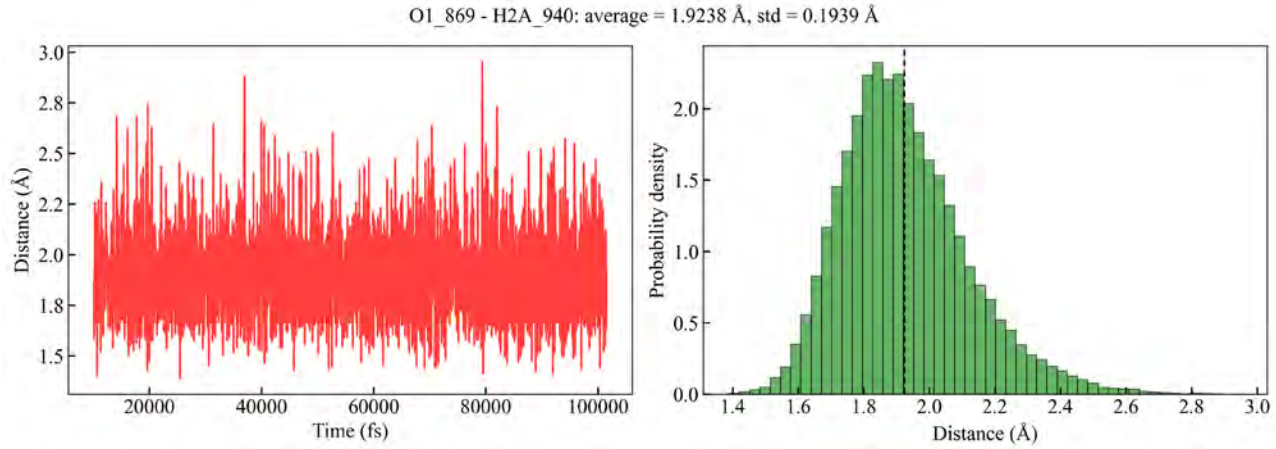
O1_748 - H2A_813

Average distance = 1.9274 Å; standard deviation = 0.1884 Å; number of points = 91387



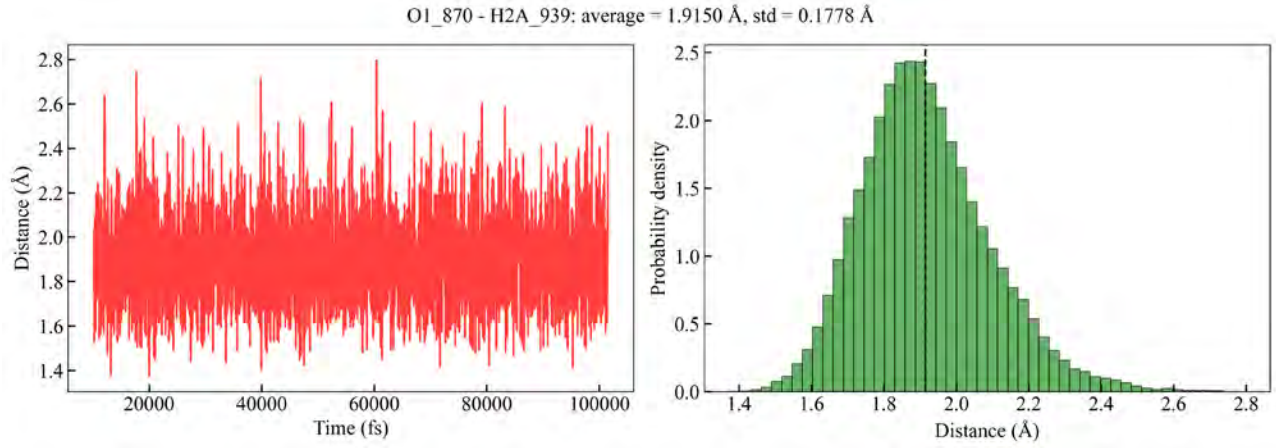
O1_869 - H2A_940

Average distance = 1.9238 Å; standard deviation = 0.1939 Å; number of points = 91387



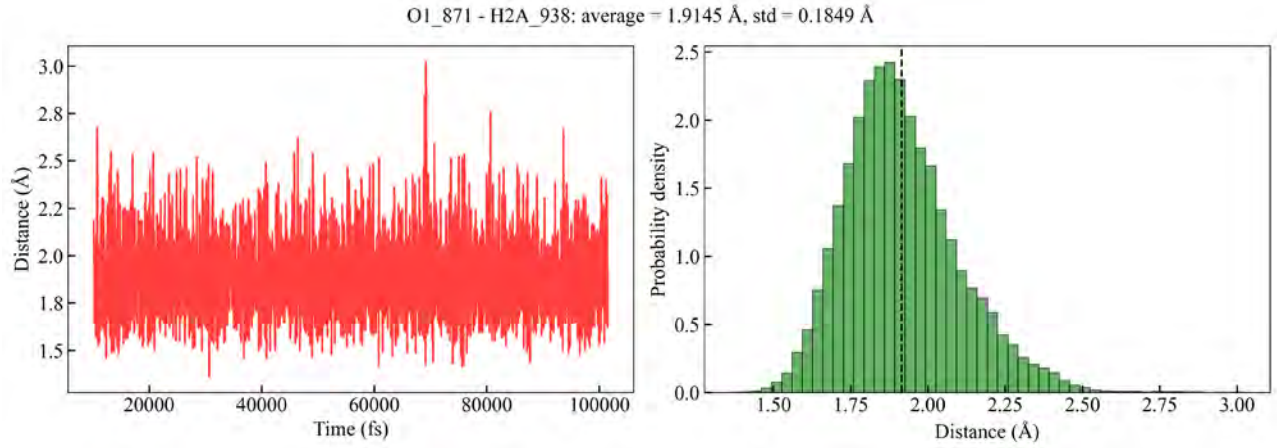
O1_870 - H2A_939

Average distance = 1.9150 Å; standard deviation = 0.1778 Å; number of points = 91387



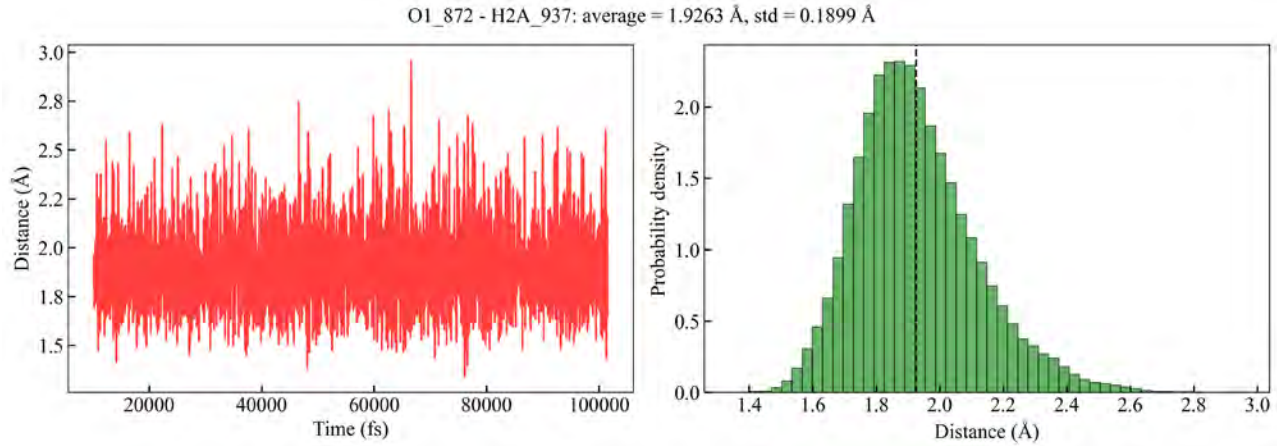
O1_871 - H2A_938

Average distance = 1.9145 Å; standard deviation = 0.1849 Å; number of points = 91387



O1_872 - H2A_937

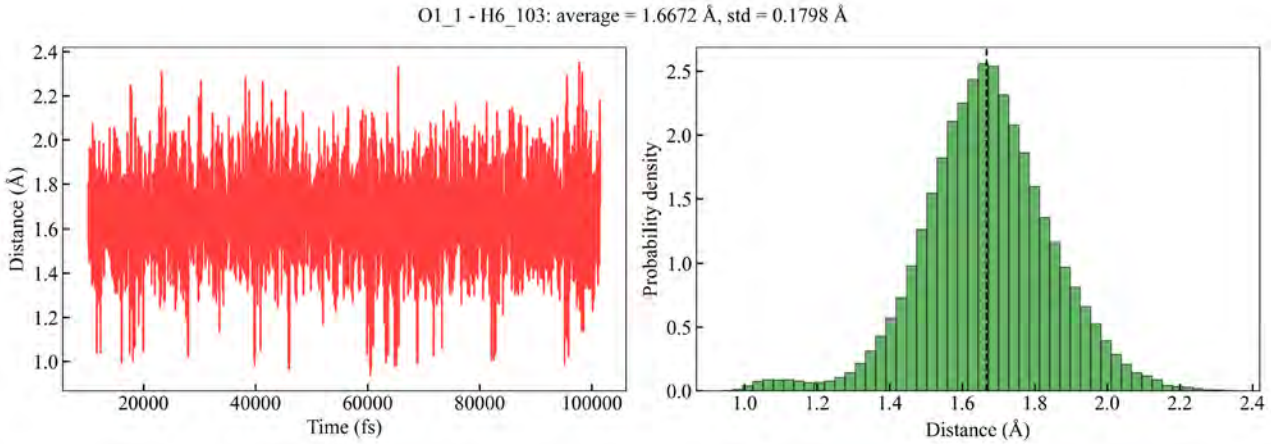
Average distance = 1.9263 Å; standard deviation = 0.1899 Å; number of points = 91387



O1 - H6

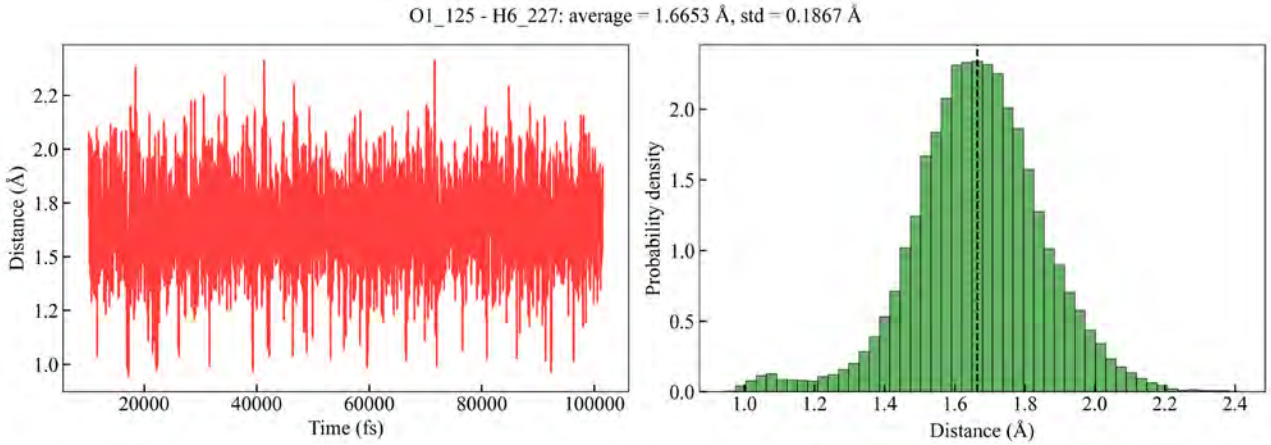
O1_1 - H6_103

Average distance = 1.6672 Å; standard deviation = 0.1798 Å; number of points = 91387



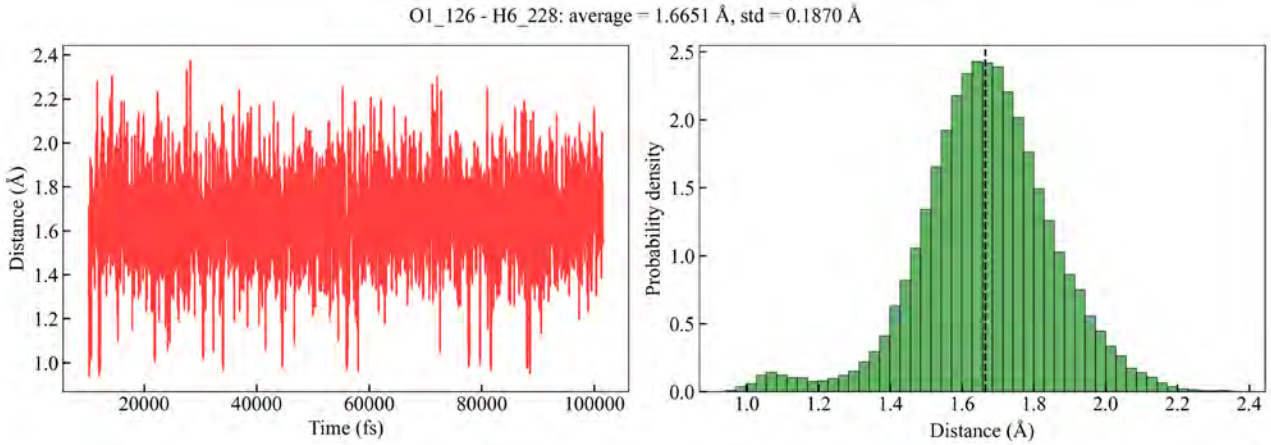
O1_125 - H6_227

Average distance = 1.6653 Å; standard deviation = 0.1867 Å; number of points = 91387



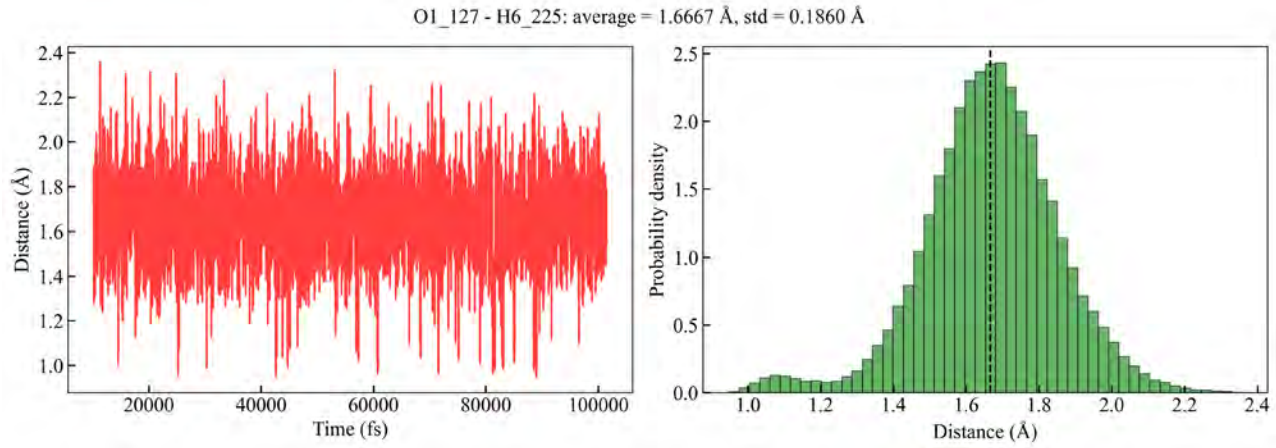
O1_126 - H6_228

Average distance = 1.6651 Å; standard deviation = 0.1870 Å; number of points = 91387



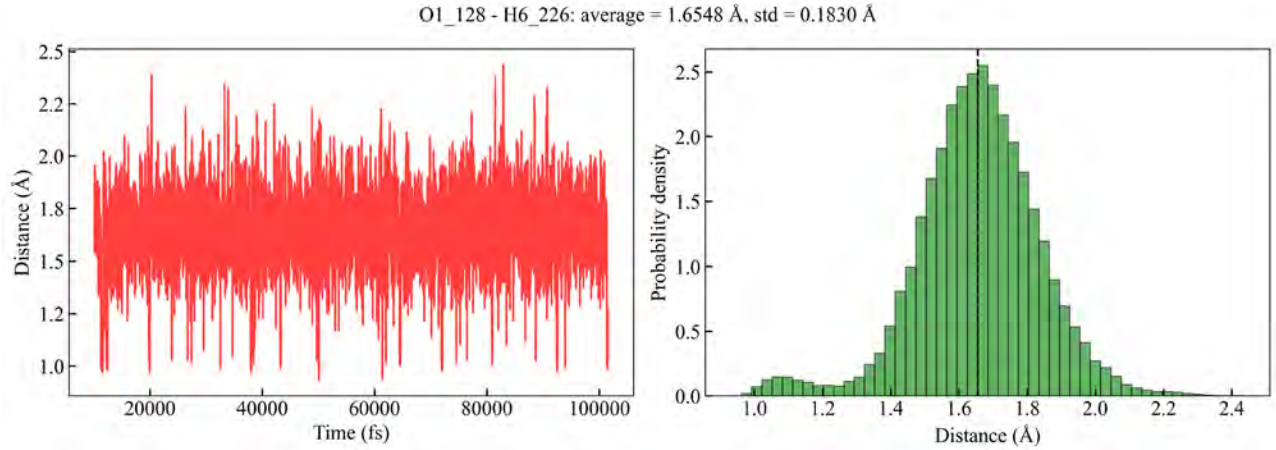
O1_127 - H6_225

Average distance = 1.6667 Å; standard deviation = 0.1860 Å; number of points = 91387



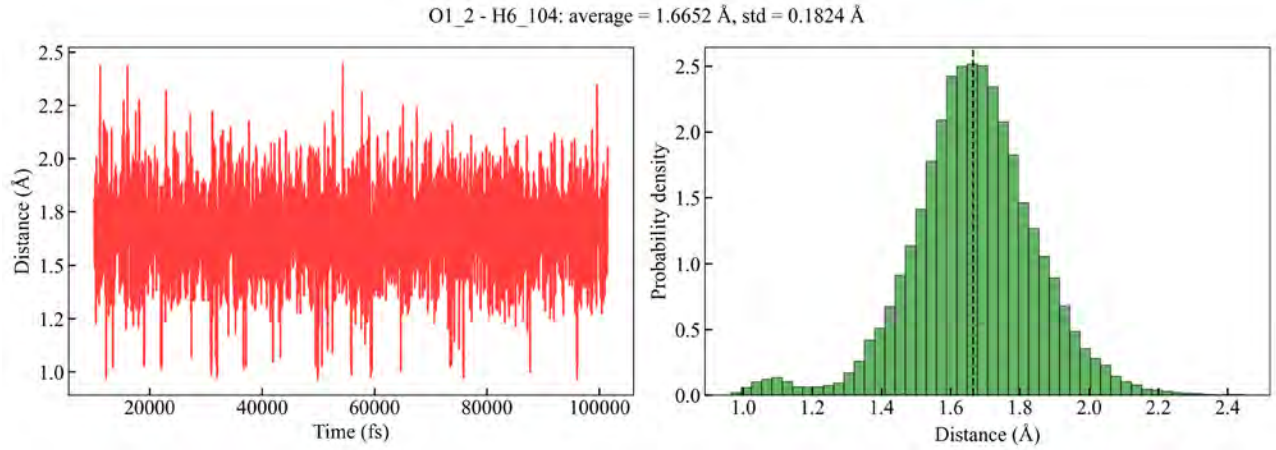
O1_128 - H6_226

Average distance = 1.6548 Å; standard deviation = 0.1830 Å; number of points = 91387



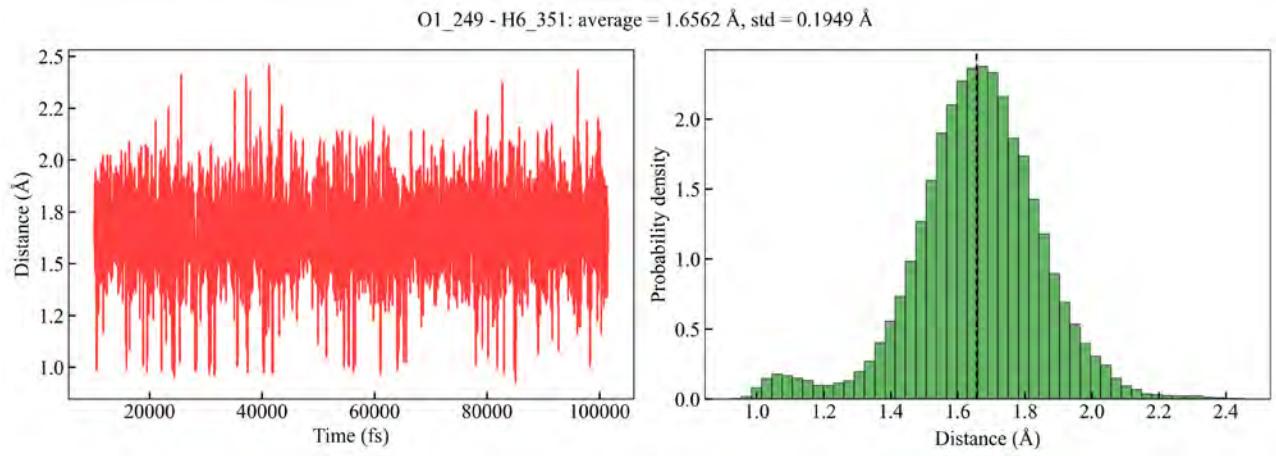
O1_2 - H6_104

Average distance = 1.6652 Å; standard deviation = 0.1824 Å; number of points = 91387



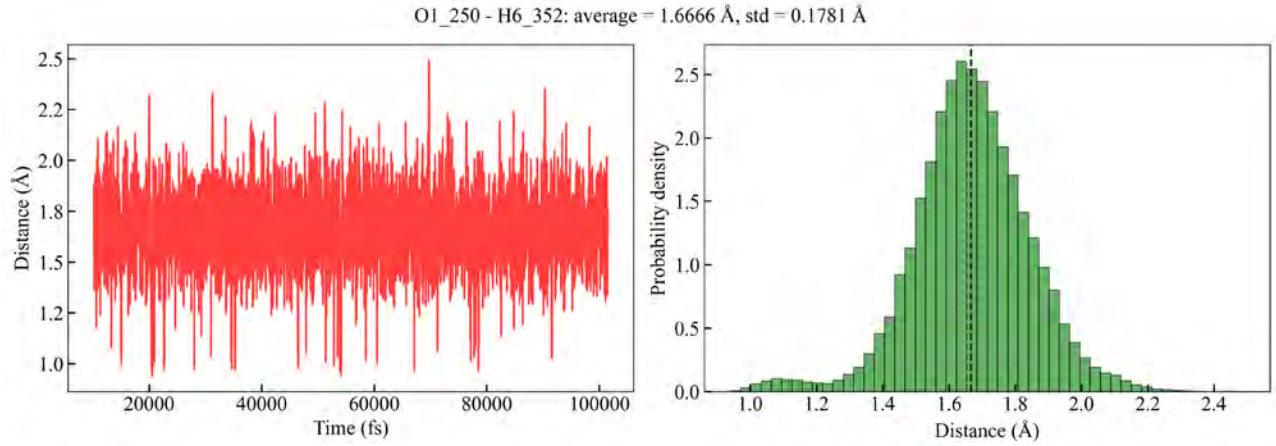
O1_249 - H6_351

Average distance = 1.6562 Å; standard deviation = 0.1949 Å; number of points = 91387



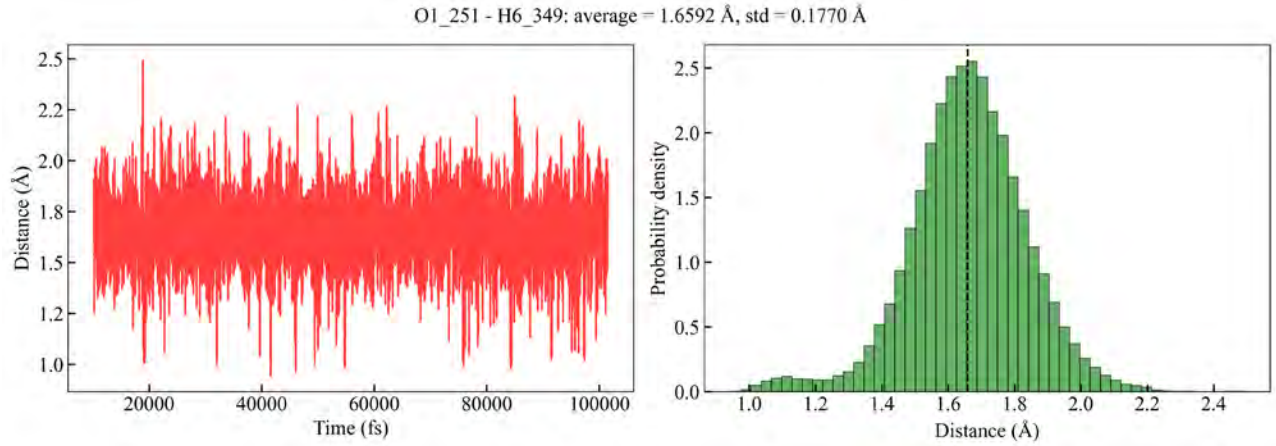
O1_250 - H6_352

Average distance = 1.6666 Å; standard deviation = 0.1781 Å; number of points = 91387



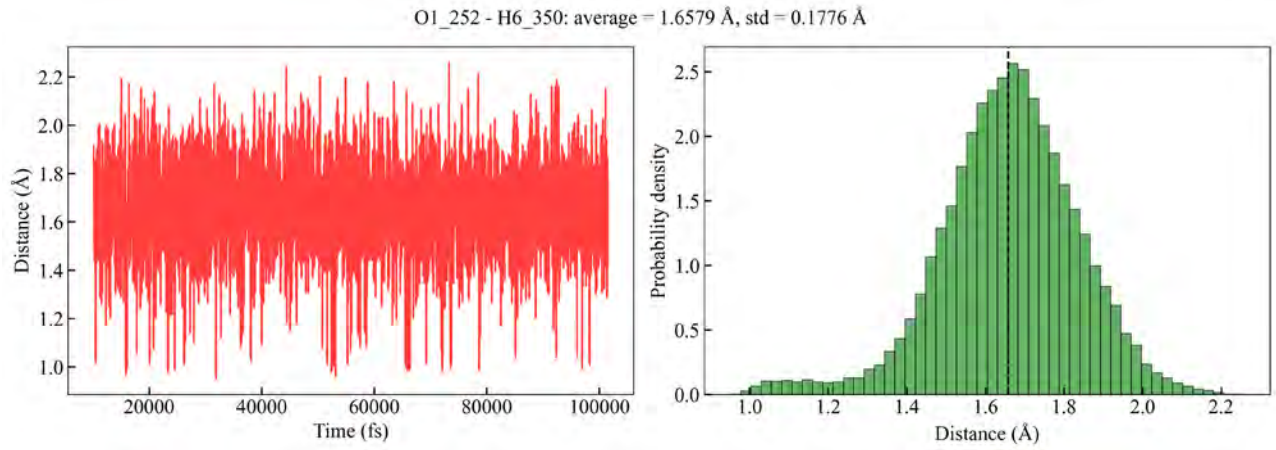
O1_251 - H6_349

Average distance = 1.6592 Å; standard deviation = 0.1770 Å; number of points = 91387



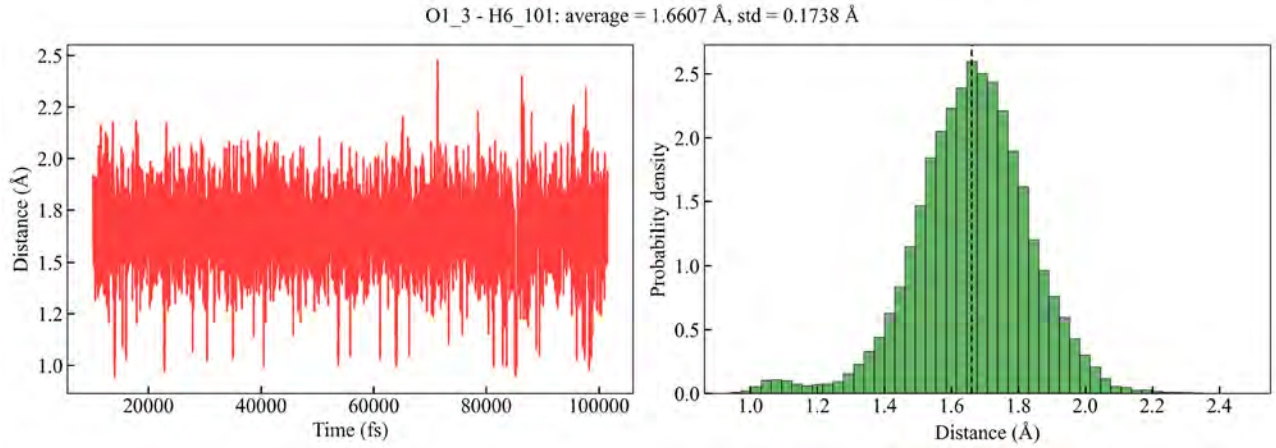
O1_252 - H6_350

Average distance = 1.6579 Å; standard deviation = 0.1776 Å; number of points = 91387



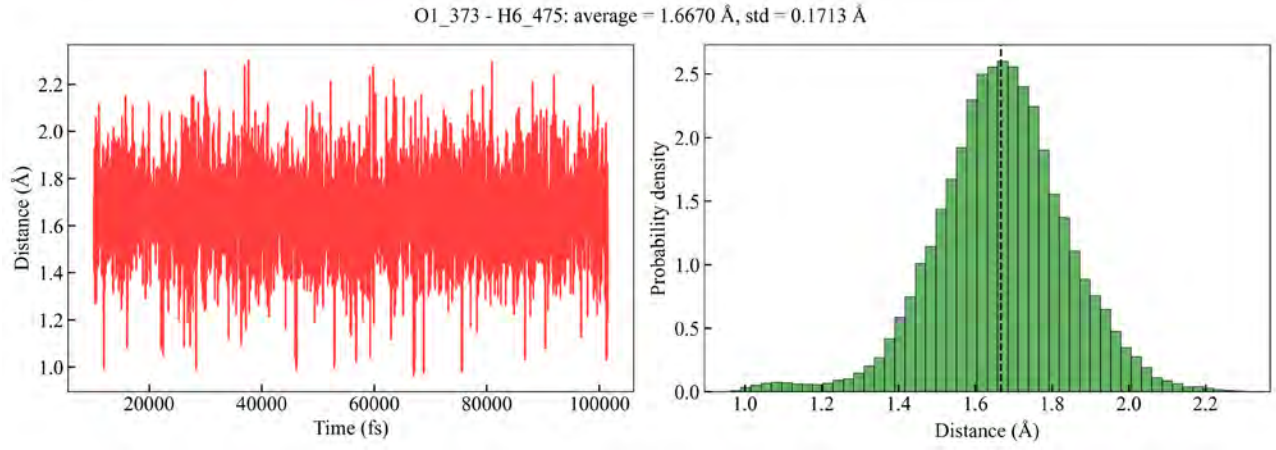
O1_3 - H6_101

Average distance = 1.6607 Å; standard deviation = 0.1738 Å; number of points = 91387



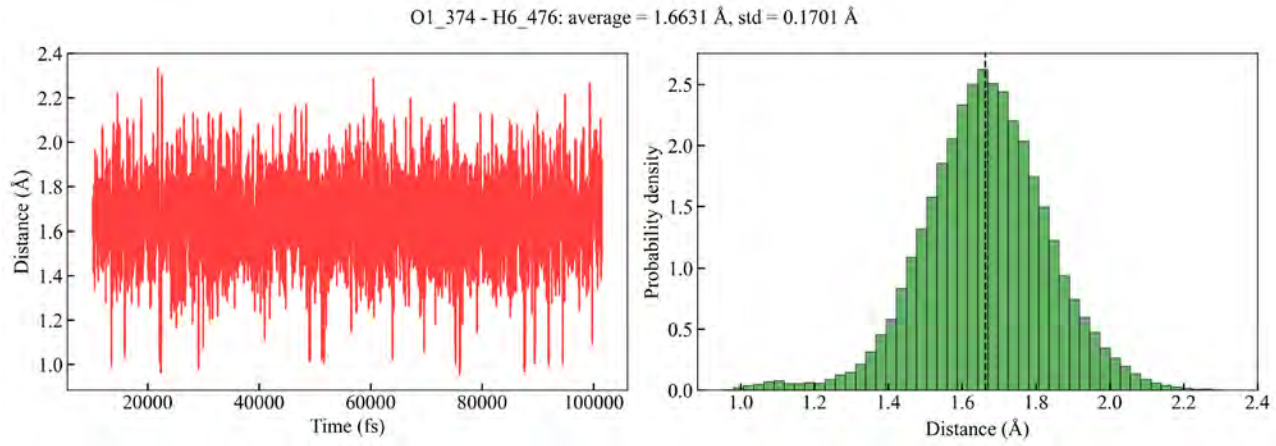
O1_373 - H6_475

Average distance = 1.6670 Å; standard deviation = 0.1713 Å; number of points = 91387



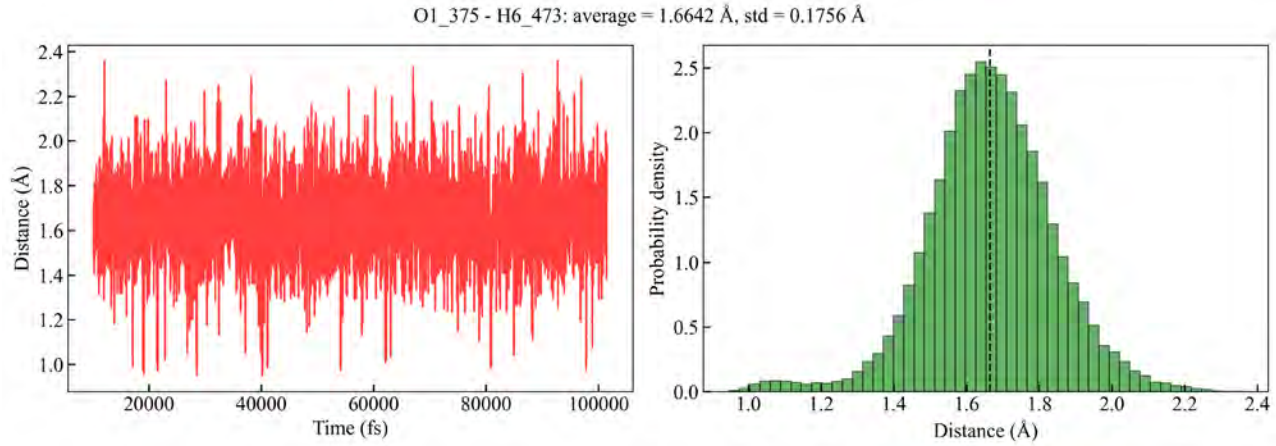
O1_374 - H6_476

Average distance = 1.6631 Å; standard deviation = 0.1701 Å; number of points = 91387



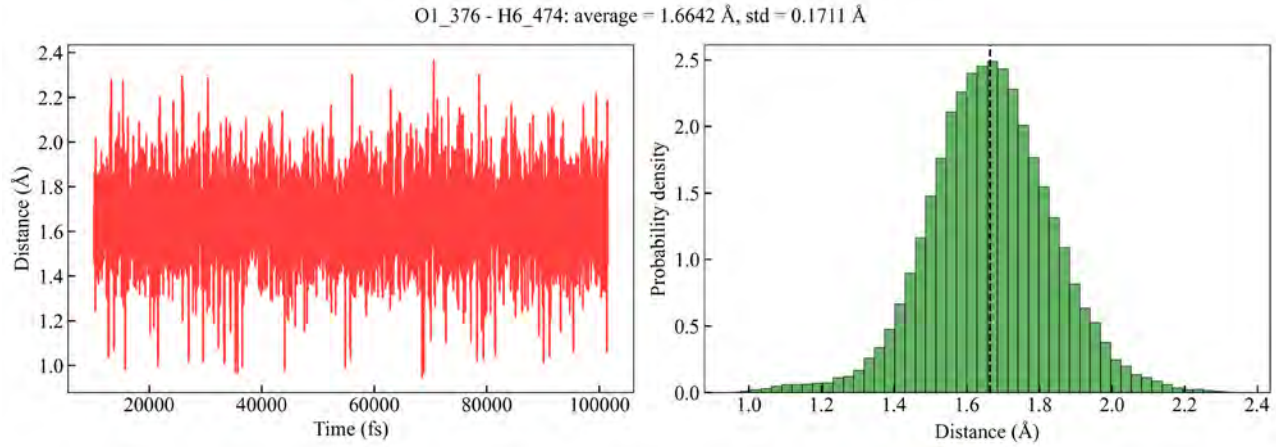
O1_375 - H6_473

Average distance = 1.6642 Å; standard deviation = 0.1756 Å; number of points = 91387



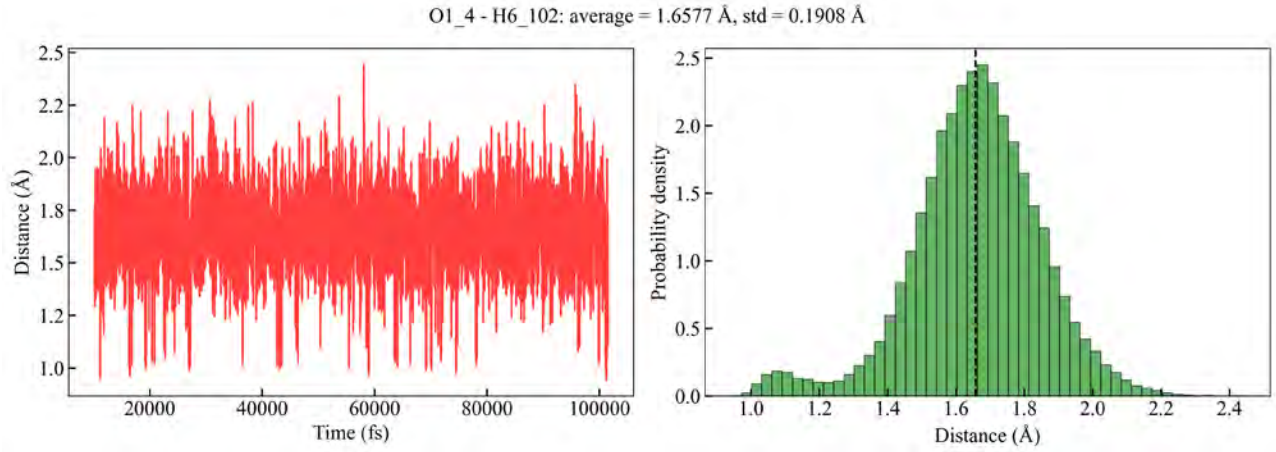
O1_376 - H6_474

Average distance = 1.6642 Å; standard deviation = 0.1711 Å; number of points = 91387



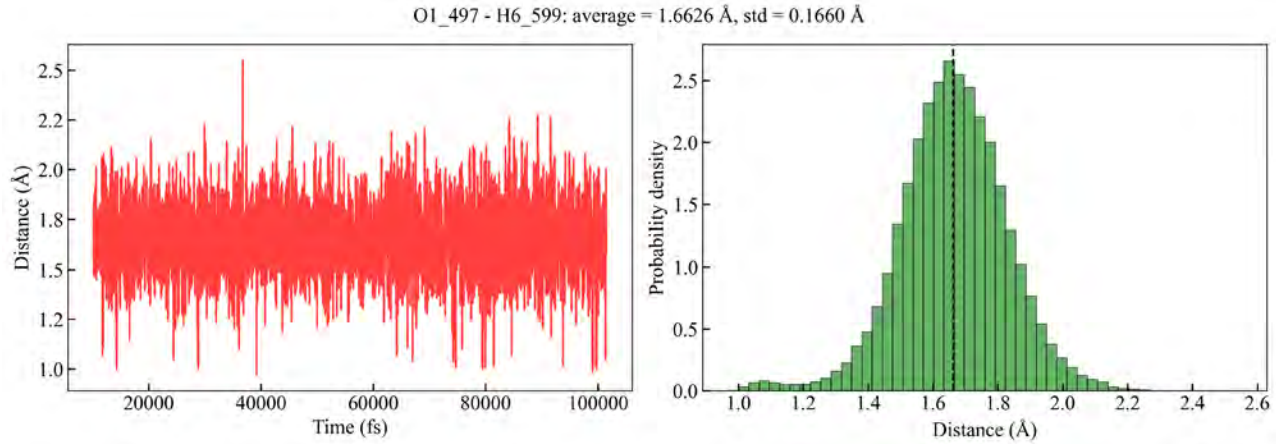
O1_4 - H6_102

Average distance = 1.6577 Å; standard deviation = 0.1908 Å; number of points = 91387



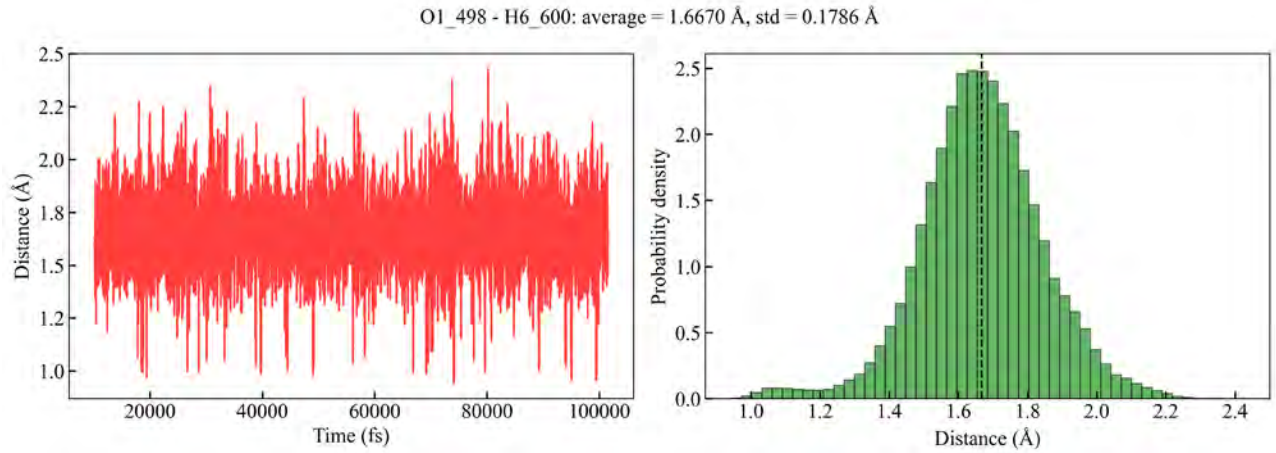
O1_497 - H6_599

Average distance = 1.6626 Å; standard deviation = 0.1660 Å; number of points = 91387



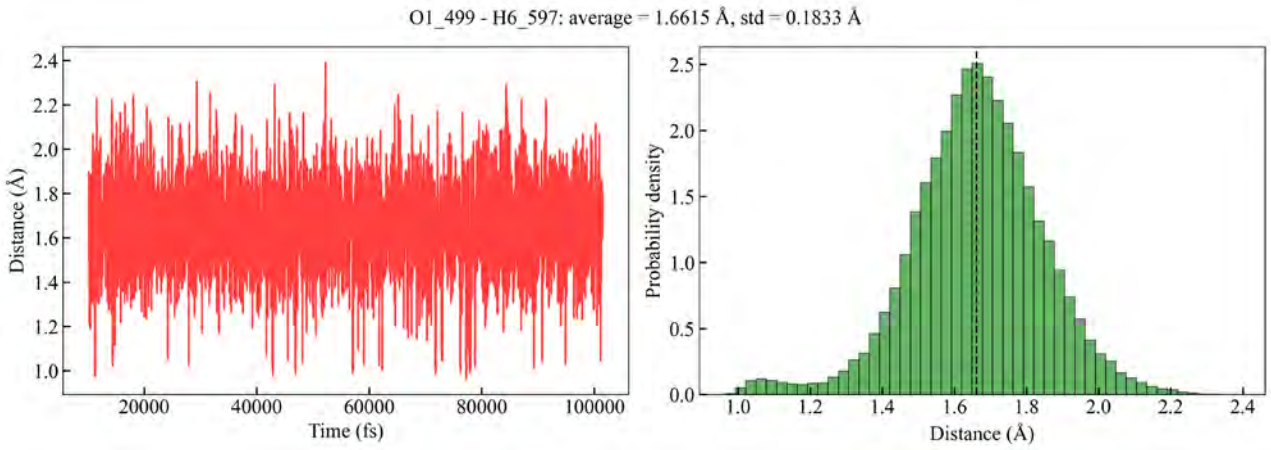
O1_498 - H6_600

Average distance = 1.6670 Å; standard deviation = 0.1786 Å; number of points = 91387



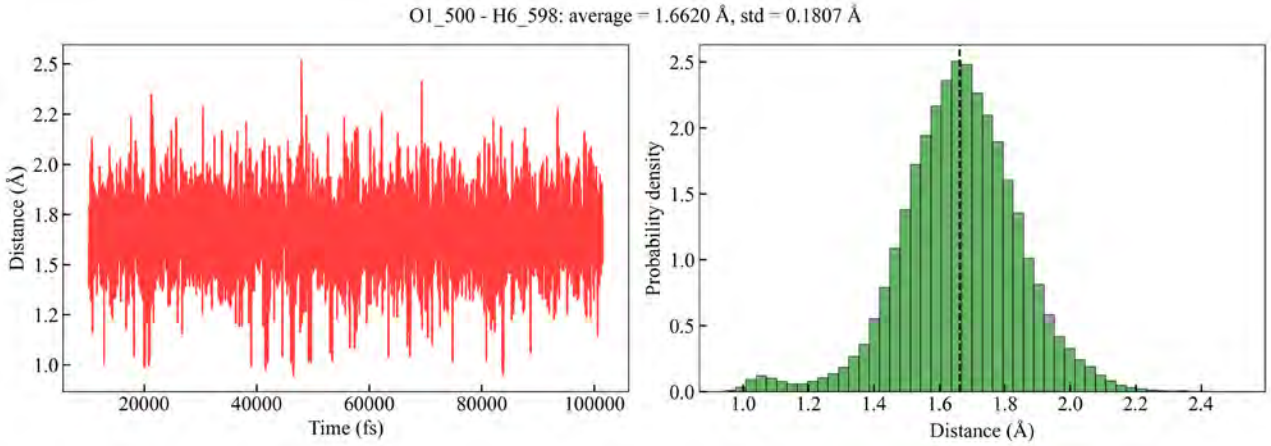
O1_499 - H6_597

Average distance = 1.6615 Å; standard deviation = 0.1833 Å; number of points = 91387



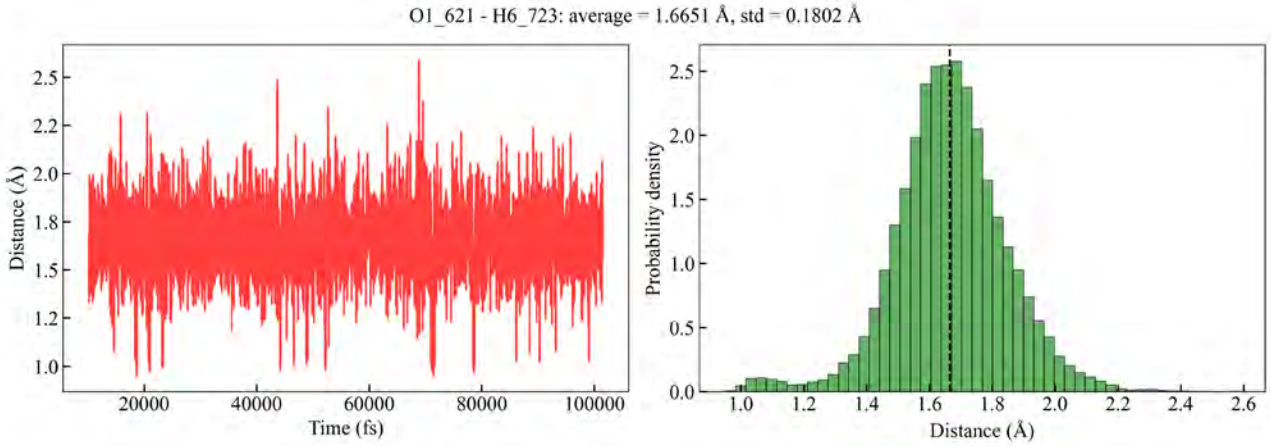
O1_500 - H6_598

Average distance = 1.6620 Å; standard deviation = 0.1807 Å; number of points = 91387



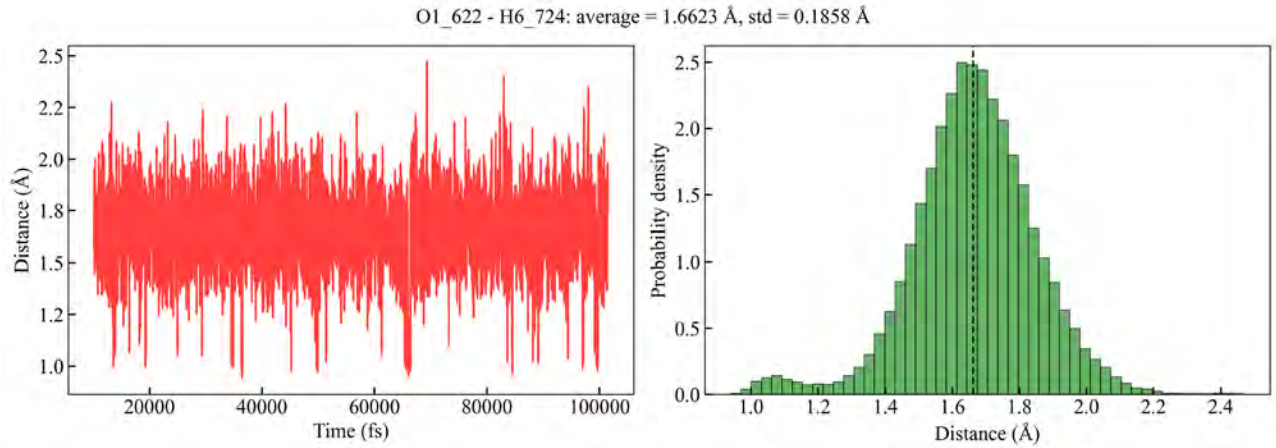
O1_621 - H6_723

Average distance = 1.6651 Å; standard deviation = 0.1802 Å; number of points = 91387



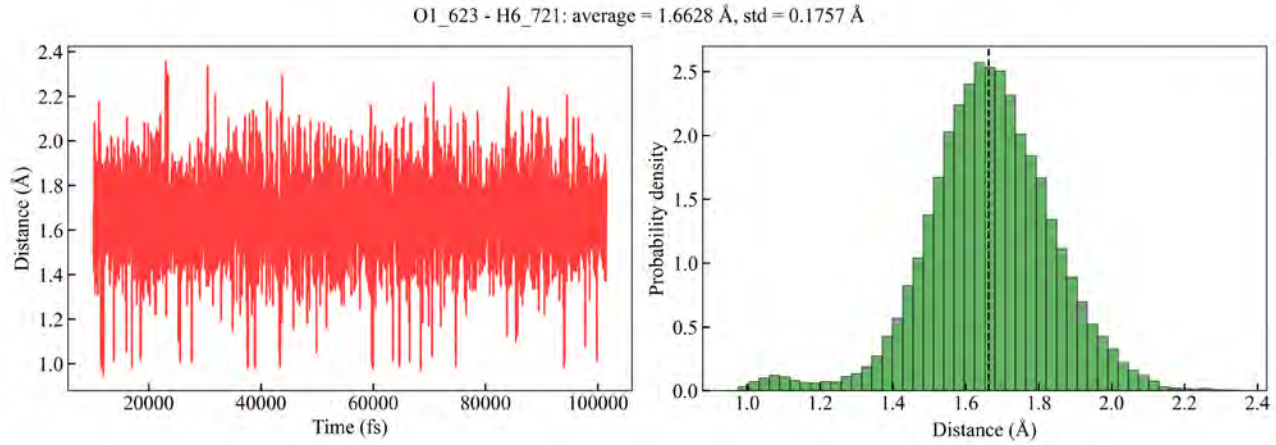
O1_622 - H6_724

Average distance = 1.6623 Å; standard deviation = 0.1858 Å; number of points = 91387



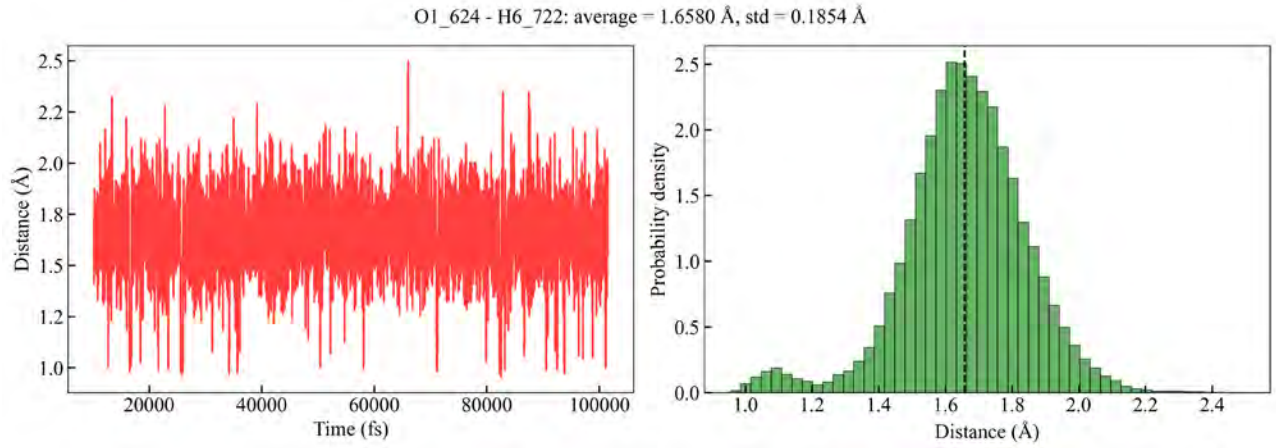
O1_623 - H6_721

Average distance = 1.6628 Å; standard deviation = 0.1757 Å; number of points = 91387



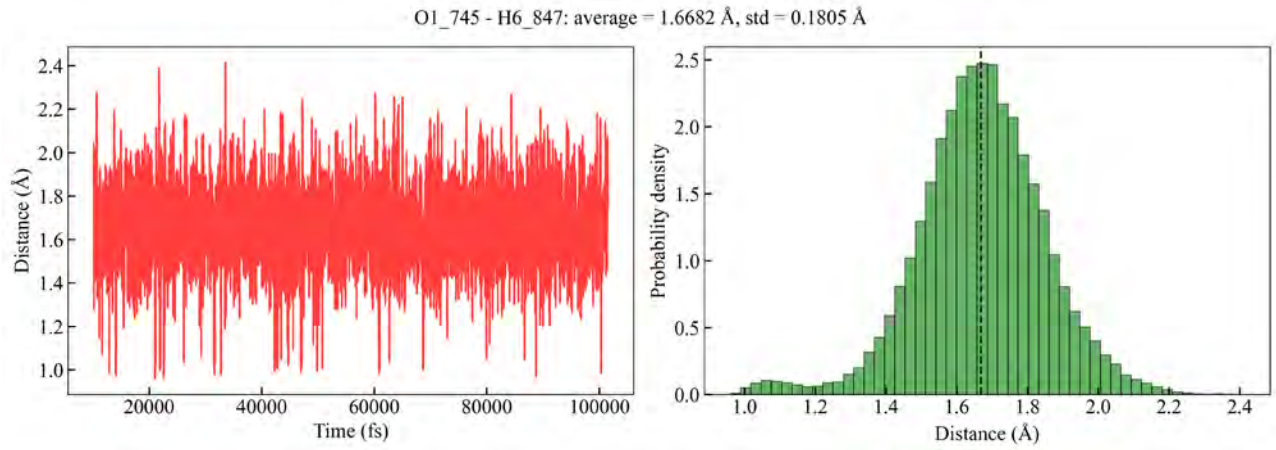
O1_624 - H6_722

Average distance = 1.6580 Å; standard deviation = 0.1854 Å; number of points = 91387



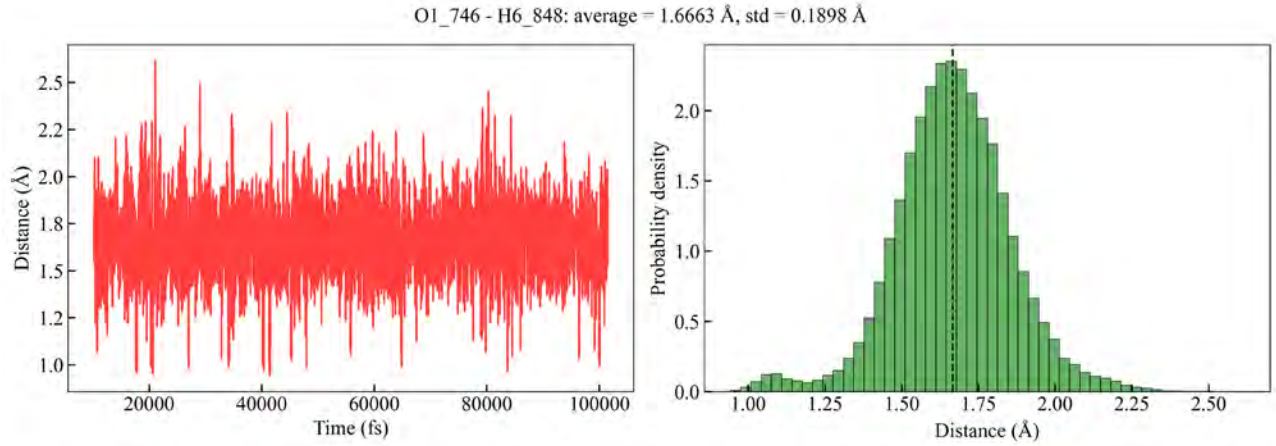
O1_745 - H6_847

Average distance = 1.6682 Å; standard deviation = 0.1805 Å; number of points = 91387



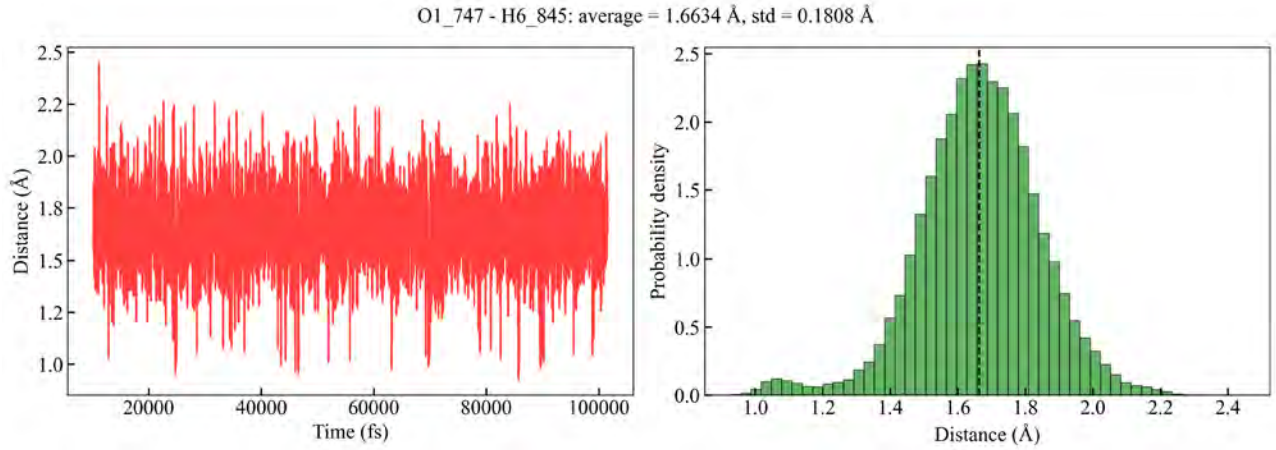
O1_746 - H6_848

Average distance = 1.6663 Å; standard deviation = 0.1898 Å; number of points = 91387



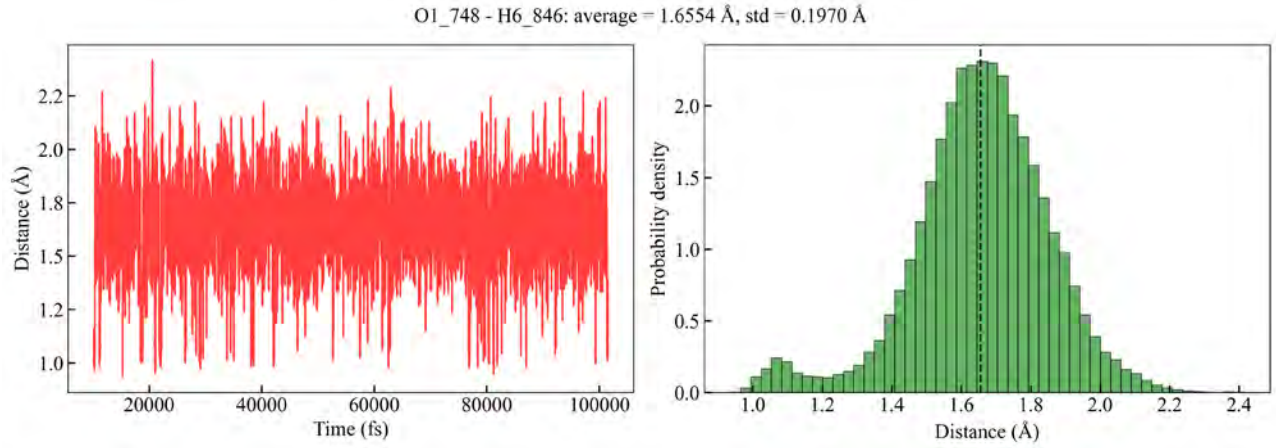
O1_747 - H6_845

Average distance = 1.6634 Å; standard deviation = 0.1808 Å; number of points = 91387



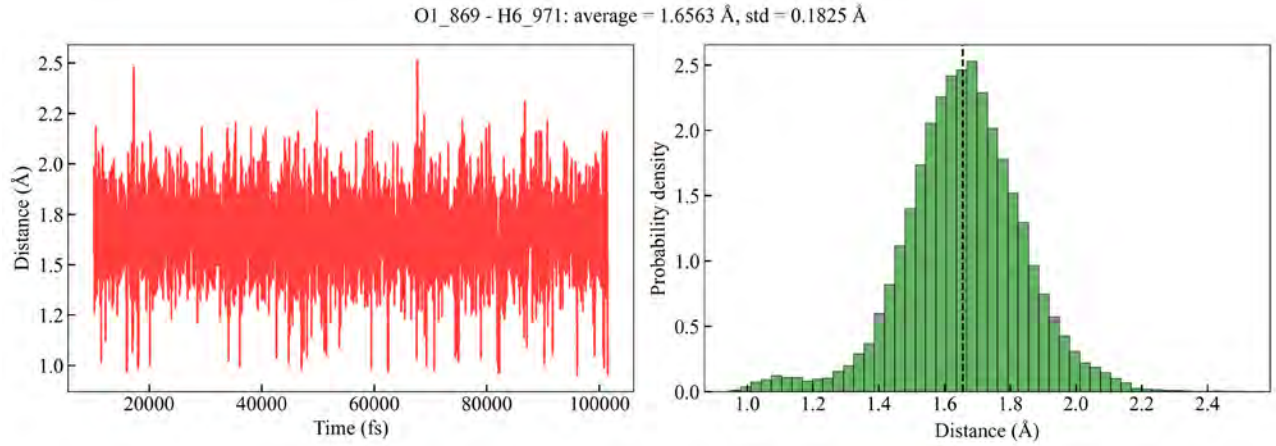
O1_748 - H6_846

Average distance = 1.6554 Å; standard deviation = 0.1970 Å; number of points = 91387



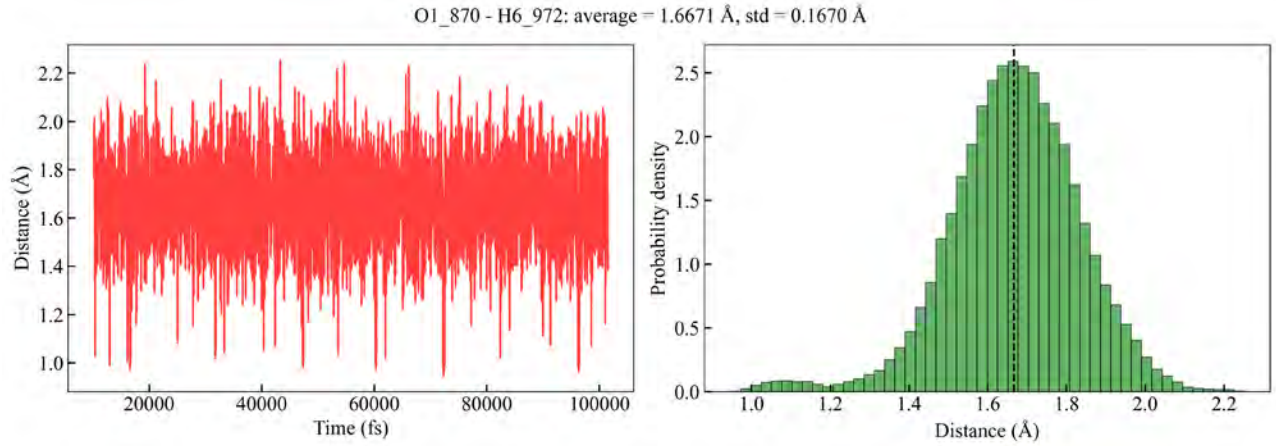
O1_869 - H6_971

Average distance = 1.6563 Å; standard deviation = 0.1825 Å; number of points = 91387



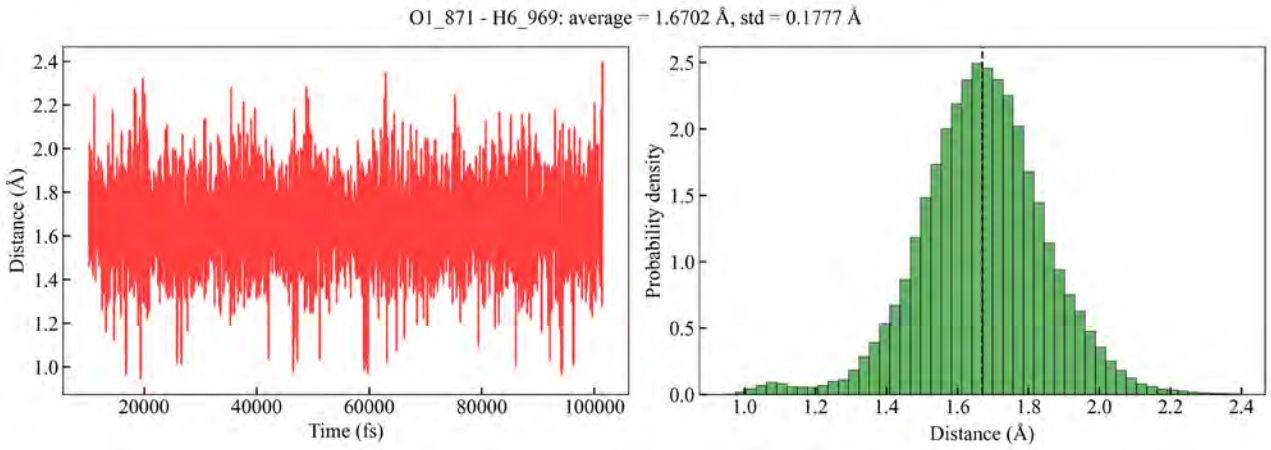
O1_870 - H6_972

Average distance = 1.6671 Å; standard deviation = 0.1670 Å; number of points = 91387



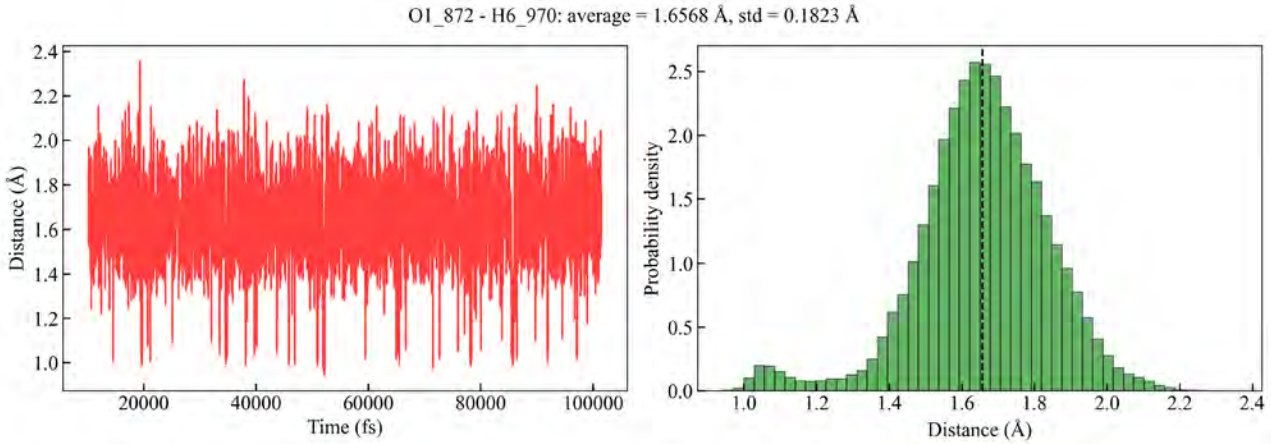
O1_871 - H6_969

Average distance = 1.6702 Å; standard deviation = 0.1777 Å; number of points = 91387



O1_872 - H6_970

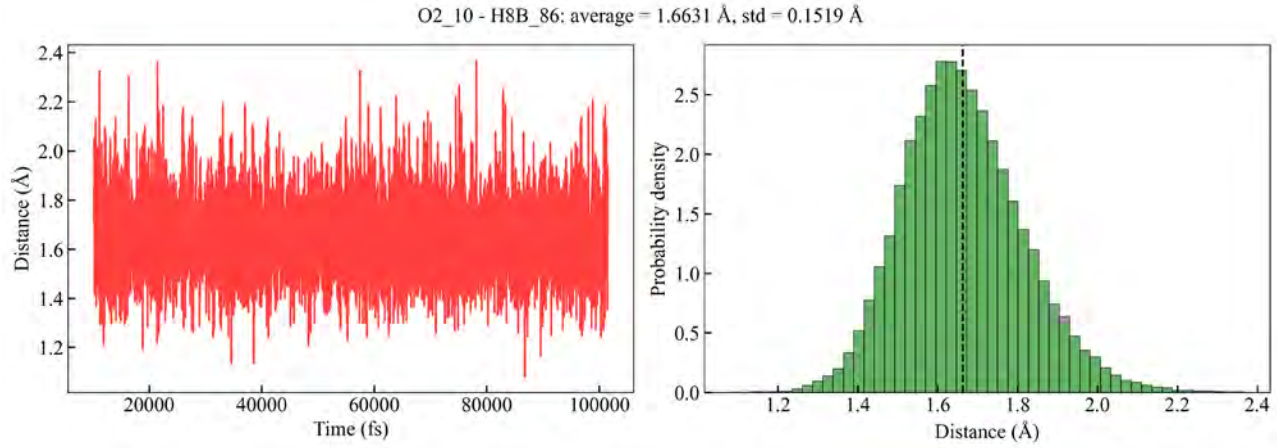
Average distance = 1.6568 Å; standard deviation = 0.1823 Å; number of points = 91387



O2 - H8B

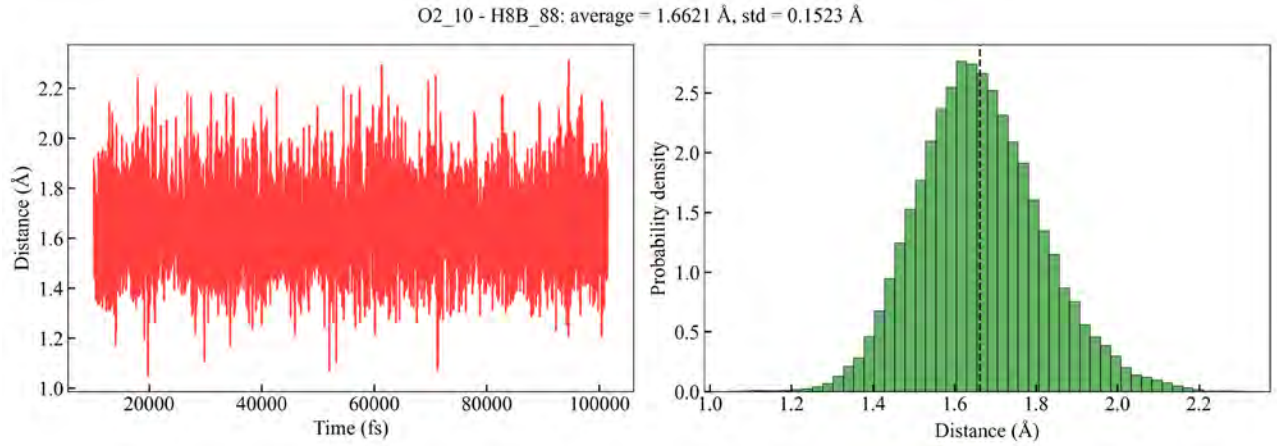
O2_10 - H8B_86

Average distance = 1.6631 Å; standard deviation = 0.1519 Å; number of points = 91387



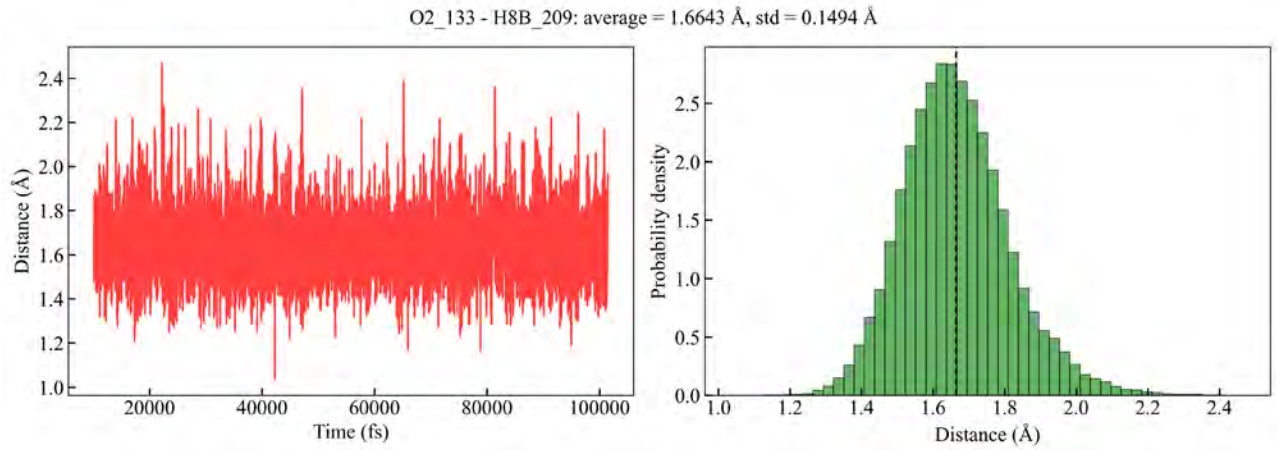
O2_10 - H8B_88

Average distance = 1.6621 Å; standard deviation = 0.1523 Å; number of points = 91387



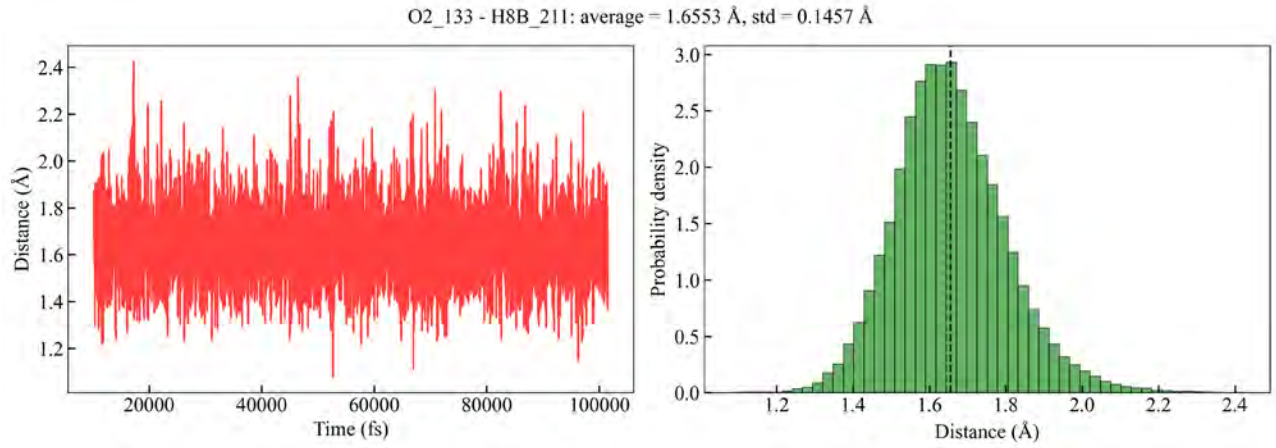
O2_133 - H8B_209

Average distance = 1.6643 Å; standard deviation = 0.1494 Å; number of points = 91387



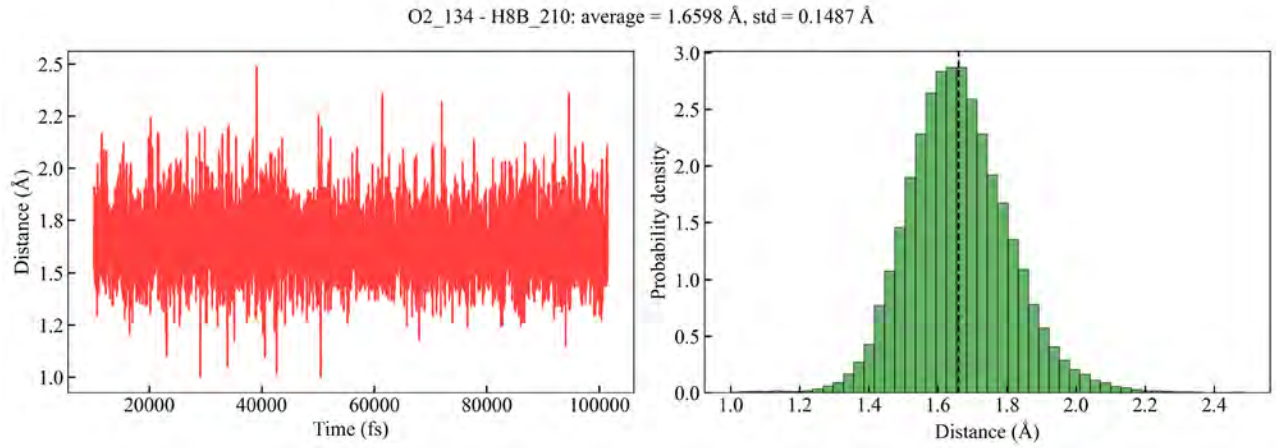
O2_133 - H8B_211

Average distance = 1.6553 Å; standard deviation = 0.1457 Å; number of points = 91387



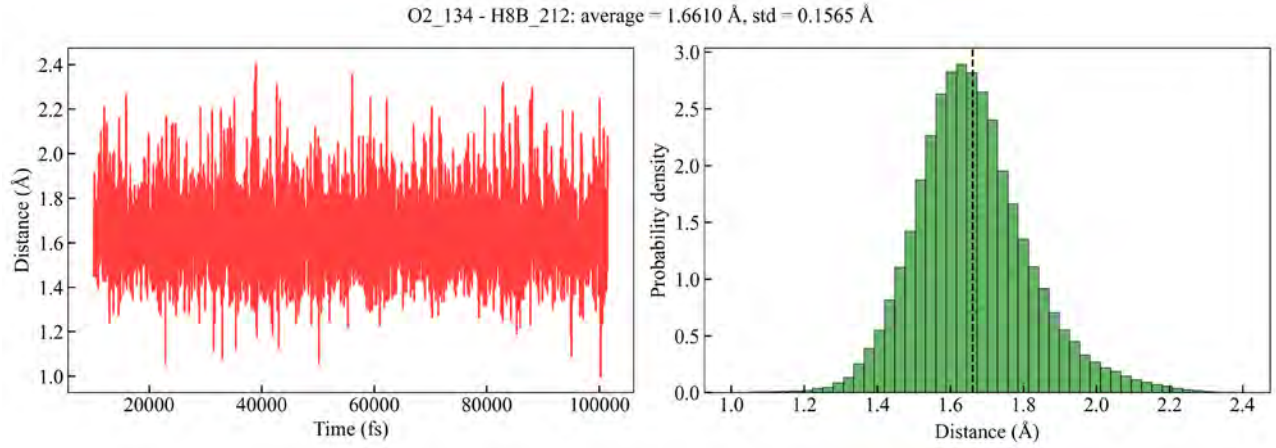
O2_134 - H8B_210

Average distance = 1.6598 Å; standard deviation = 0.1487 Å; number of points = 91387



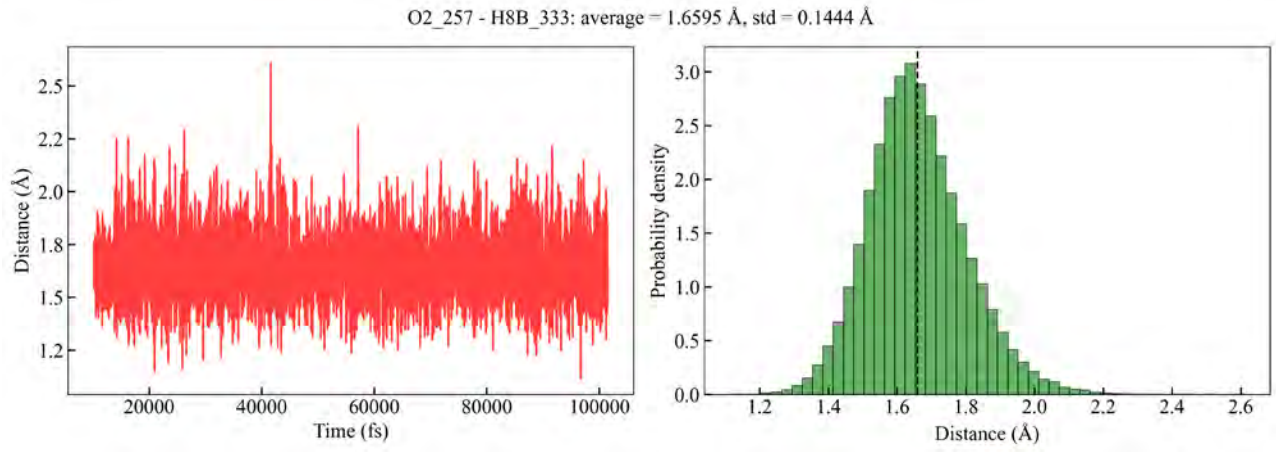
O2_134 - H8B_212

Average distance = 1.6610 Å; standard deviation = 0.1565 Å; number of points = 91387



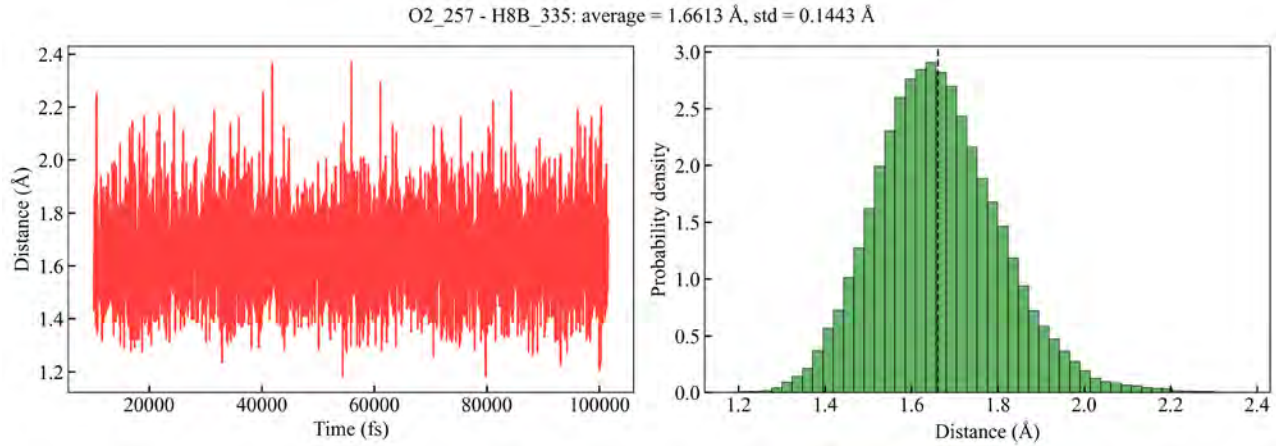
O2_257 - H8B_333

Average distance = 1.6595 Å; standard deviation = 0.1444 Å; number of points = 91387



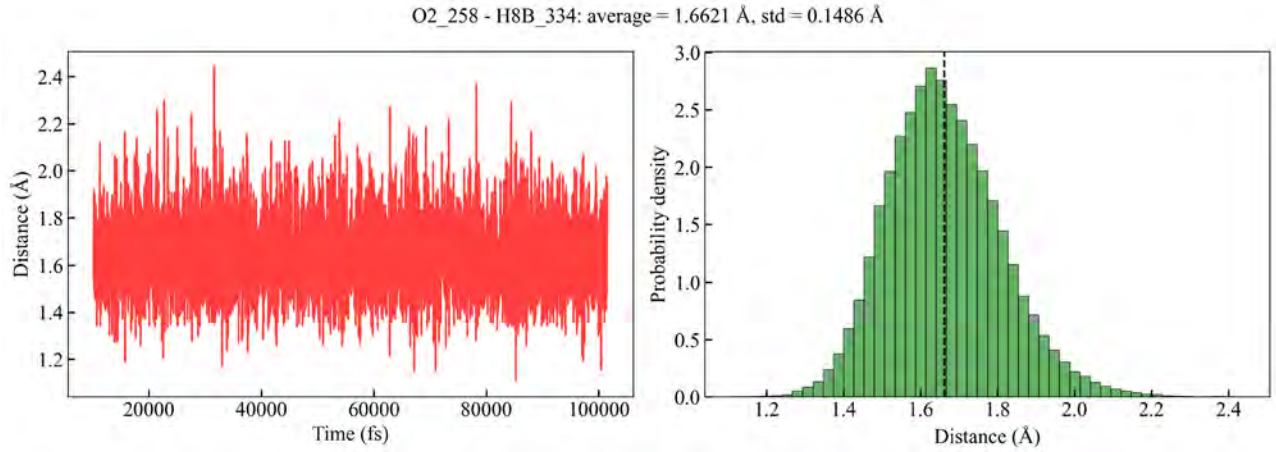
O2_257 - H8B_335

Average distance = 1.6613 Å; standard deviation = 0.1443 Å; number of points = 91387



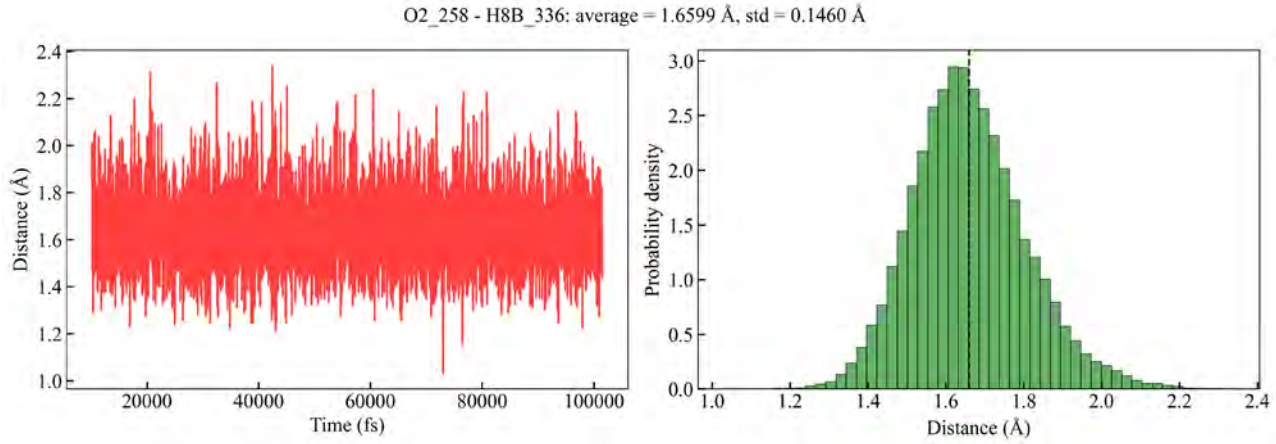
O2_258 - H8B_334

Average distance = 1.6621 Å; standard deviation = 0.1486 Å; number of points = 91387



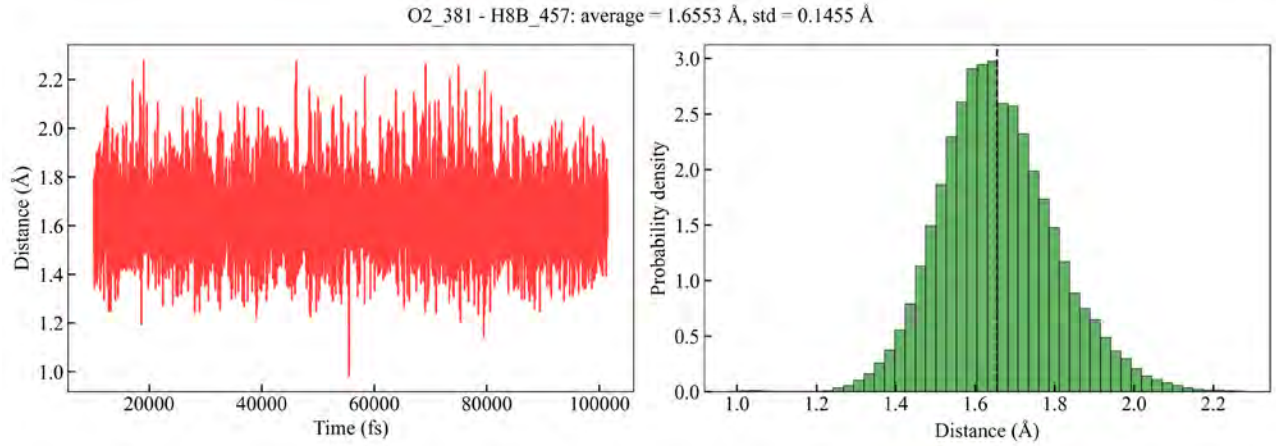
O2_258 - H8B_336

Average distance = 1.6599 Å; standard deviation = 0.1460 Å; number of points = 91387



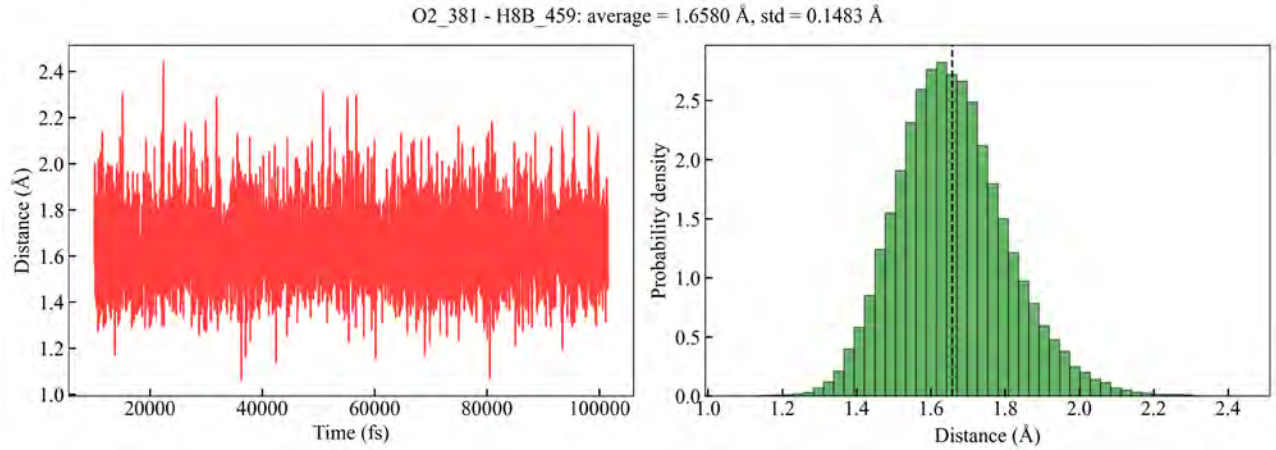
O2_381 - H8B_457

Average distance = 1.6553 Å; standard deviation = 0.1455 Å; number of points = 91387



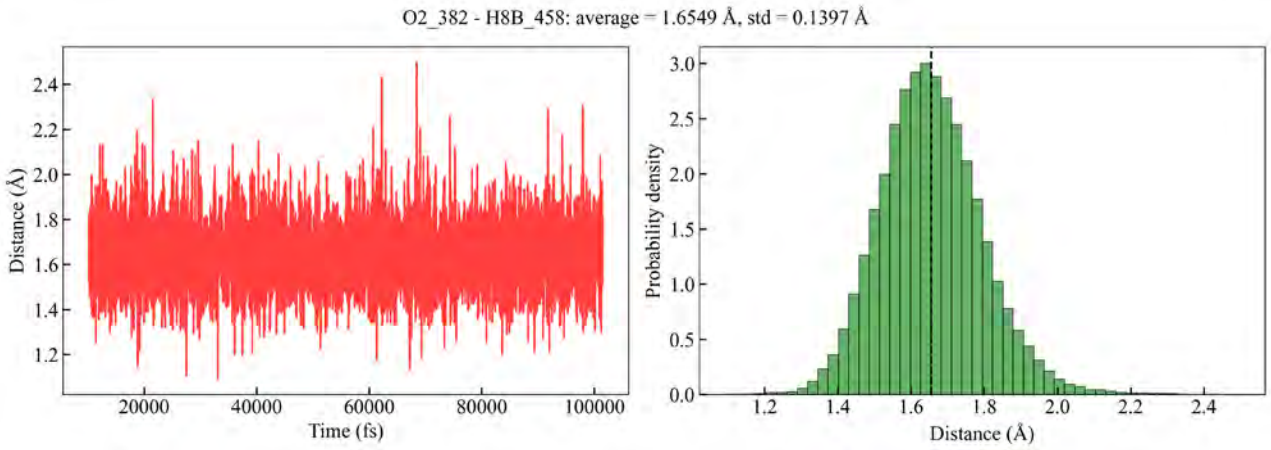
O2_381 - H8B_459

Average distance = 1.6580 Å; standard deviation = 0.1483 Å; number of points = 91387



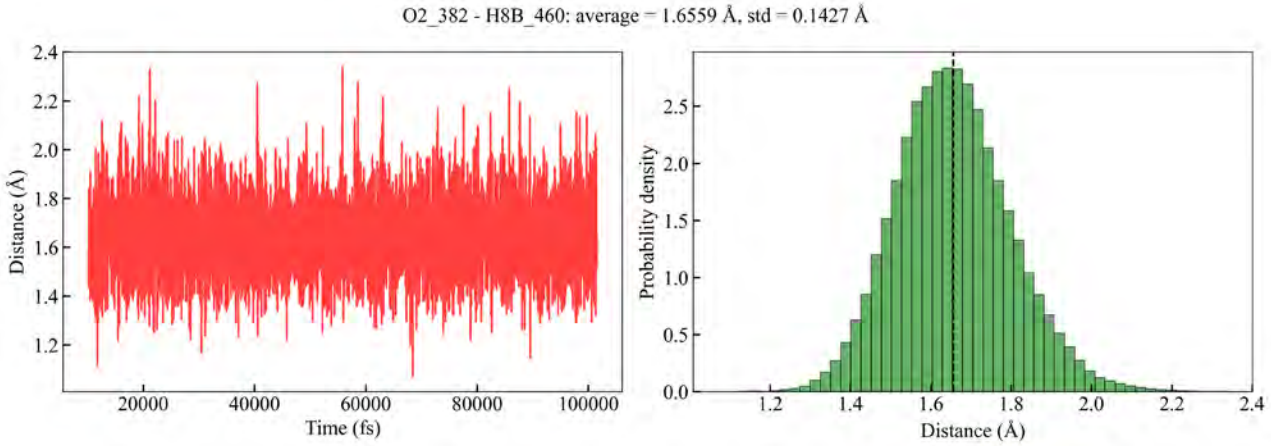
O2_382 - H8B_458

Average distance = 1.6549 Å; standard deviation = 0.1397 Å; number of points = 91387



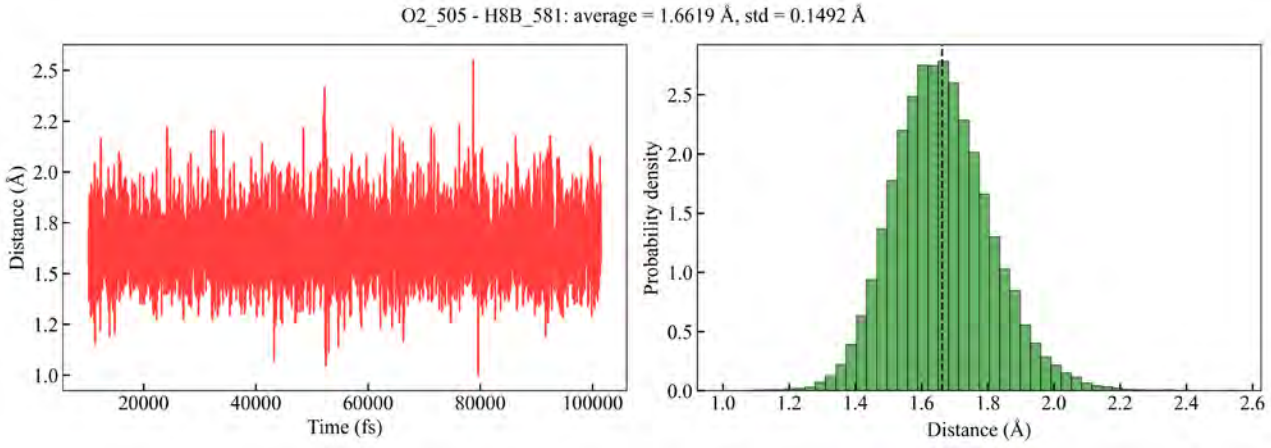
O2_382 - H8B_460

Average distance = 1.6559 Å; standard deviation = 0.1427 Å; number of points = 91387



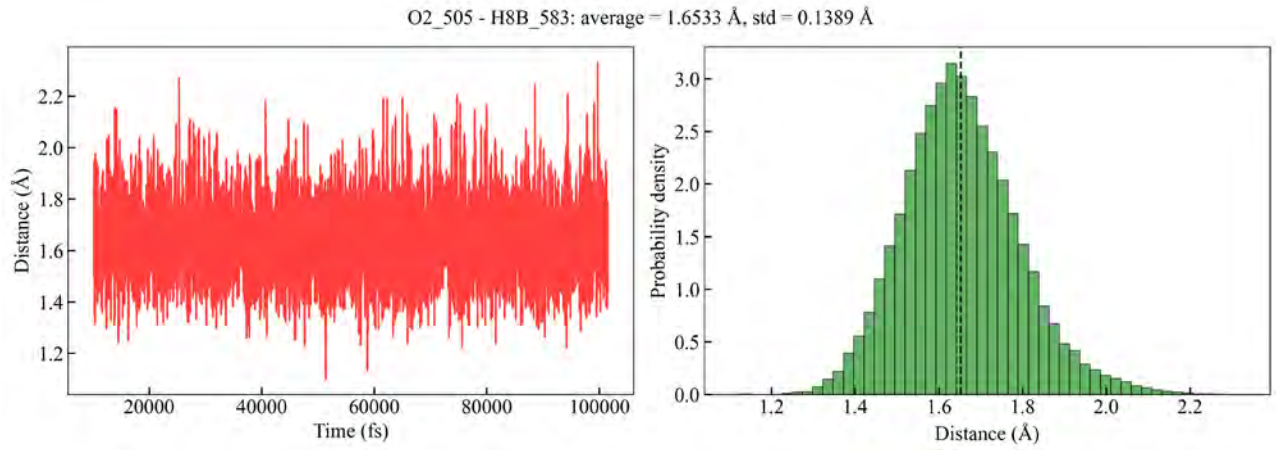
O2_505 - H8B_581

Average distance = 1.6619 Å; standard deviation = 0.1492 Å; number of points = 91387



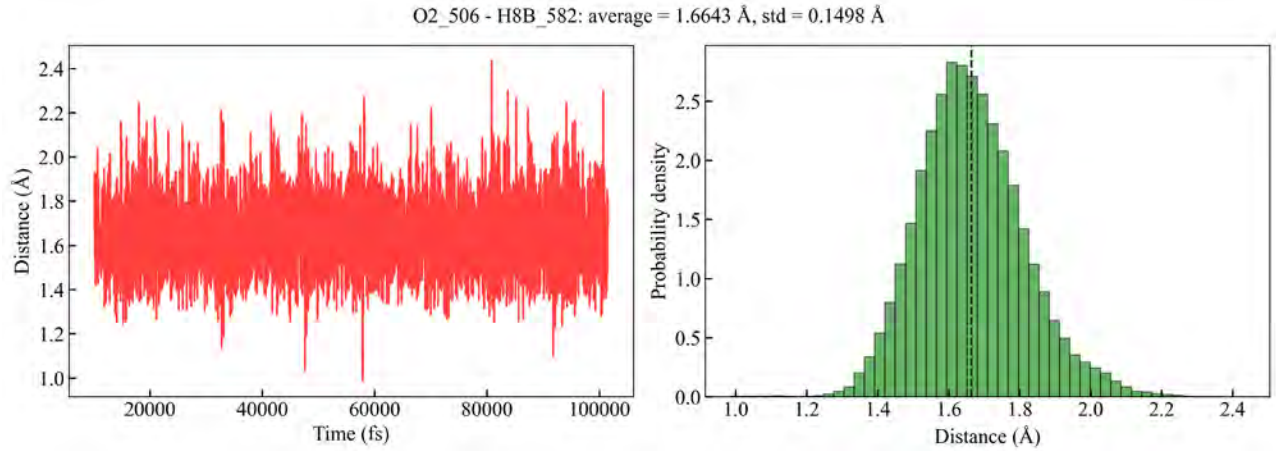
O2_505 - H8B_583

Average distance = 1.6533 Å; standard deviation = 0.1389 Å; number of points = 91387



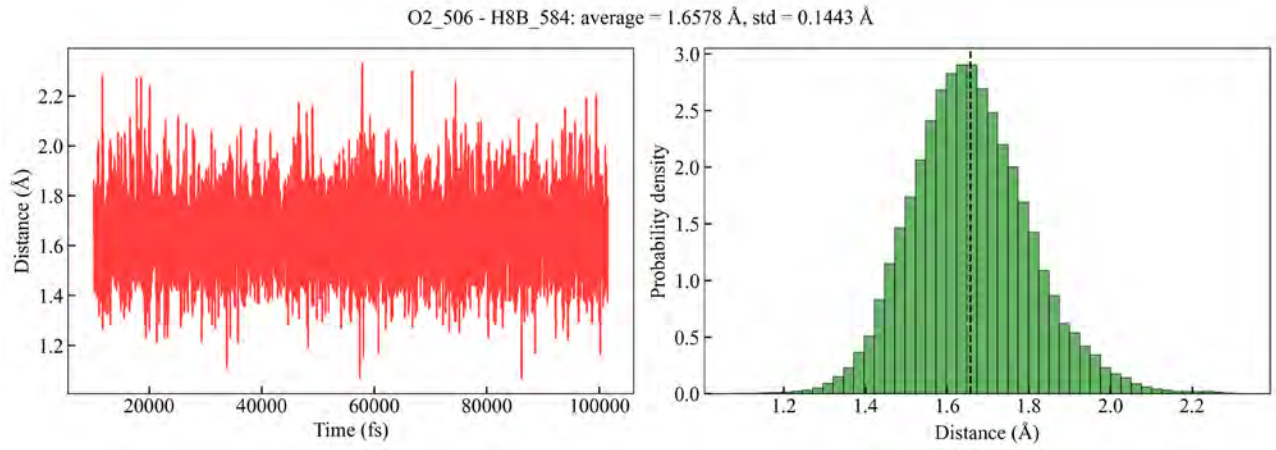
O2_506 - H8B_582

Average distance = 1.6643 Å; standard deviation = 0.1498 Å; number of points = 91387



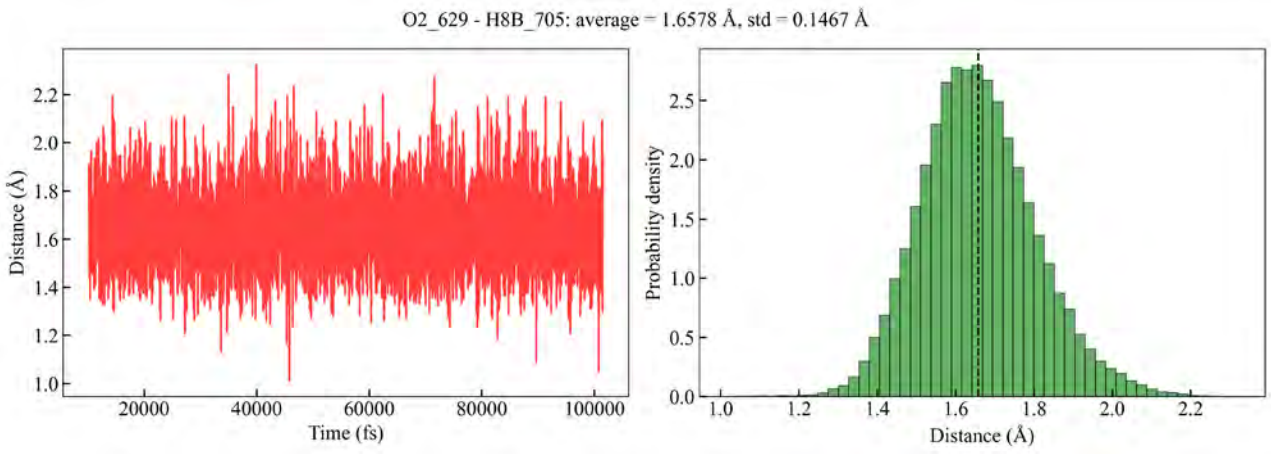
O2_506 - H8B_584

Average distance = 1.6578 Å; standard deviation = 0.1443 Å; number of points = 91387



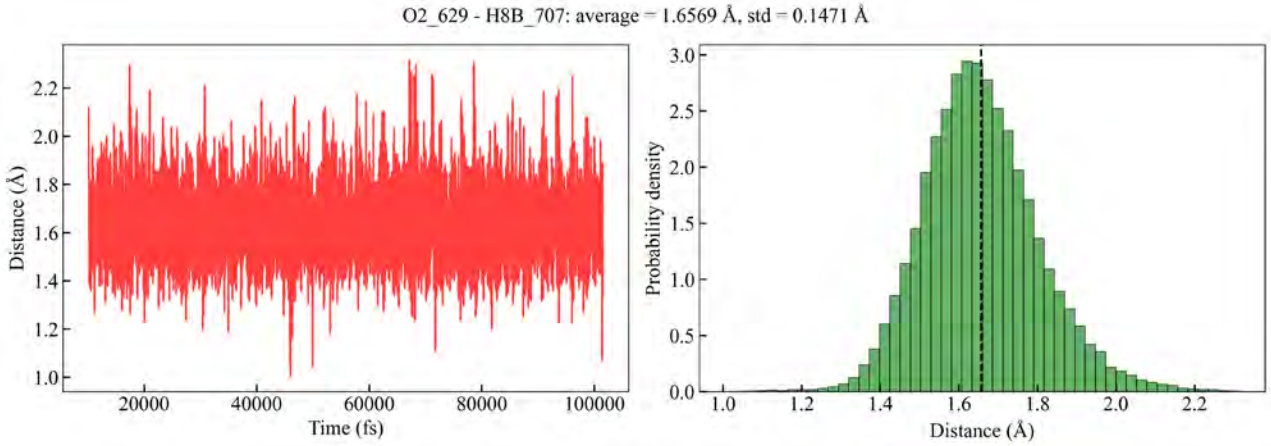
O2_629 - H8B_705

Average distance = 1.6578 Å; standard deviation = 0.1467 Å; number of points = 91387



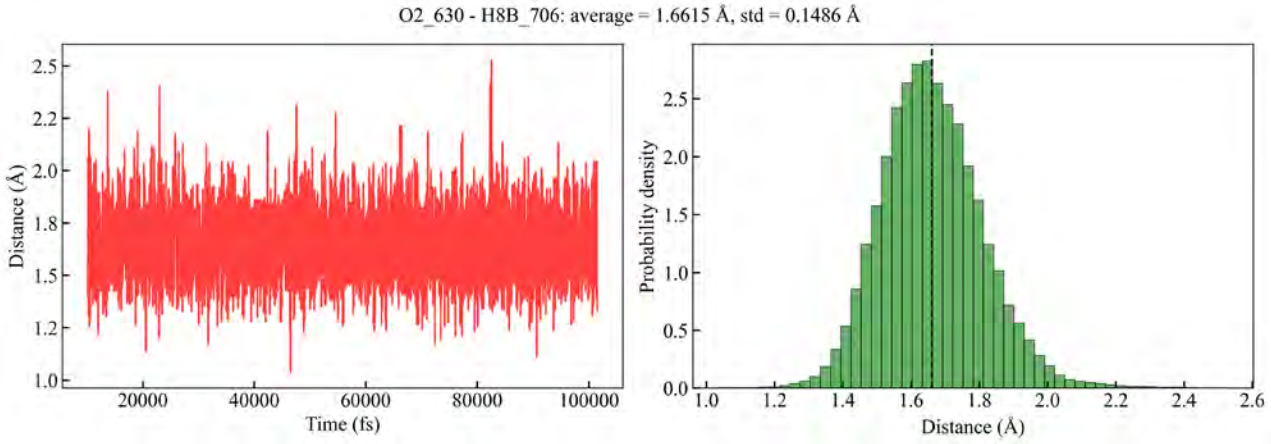
O2_629 - H8B_707

Average distance = 1.6569 Å; standard deviation = 0.1471 Å; number of points = 91387



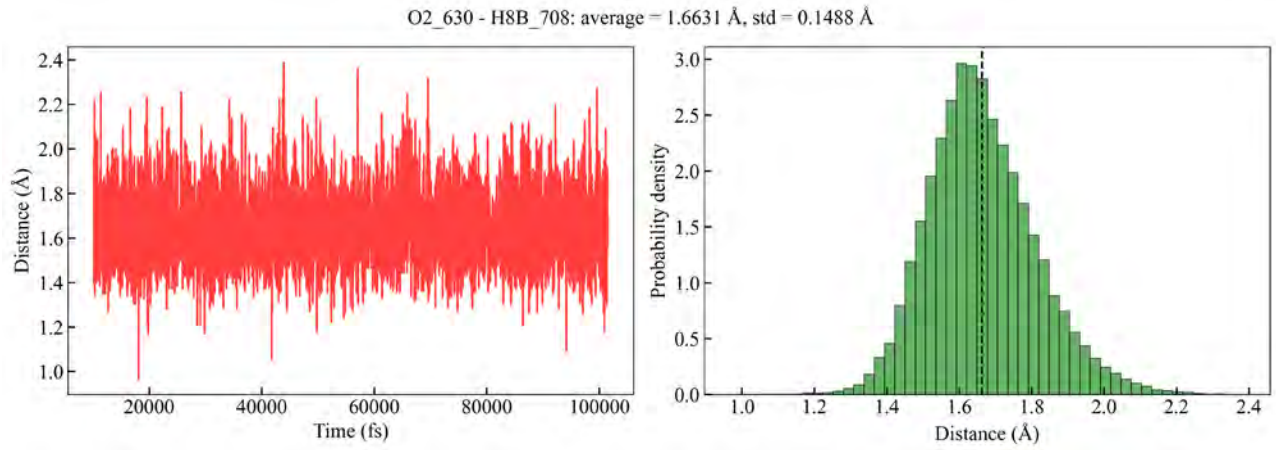
O2_630 - H8B_706

Average distance = 1.6615 Å; standard deviation = 0.1486 Å; number of points = 91387



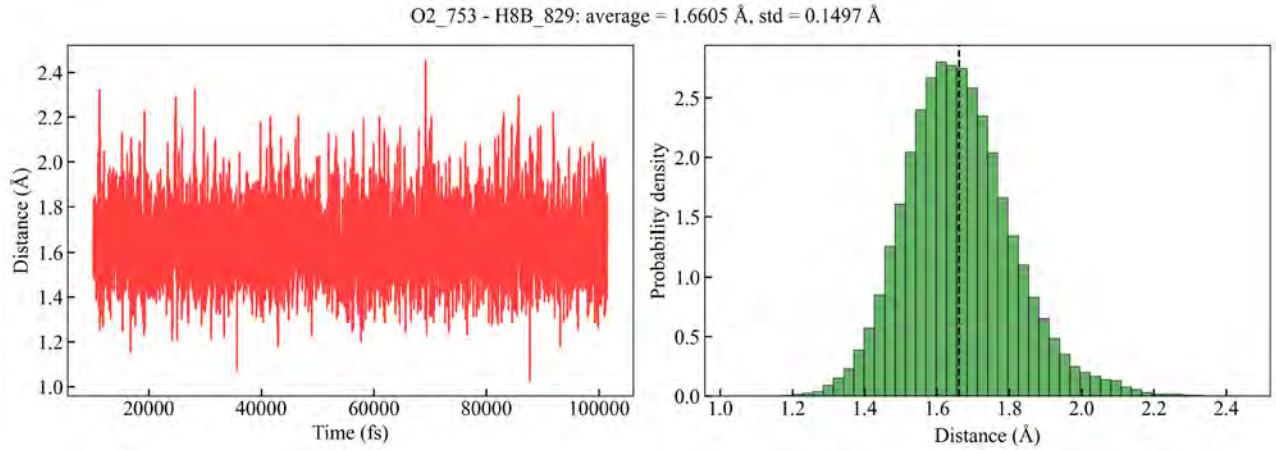
O2_630 - H8B_708

Average distance = 1.6631 Å; standard deviation = 0.1488 Å; number of points = 91387



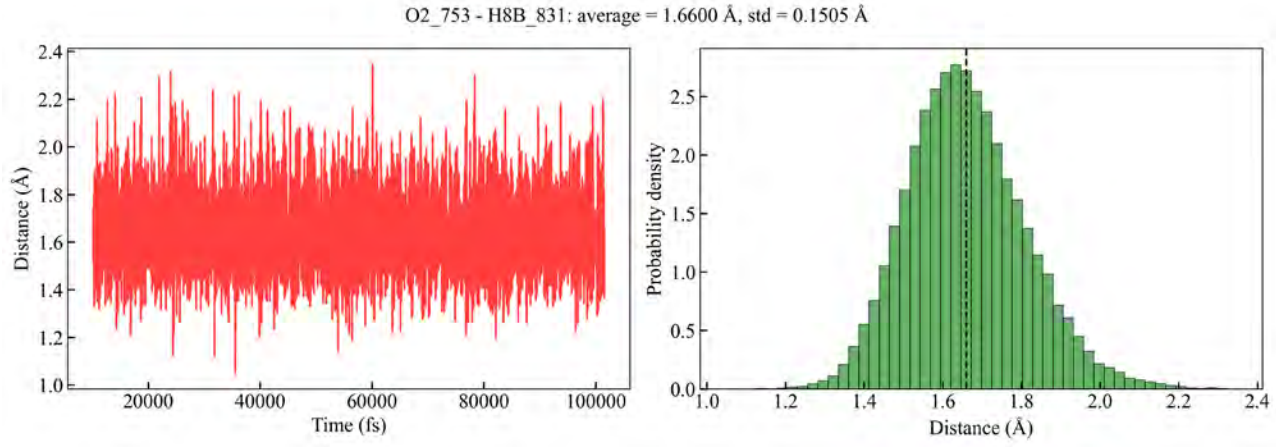
O2_753 - H8B_829

Average distance = 1.6605 Å; standard deviation = 0.1497 Å; number of points = 91387



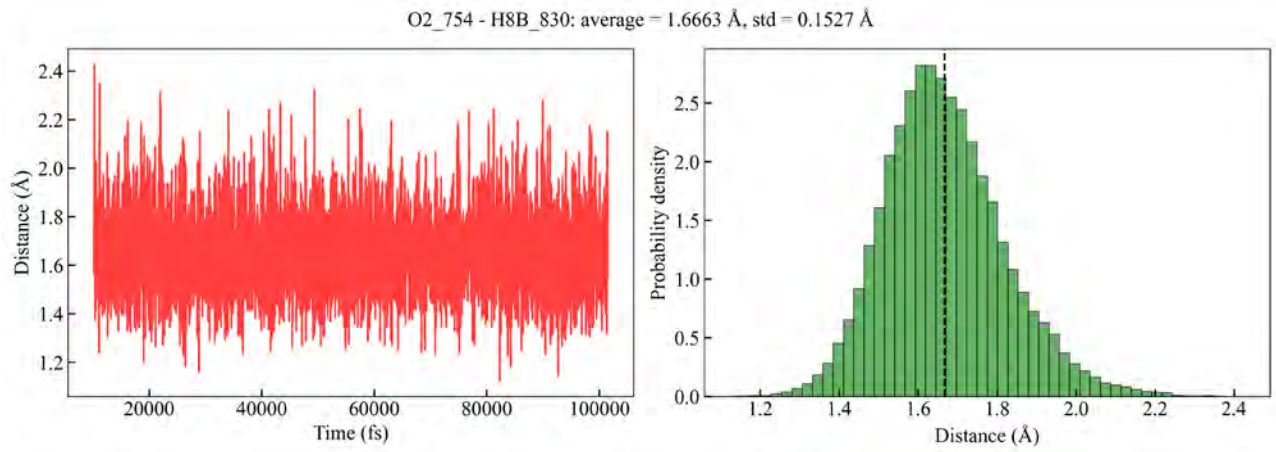
O2_753 - H8B_831

Average distance = 1.6600 Å; standard deviation = 0.1505 Å; number of points = 91387



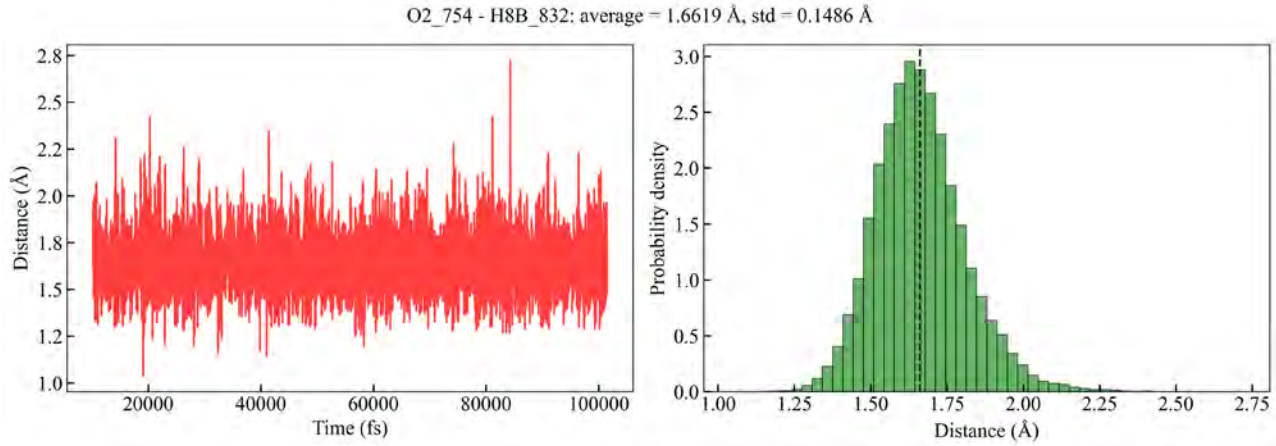
O2_754 - H8B_830

Average distance = 1.6663 Å; standard deviation = 0.1527 Å; number of points = 91387



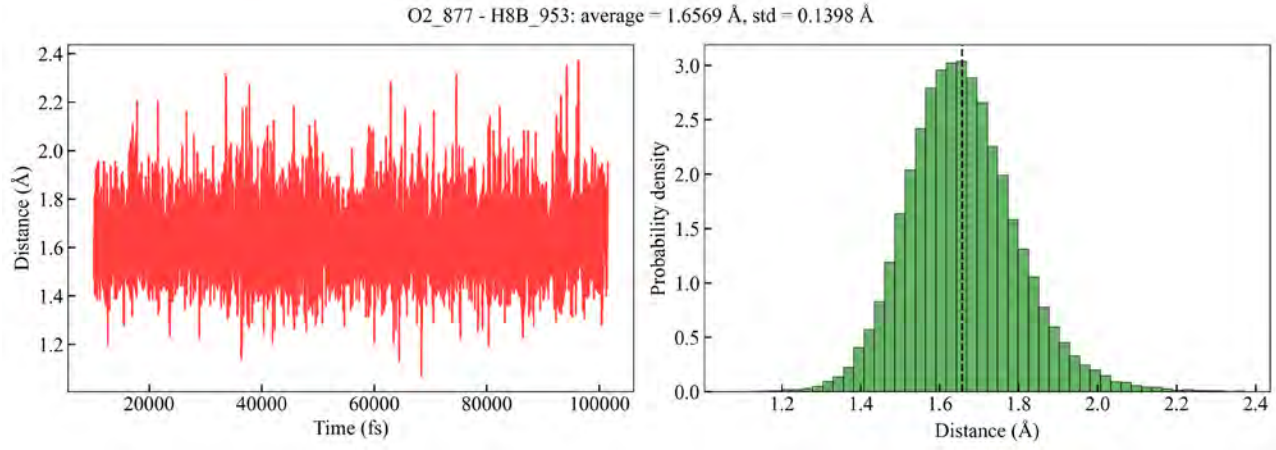
O2_754 - H8B_832

Average distance = 1.6619 Å; standard deviation = 0.1486 Å; number of points = 91387



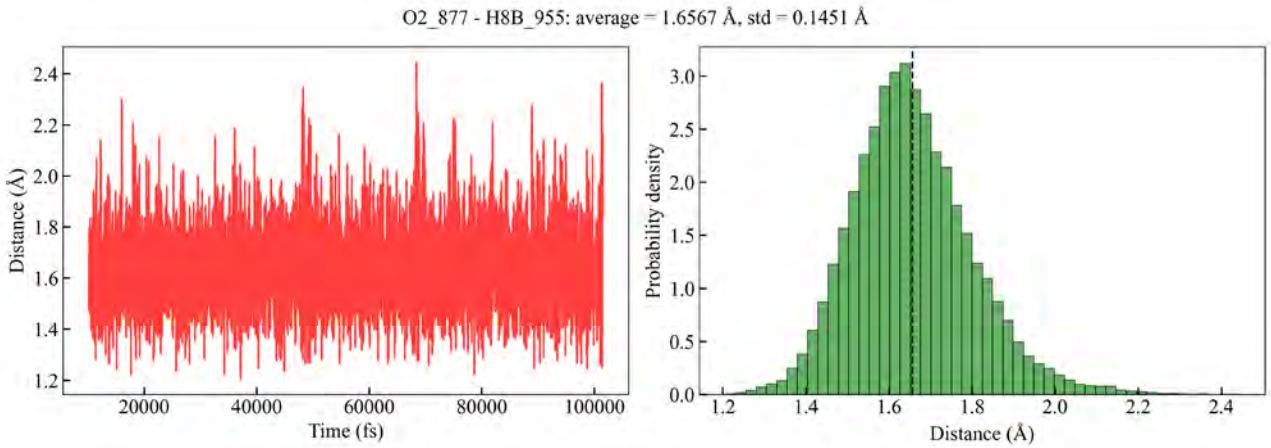
O2_877 - H8B_953

Average distance = 1.6569 Å; standard deviation = 0.1398 Å; number of points = 91387



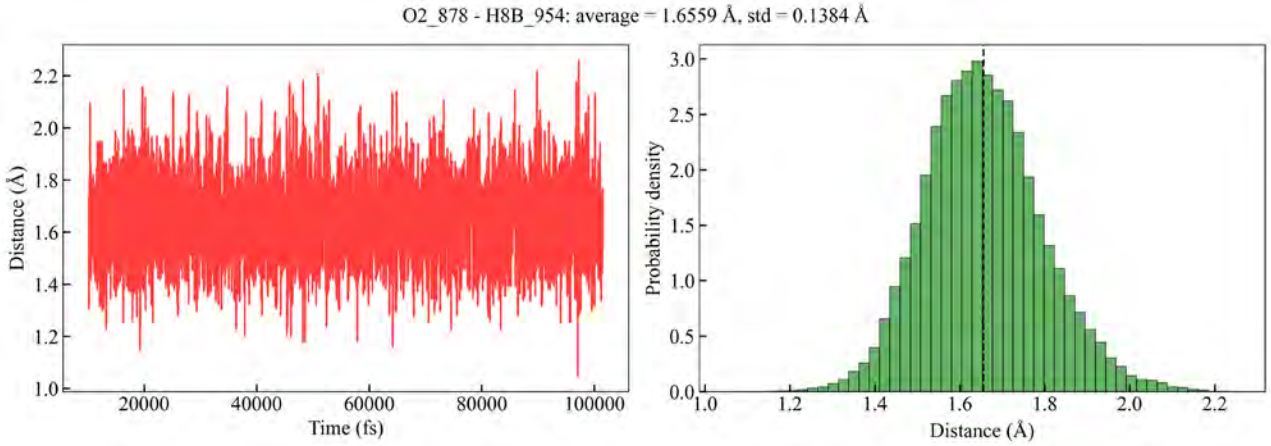
O2_877 - H8B_955

Average distance = 1.6567 Å; standard deviation = 0.1451 Å; number of points = 91387



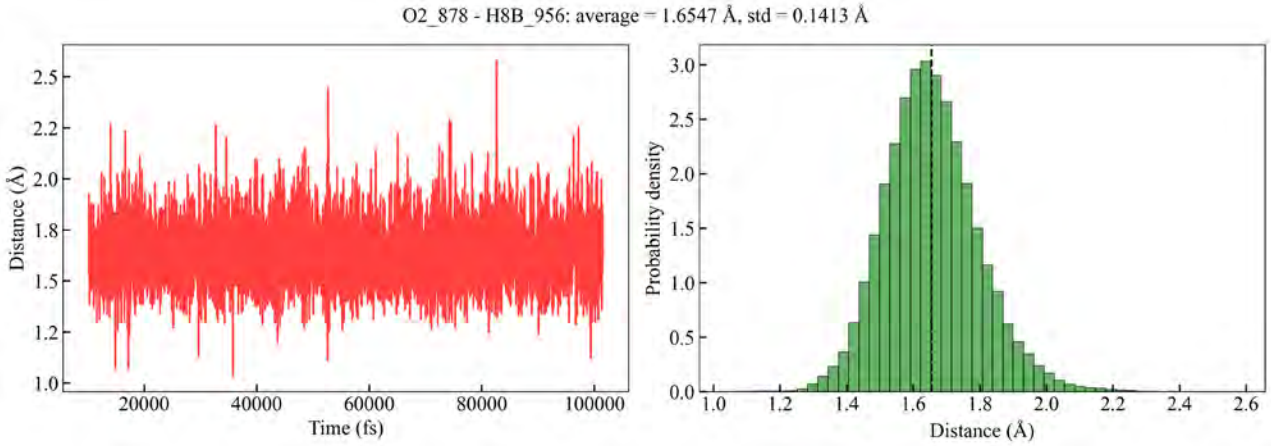
O2_878 - H8B_954

Average distance = 1.6559 Å; standard deviation = 0.1384 Å; number of points = 91387



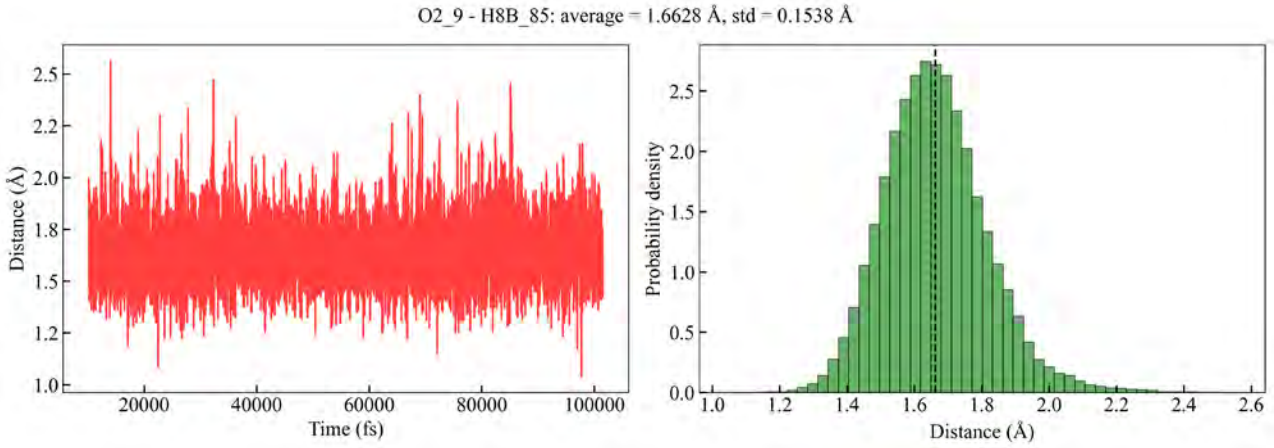
O2_878 - H8B_956

Average distance = 1.6547 Å; standard deviation = 0.1413 Å; number of points = 91387



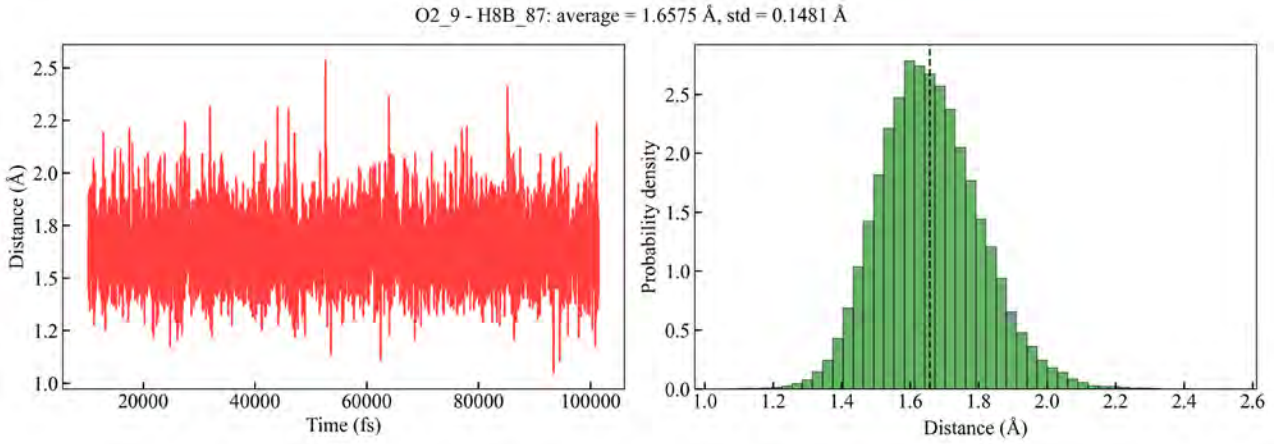
O2_9 - H8B_85

Average distance = 1.6628 Å; standard deviation = 0.1538 Å; number of points = 91387



O2_9 - H8B_87

Average distance = 1.6575 Å; standard deviation = 0.1481 Å; number of points = 91387



3.2.3. P1 at 453 K - Bond Distance Analysis at the surface

Table S20. Individual time-averaged hydrogen-involving atomic distances for all equivalent proton environments in the P1 surface AIMD trajectory at 453 K.

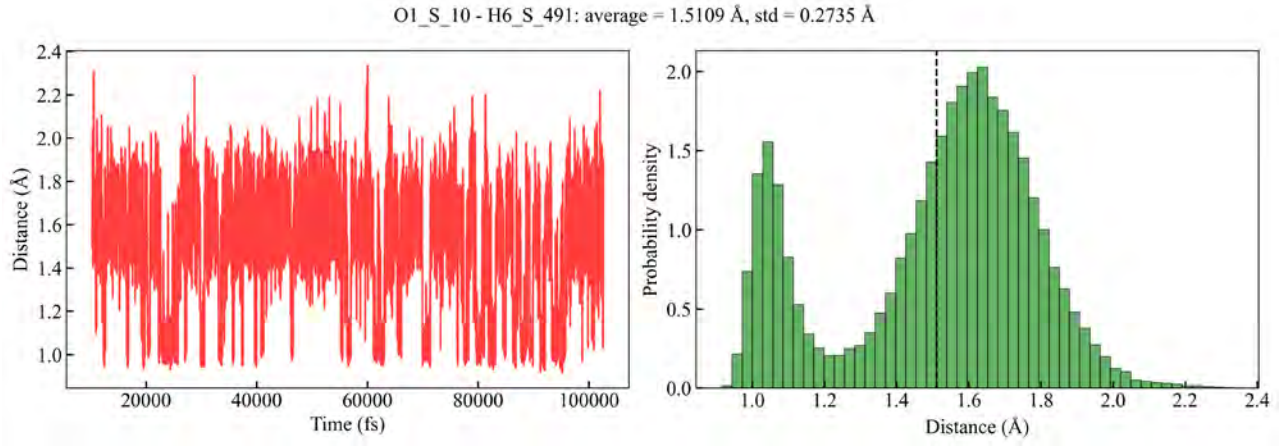
Bond type	Average distance (Å)	Standard dev. σ (Å)	Number of points
O1_S_10 - H6_S_491	1.5109	0.2735	92369
O1_S_11 - H6_S_490	1.5392	0.2688	92369
O1_S_12 - H6_S_489	1.5146	0.2808	92369
O1_S_21 - H6_S_469	1.2404	0.2935	92369
O1_S_22 - H6_S_470	1.2470	0.2893	92369
O1_S_23 - H6_S_471	1.2095	0.2725	92369
O1_S_24 - H6_S_472	1.2053	0.2701	92369
O1_S_25 - H6_S_475	1.2027	0.2679	92369
O1_S_26 - H6_S_476	1.2089	0.2706	92369
O1_S_27 - H6_S_473	1.1939	0.2630	92369
O1_S_28 - H6_S_474	1.2135	0.2781	92369
O1_S_5 - H6_S_486	1.4995	0.2848	92369
O1_S_6 - H6_S_485	1.4856	0.2895	92369
O1_S_7 - H6_S_488	1.5218	0.2677	92369
O1_S_8 - H6_S_487	1.5247	0.2707	92369
O1_S_9 - H6_S_492	1.5319	0.2740	92369
O2_S_69 - H8B_S_390	1.7230	0.1662	92369
O2_S_71 - H8B_S_392	1.7174	0.1706	92369
O2_S_72 - H8B_S_391	1.7192	0.1698	92369
O2_S_74 - H8B_S_395	1.7203	0.1769	92369

Bond Distance Plots

O1 - H6

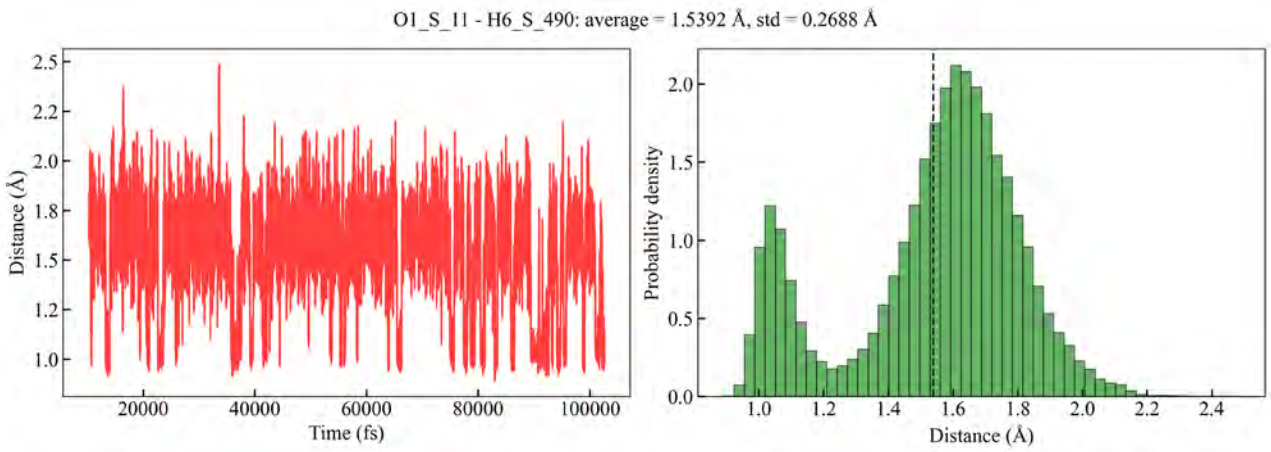
O1_S_10 - H6_S_491

Average distance = 1.5109 Å; standard deviation = 0.2735 Å; number of points = 92369



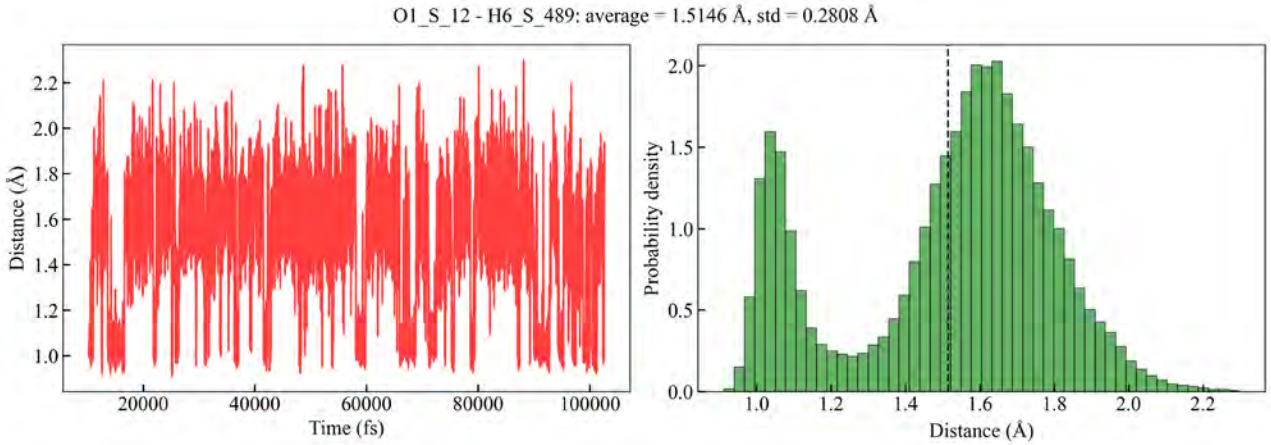
O1_S_11 - H6_S_490

Average distance = 1.5392 Å; standard deviation = 0.2688 Å; number of points = 92369



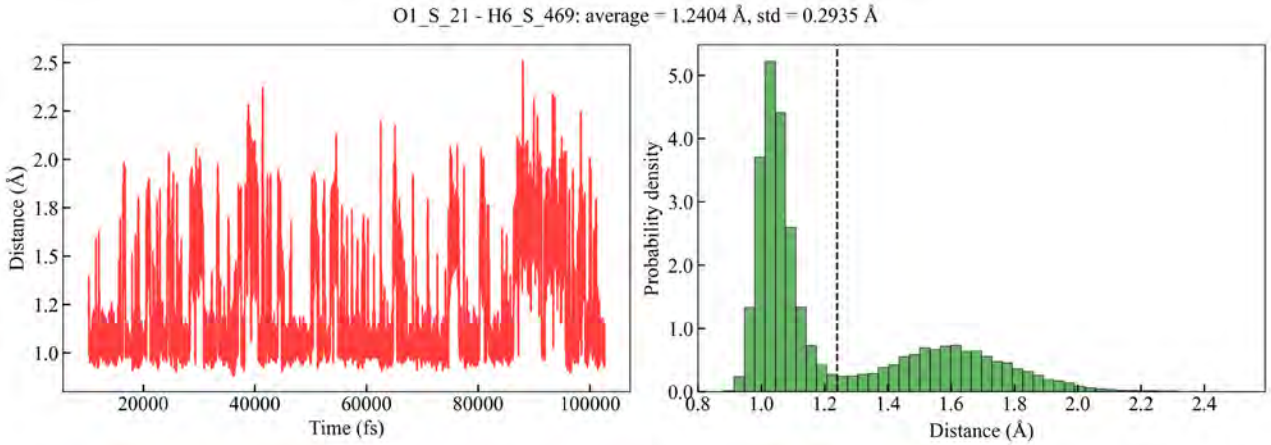
O1_S_12 - H6_S_489

Average distance = 1.5146 Å; standard deviation = 0.2808 Å; number of points = 92369



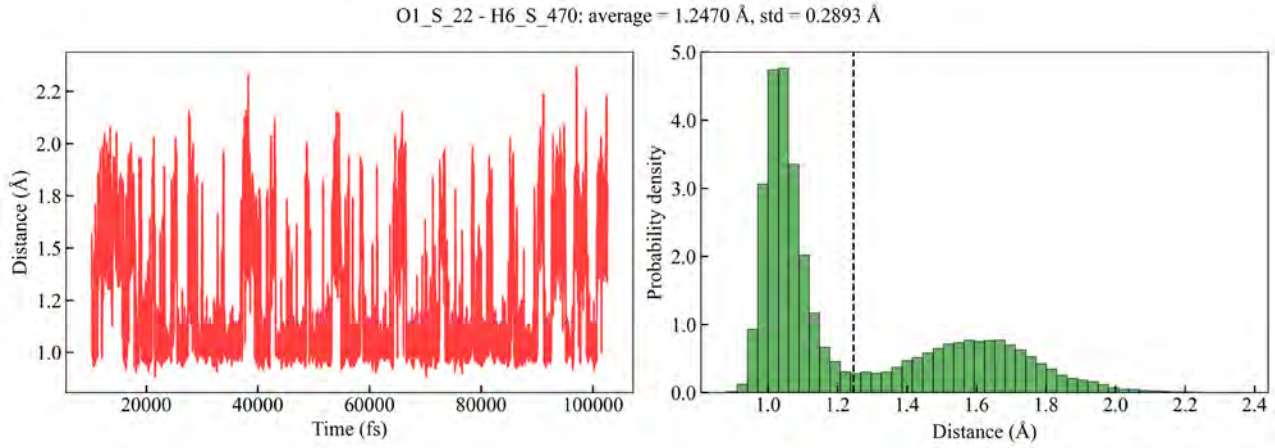
O1_S_21 - H6_S_469

Average distance = 1.2404 Å; standard deviation = 0.2935 Å; number of points = 92369



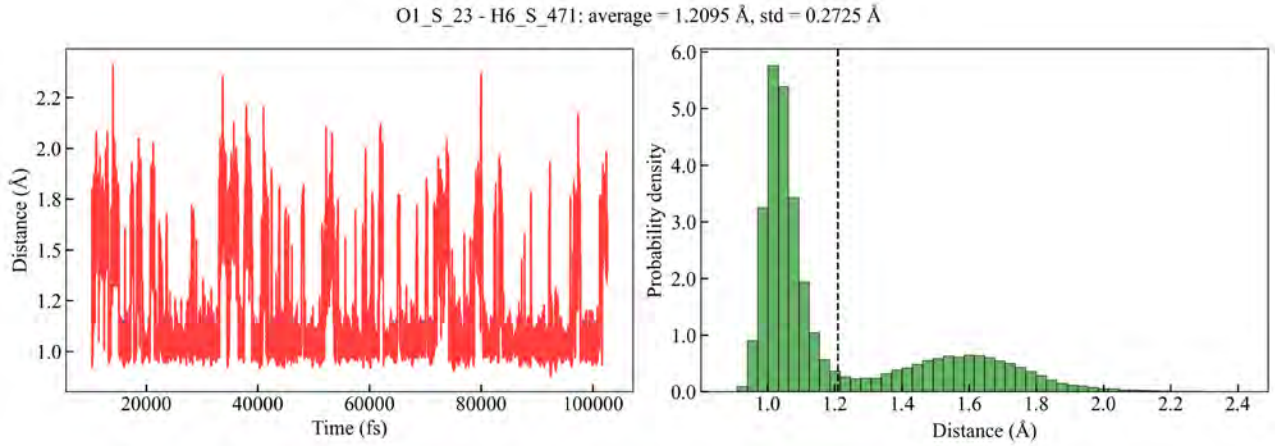
O1_S_22 - H6_S_470

Average distance = 1.2470 Å; standard deviation = 0.2893 Å; number of points = 92369



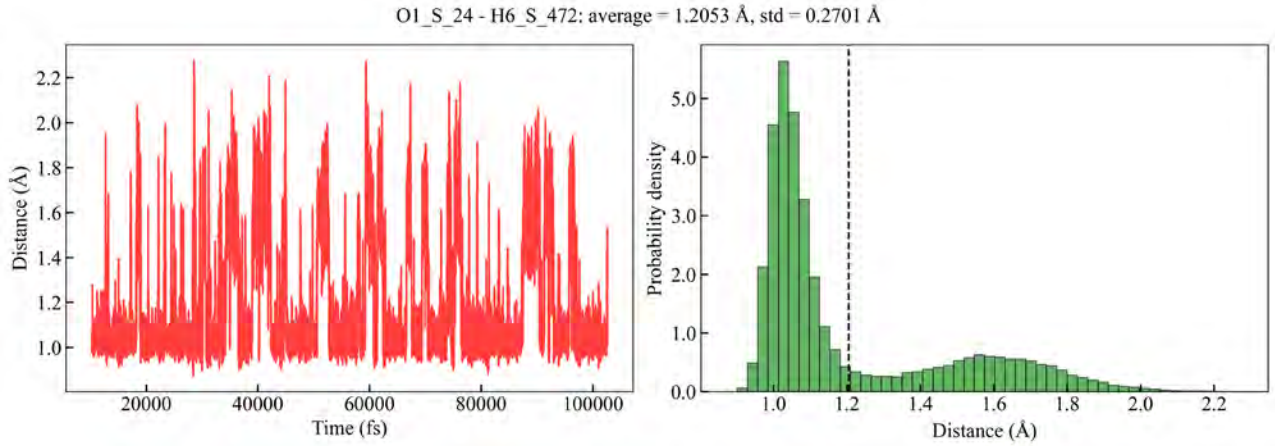
O1_S_23 - H6_S_471

Average distance = 1.2095 Å; standard deviation = 0.2725 Å; number of points = 92369



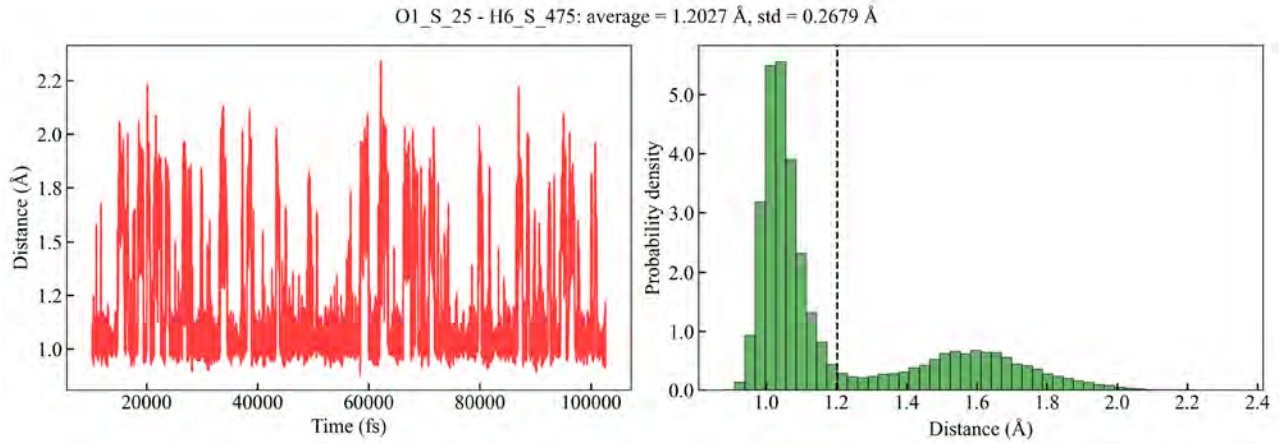
O1_S_24 - H6_S_472

Average distance = 1.2053 Å; standard deviation = 0.2701 Å; number of points = 92369



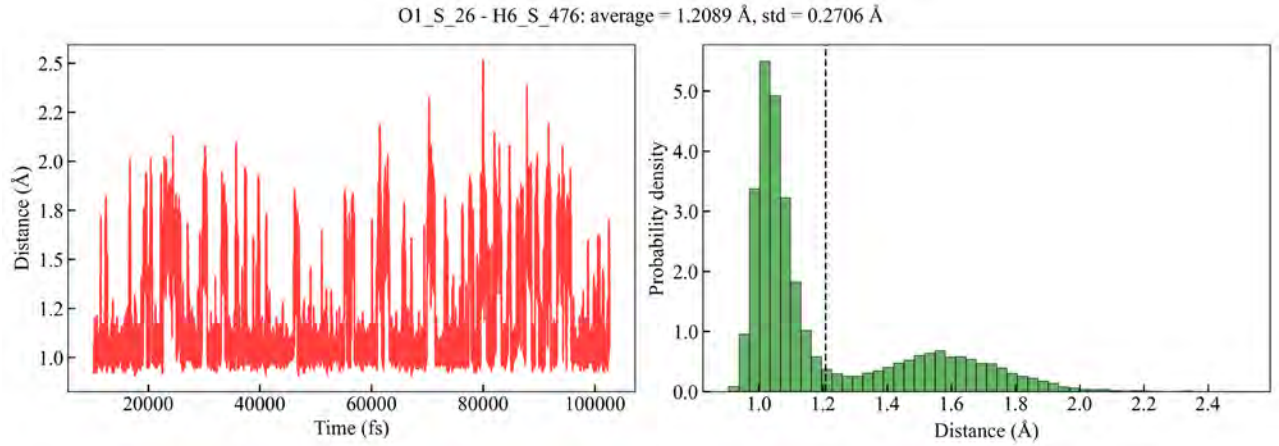
O1_S_25 - H6_S_475

Average distance = 1.2027 Å; standard deviation = 0.2679 Å; number of points = 92369



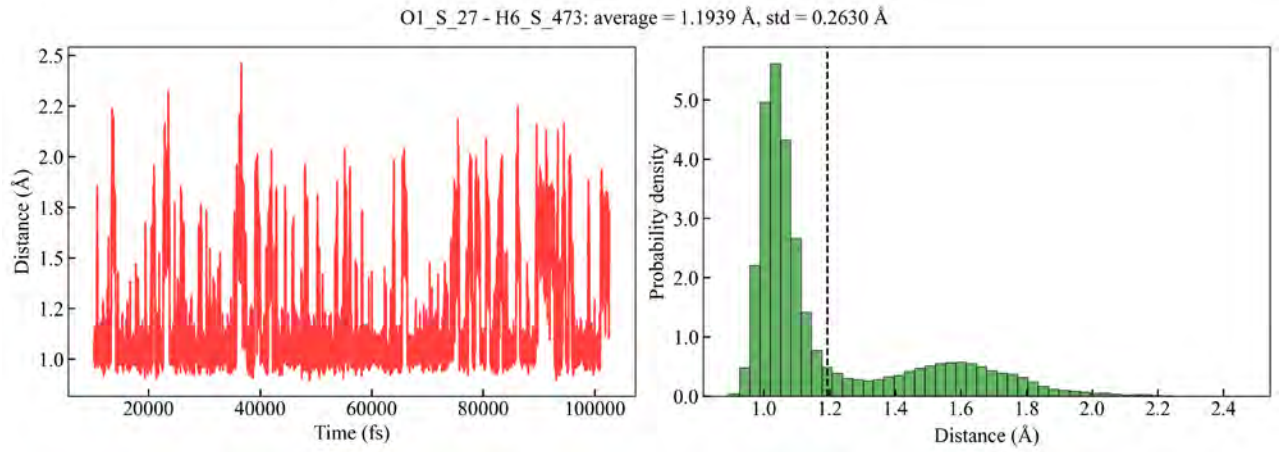
O1_S_26 - H6_S_476

Average distance = 1.2089 Å; standard deviation = 0.2706 Å; number of points = 92369



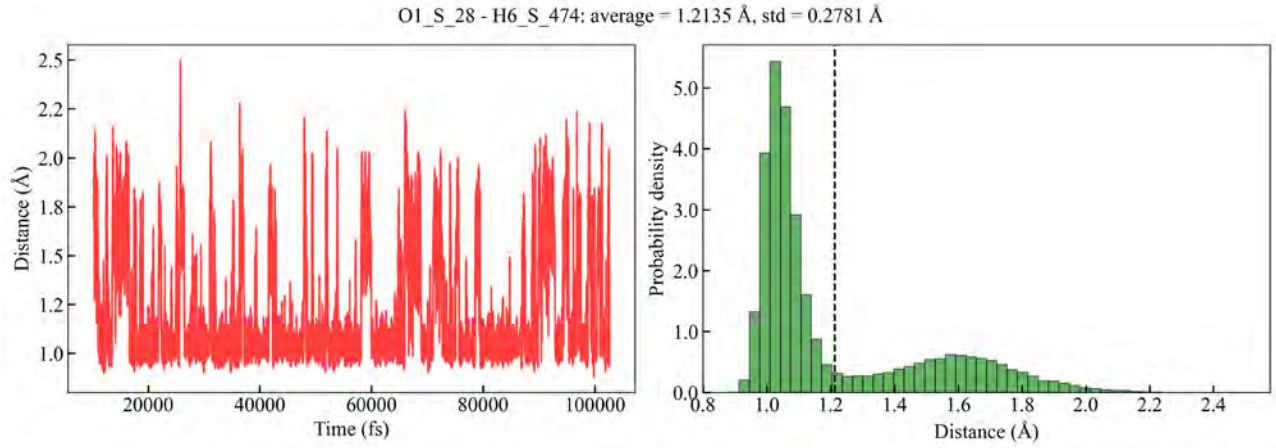
O1_S_27 - H6_S_473

Average distance = 1.1939 Å; standard deviation = 0.2630 Å; number of points = 92369



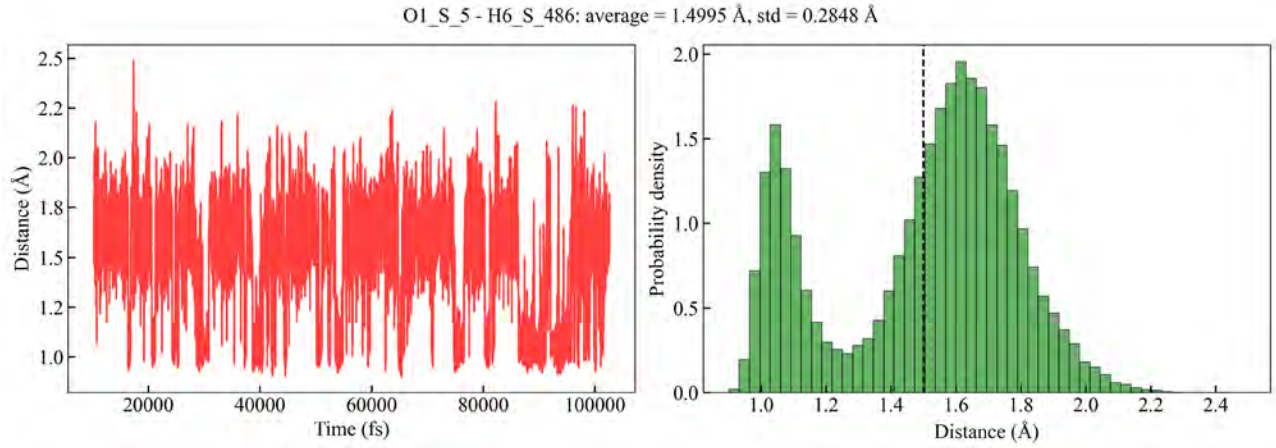
O1_S_28 - H6_S_474

Average distance = 1.2135 Å; standard deviation = 0.2781 Å; number of points = 92369



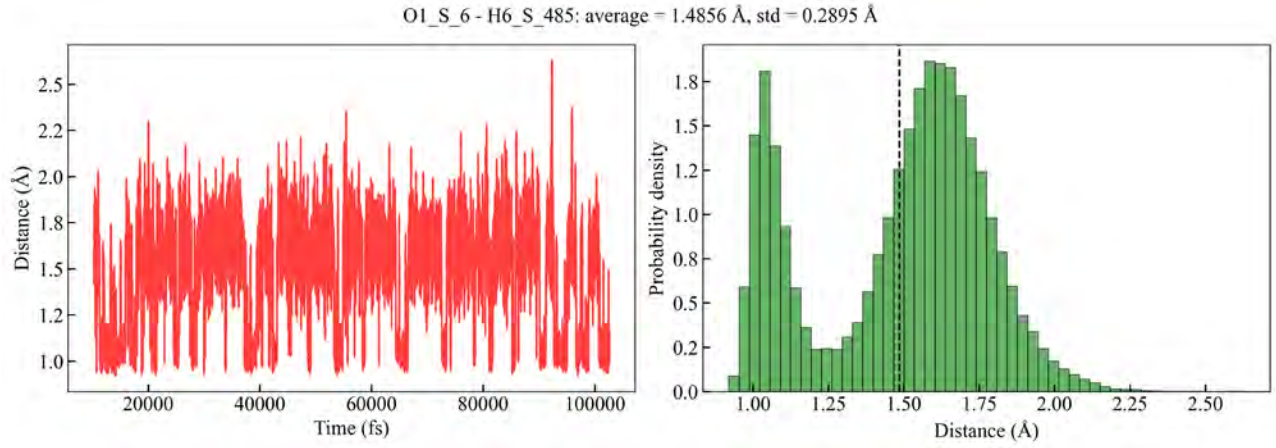
O1_S_5 - H6_S_486

Average distance = 1.4995 Å; standard deviation = 0.2848 Å; number of points = 92369



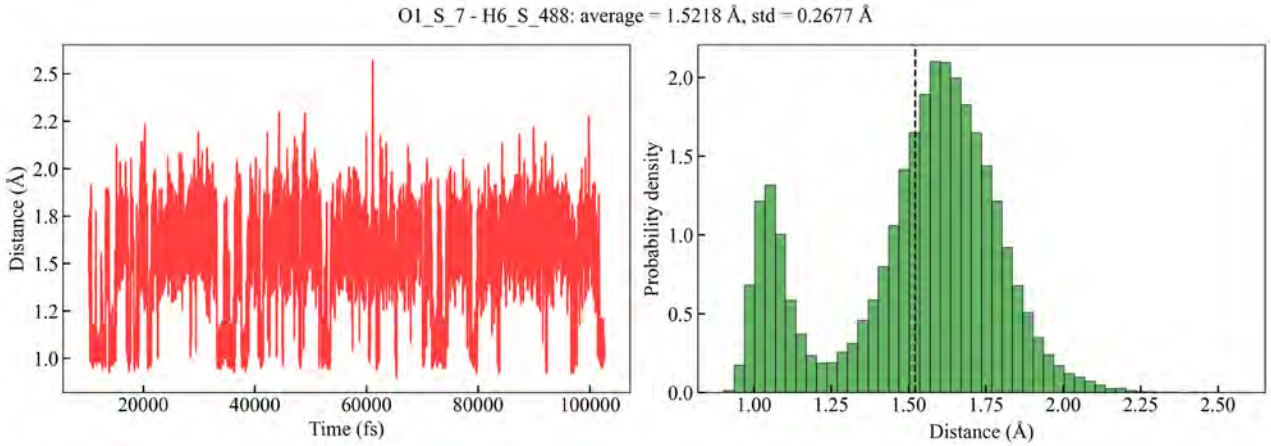
O1_S_6 - H6_S_485

Average distance = 1.4856 Å; standard deviation = 0.2895 Å; number of points = 92369



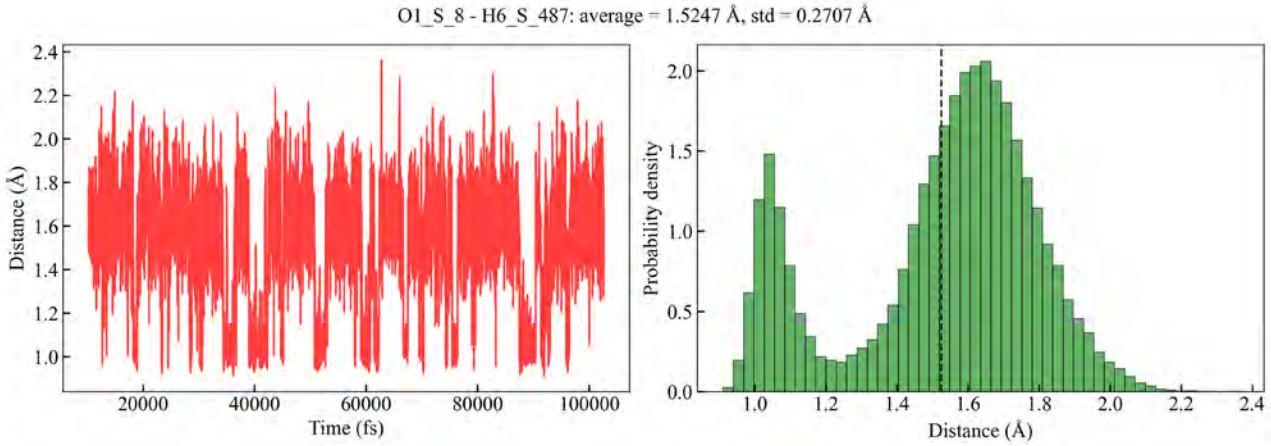
O1_S_7 - H6_S_488

Average distance = 1.5218 Å; standard deviation = 0.2677 Å; number of points = 92369



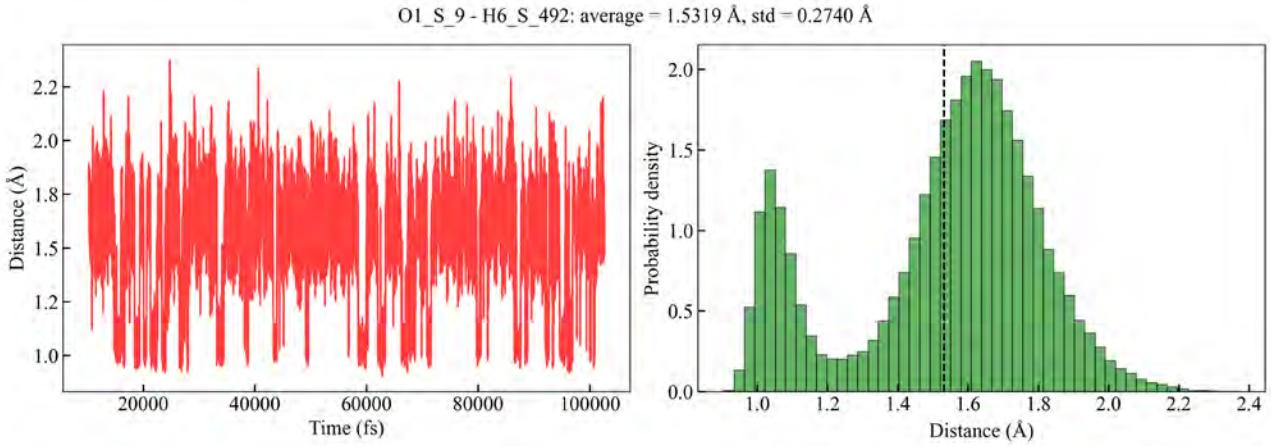
O1_S_8 - H6_S_487

Average distance = 1.5247 Å; standard deviation = 0.2707 Å; number of points = 92369



O1_S_9 - H6_S_492

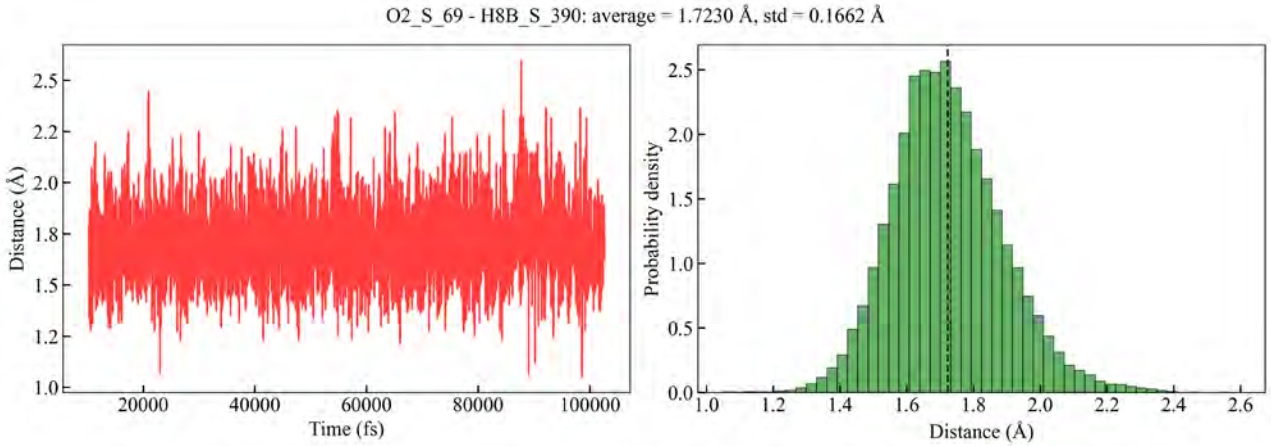
Average distance = 1.5319 Å; standard deviation = 0.2740 Å; number of points = 92369



O2 - H8B

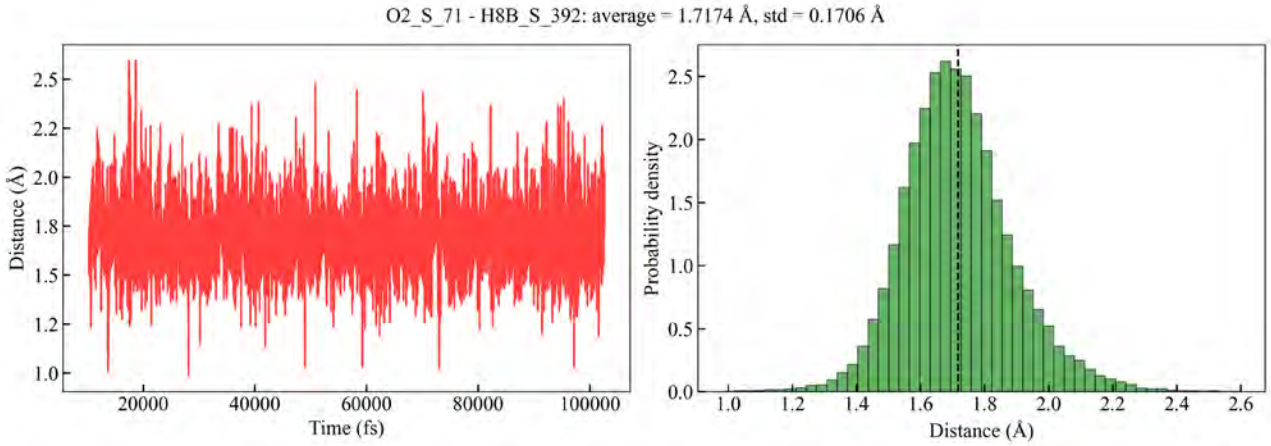
O2_S_69 - H8B_S_390

Average distance = 1.7230 Å; standard deviation = 0.1662 Å; number of points = 92369



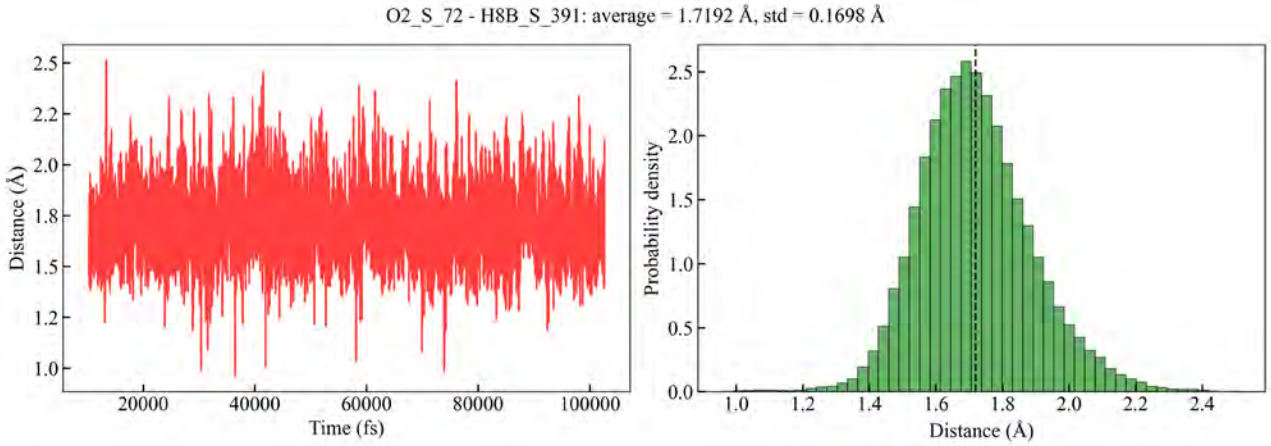
O2_S_71 - H8B_S_392

Average distance = 1.7174 Å; standard deviation = 0.1706 Å; number of points = 92369



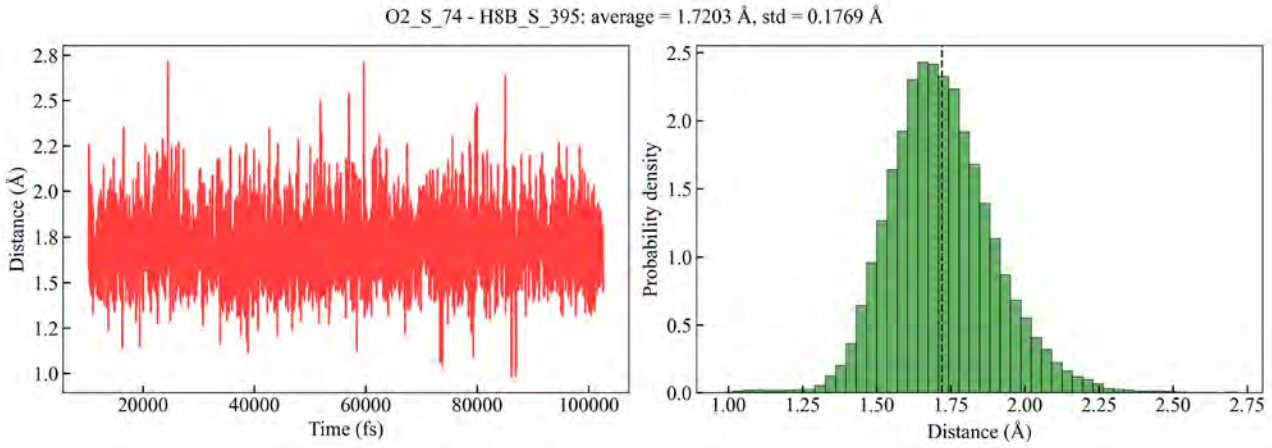
O2_S_72 - H8B_S_391

Average distance = 1.7192 Å; standard deviation = 0.1698 Å; number of points = 92369



O2_S_74 - H8B_S_395

Average distance = 1.7203 Å; standard deviation = 0.1769 Å; number of points = 92369



3.2.4. P3 at 320 K - Bond Distance Analysis

Table S21. Individual time-averaged hydrogen-involving atomic distances for all equivalent proton environments in the P3 bulk AIMD trajectory at 320 K.

Bond type	Average distance (Å)	Standard dev. σ (Å)	Number of points
O1_10 - H2D1_93	1.9460	0.1844	110177
O1_11 - H2D1_96	1.9390	0.1802	110177
O1_12 - H2D1_95	1.9436	0.1810	110177
O1_157 - H2D1_242	1.9434	0.1847	110177
O1_158 - H2D1_241	1.9436	0.1836	110177
O1_159 - H2D1_244	1.9457	0.1815	110177
O1_160 - H2D1_243	1.9480	0.1906	110177
O1_305 - H2D1_390	1.9488	0.1818	110177
O1_306 - H2D1_389	1.9443	0.1855	110177
O1_307 - H2D1_392	1.9461	0.1867	110177
O1_308 - H2D1_391	1.9524	0.1930	110177
O1_453 - H2D1_538	1.9421	0.1828	110177
O1_454 - H2D1_537	1.9494	0.1894	110177
O1_455 - H2D1_540	1.9537	0.1947	110177
O1_456 - H2D1_539	1.9472	0.1935	110177
O1_601 - H2D1_686	1.9422	0.1802	110177
O1_602 - H2D1_685	1.9445	0.1836	110177
O1_603 - H2D1_688	1.9456	0.1905	110177
O1_604 - H2D1_687	1.9441	0.1785	110177
O1_749 - H2D1_834	1.9411	0.1820	110177
O1_750 - H2D1_833	1.9500	0.1903	110177
O1_751 - H2D1_836	1.9468	0.1896	110177
O1_752 - H2D1_835	1.9398	0.1754	110177
O1_9 - H2D1_94	1.9501	0.1883	110177
O1_10 - H6_110	1.7515	0.1437	110177
O1_11 - H6_259	1.7577	0.1450	110177
O1_12 - H6_260	1.7551	0.1481	110177
O1_157 - H6_257	1.7527	0.1421	110177
O1_158 - H6_258	1.7540	0.1450	110177
O1_159 - H6_111	1.7512	0.1361	110177
O1_160 - H6_112	1.7542	0.1459	110177
O1_305 - H6_405	1.7538	0.1436	110177
O1_306 - H6_406	1.7546	0.1467	110177
O1_307 - H6_555	1.7517	0.1430	110177
O1_308 - H6_556	1.7504	0.1419	110177
O1_453 - H6_553	1.7534	0.1418	110177
O1_454 - H6_554	1.7586	0.1527	110177
O1_455 - H6_407	1.7538	0.1483	110177
O1_456 - H6_408	1.7564	0.1468	110177
O1_601 - H6_701	1.7564	0.1418	110177
O1_602 - H6_702	1.7565	0.1450	110177
O1_603 - H6_851	1.7554	0.1482	110177
O1_604 - H6_852	1.7506	0.1392	110177
O1_749 - H6_849	1.7567	0.1504	110177
O1_750 - H6_850	1.7543	0.1528	110177
O1_751 - H6_703	1.7565	0.1475	110177
O1_752 - H6_704	1.7568	0.1383	110177
O1_9 - H6_109	1.7516	0.1445	110177
O1_10 - H7_138	3.0120	0.2972	110177

O1_11 - H7_139	2.0066	0.2598	110177
O1_12 - H7_140	1.9976	0.2589	110177
O1_157 - H7_285	1.9931	0.2559	110177
O1_158 - H7_286	1.9992	0.2602	110177
O1_159 - H7_287	1.9975	0.2521	110177
O1_160 - H7_288	2.0133	0.3275	110177
O1_305 - H7_433	2.0054	0.2803	110177
O1_306 - H7_434	2.0042	0.2623	110177
O1_307 - H7_435	3.0236	0.2520	110177
O1_308 - H7_436	2.0016	0.2600	110177
O1_453 - H7_581	2.0678	0.3631	110177
O1_454 - H7_582	1.9898	0.2492	110177
O1_455 - H7_583	1.9958	0.2583	110177
O1_456 - H7_584	1.9996	0.2646	110177
O1_601 - H7_729	2.0013	0.2607	110177
O1_602 - H7_730	2.0045	0.2672	110177
O1_603 - H7_731	1.9911	0.2533	110177
O1_604 - H7_732	2.0061	0.2658	110177
O1_749 - H7_877	2.0059	0.2650	110177
O1_750 - H7_878	2.0080	0.2770	110177
O1_751 - H7_879	1.9954	0.2529	110177
O1_752 - H7_880	1.9919	0.2544	110177
O1_9 - H7_137	1.9948	0.2619	110177
O2_1 - H1_135	1.7955	0.1521	110177
O2_149 - H1_283	1.7956	0.1521	110177
O2_150 - H1_284	1.7949	0.1509	110177
O2_151 - H1_281	1.7960	0.1524	110177
O2_152 - H1_282	1.8036	0.1619	110177
O2_297 - H1_431	1.7952	0.1552	110177
O2_298 - H1_432	1.7984	0.1524	110177
O2_299 - H1_429	1.7982	0.1590	110177
O2_3 - H1_133	1.7920	0.1524	110177
O2_300 - H1_430	1.7978	0.1554	110177
O2_4 - H1_134	1.7940	0.1501	110177
O2_445 - H1_579	1.8007	0.1604	110177
O2_446 - H1_580	1.7947	0.1543	110177
O2_447 - H1_577	1.7964	0.1545	110177
O2_448 - H1_578	1.7992	0.1542	110177
O2_593 - H1_727	1.7940	0.1495	110177
O2_594 - H1_728	1.8058	0.1631	110177
O2_595 - H1_725	1.7949	0.1561	110177
O2_596 - H1_726	1.7982	0.1553	110177
O2_741 - H1_875	1.7965	0.1563	110177
O2_742 - H1_876	1.7998	0.1581	110177
O2_743 - H1_873	1.7950	0.1504	110177
O2_744 - H1_874	1.7948	0.1566	110177
O2_1 - H1A_114	1.7539	0.1468	110177
O2_149 - H1A_262	1.7499	0.1436	110177
O2_150 - H1A_261	1.7492	0.1427	110177
O2_151 - H1A_264	1.7482	0.1403	110177
O2_152 - H1A_263	1.7480	0.1440	110177
O2_2 - H1A_113	1.7500	0.1437	110177
O2_297 - H1A_410	1.7502	0.1477	110177

O2_298 - H1A_409	1.7520	0.1465	110177
O2_299 - H1A_412	1.7474	0.1407	110177
O2_3 - H1A_116	1.7547	0.1518	110177
O2_300 - H1A_411	1.7523	0.1460	110177
O2_4 - H1A_115	1.7493	0.1452	110177
O2_445 - H1A_558	1.7491	0.1440	110177
O2_446 - H1A_557	1.7506	0.1493	110177
O2_447 - H1A_560	1.7534	0.1480	110177
O2_448 - H1A_559	1.7480	0.1442	110177
O2_593 - H1A_706	1.7496	0.1456	110177
O2_594 - H1A_705	1.7490	0.1436	110177
O2_595 - H1A_708	1.7533	0.1459	110177
O2_596 - H1A_707	1.7480	0.1412	110177
O2_741 - H1A_854	1.7499	0.1460	110177
O2_742 - H1A_853	1.7480	0.1439	110177
O2_743 - H1A_856	1.7486	0.1425	110177
O2_744 - H1A_855	1.7514	0.1451	110177
O2_1 - H3_84	1.9252	0.1719	110177
O2_149 - H3_232	1.9227	0.1683	110177
O2_150 - H3_231	1.9216	0.1702	110177
O2_151 - H3_230	1.9203	0.1643	110177
O2_152 - H3_229	1.9202	0.1687	110177
O2_2 - H3_83	1.9244	0.1706	110177
O2_297 - H3_380	1.9233	0.1707	110177
O2_298 - H3_379	1.9229	0.1701	110177
O2_299 - H3_378	1.9285	0.1748	110177
O2_3 - H3_82	1.9220	0.1717	110177
O2_300 - H3_377	1.9223	0.1742	110177
O2_4 - H3_81	1.9216	0.1695	110177
O2_445 - H3_528	1.9178	0.1641	110177
O2_446 - H3_527	1.9244	0.1699	110177
O2_447 - H3_526	1.9250	0.1720	110177
O2_448 - H3_525	1.9242	0.1675	110177
O2_593 - H3_676	1.9206	0.1652	110177
O2_594 - H3_675	1.9180	0.1676	110177
O2_595 - H3_674	1.9233	0.1658	110177
O2_596 - H3_673	1.9220	0.1684	110177
O2_741 - H3_824	1.9226	0.1689	110177
O2_742 - H3_823	1.9240	0.1706	110177
O2_743 - H3_822	1.9267	0.1681	110177
O2_744 - H3_821	1.9189	0.1627	110177
O3_153 - H2_289	1.7765	0.1556	110177
O3_154 - H2_290	1.7761	0.1555	110177
O3_155 - H2_291	1.7700	0.1461	110177
O3_156 - H2_292	1.7764	0.1502	110177
O3_301 - H2_437	1.7755	0.1585	110177
O3_302 - H2_438	1.7788	0.1566	110177
O3_303 - H2_439	1.7783	0.1610	110177
O3_304 - H2_440	1.7797	0.1576	110177
O3_449 - H2_585	1.7685	0.1479	110177
O3_450 - H2_586	1.7746	0.1554	110177
O3_451 - H2_587	1.7683	0.1491	110177
O3_452 - H2_588	1.7723	0.1504	110177

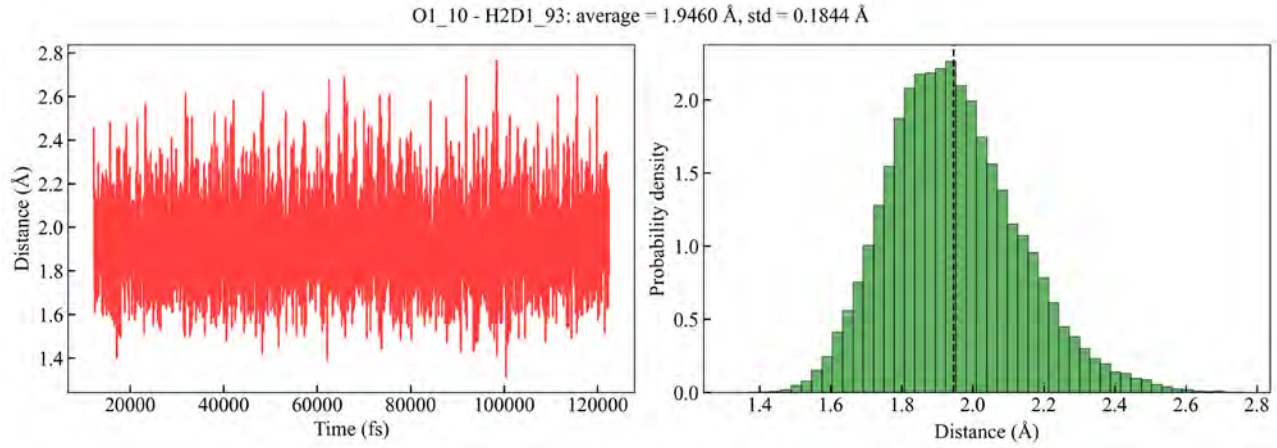
O3_5 - H2_141	1.7750	0.1528	110177
O3_597 - H2_733	1.7686	0.1461	110177
O3_598 - H2_734	1.7753	0.1533	110177
O3_599 - H2_735	1.7765	0.1609	110177
O3_6 - H2_142	1.7755	0.1530	110177
O3_7 - H2_143	1.7710	0.1513	110177
O3_745 - H2_881	1.7781	0.1559	110177
O3_746 - H2_882	1.7722	0.1479	110177
O3_747 - H2_883	1.7789	0.1596	110177
O3_748 - H2_884	1.7696	0.1468	110177
O3_8 - H2_144	1.7686	0.1465	110177
O3_153 - H8B_245	1.6861	0.1089	110177
O3_154 - H8B_246	1.6903	0.1131	110177
O3_155 - H8B_247	1.6879	0.1130	110177
O3_156 - H8B_248	1.6904	0.1170	110177
O3_301 - H8B_393	1.6859	0.1105	110177
O3_302 - H8B_394	1.6868	0.1088	110177
O3_303 - H8B_395	1.6868	0.1131	110177
O3_304 - H8B_396	1.6868	0.1117	110177
O3_449 - H8B_541	1.6868	0.1125	110177
O3_450 - H8B_542	1.6873	0.1119	110177
O3_451 - H8B_543	1.6853	0.1094	110177
O3_452 - H8B_544	1.6861	0.1108	110177
O3_5 - H8B_97	1.6868	0.1115	110177
O3_597 - H8B_689	1.6885	0.1128	110177
O3_598 - H8B_690	1.6873	0.1130	110177
O3_599 - H8B_691	1.6878	0.1141	110177
O3_6 - H8B_98	1.6849	0.1081	110177
O3_600 - H8B_692	1.6858	0.1096	110177
O3_7 - H8B_99	1.6866	0.1099	110177
O3_745 - H8B_837	1.6894	0.1145	110177
O3_746 - H8B_838	1.6902	0.1165	110177
O3_747 - H8B_839	1.6895	0.1143	110177
O3_748 - H8B_840	1.6867	0.1135	110177
O3_8 - H8B_100	1.6859	0.1102	110177

Bond Distance Plots

O1 - H2D1

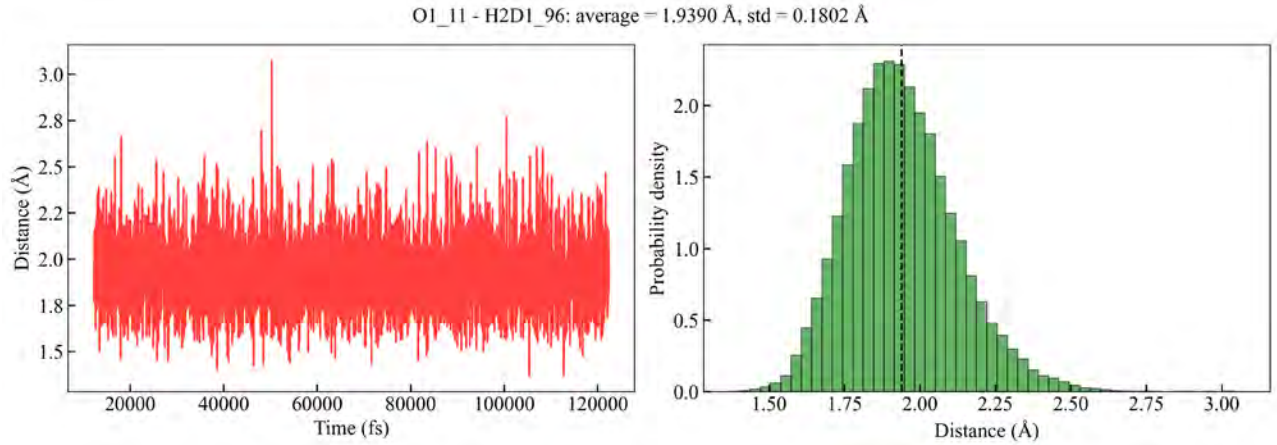
O1_10 - H2D1_93

Average distance = 1.9460 Å; standard deviation = 0.1844 Å; number of points = 110177



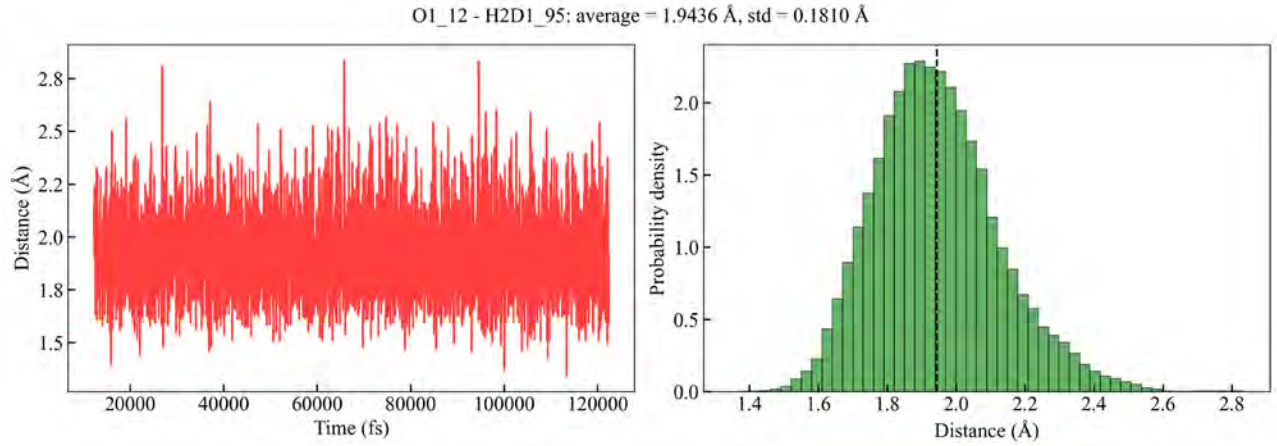
O1_11 - H2D1_96

Average distance = 1.9390 Å; standard deviation = 0.1802 Å; number of points = 110177



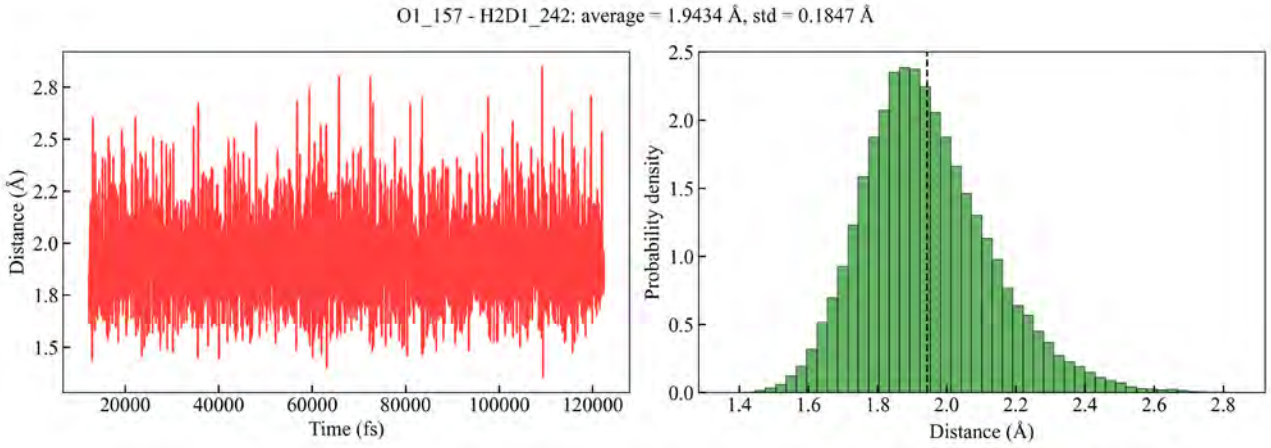
O1_12 - H2D1_95

Average distance = 1.9436 Å; standard deviation = 0.1810 Å; number of points = 110177



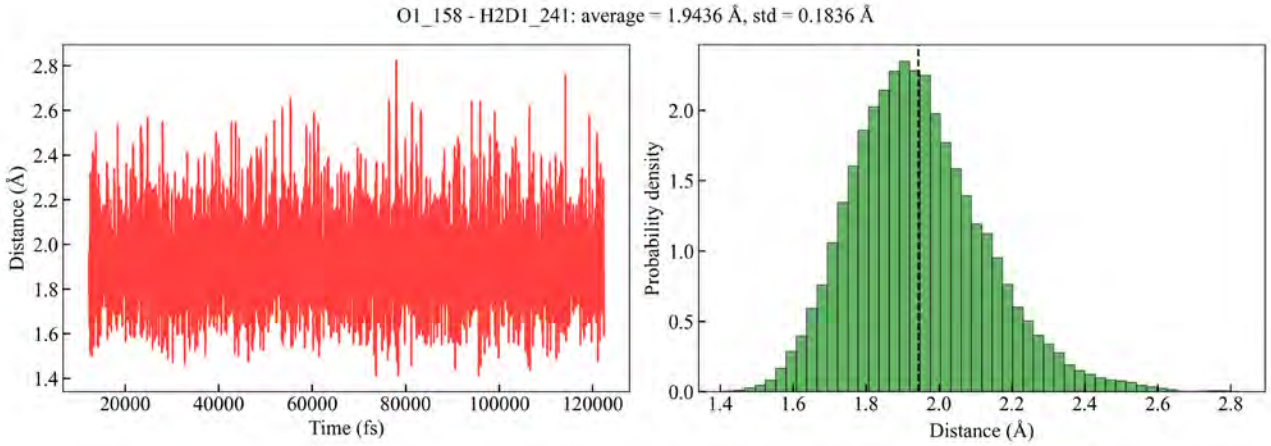
O1_157 - H2D1_242

Average distance = 1.9434 Å; standard deviation = 0.1847 Å; number of points = 110177



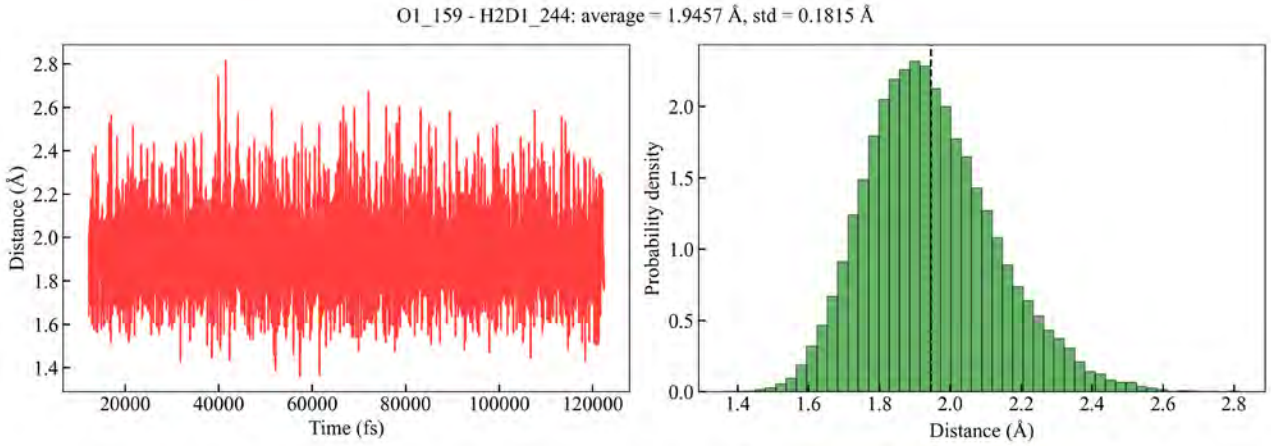
O1_158 - H2D1_241

Average distance = 1.9436 Å; standard deviation = 0.1836 Å; number of points = 110177



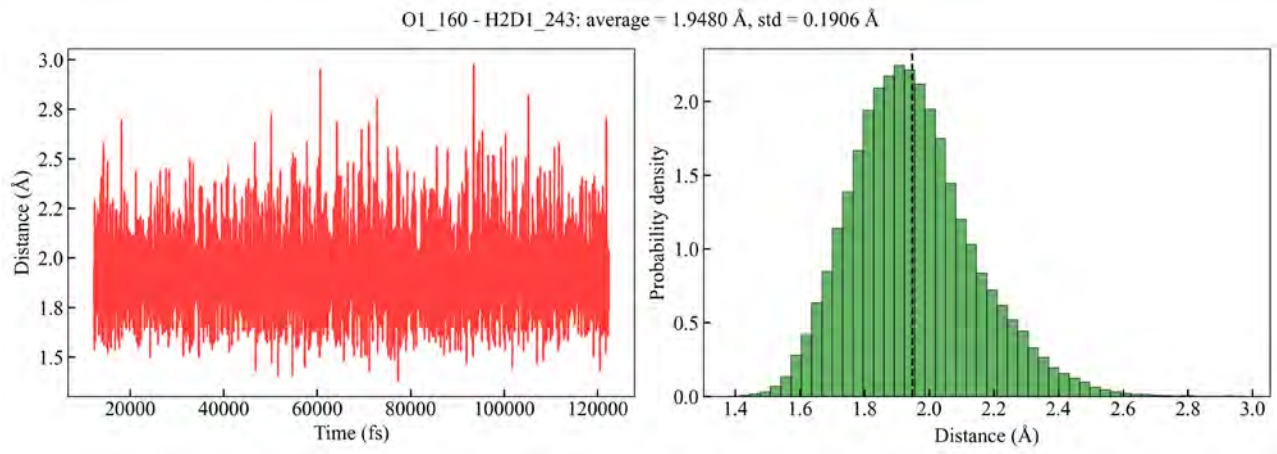
O1_159 - H2D1_244

Average distance = 1.9457 Å; standard deviation = 0.1815 Å; number of points = 110177



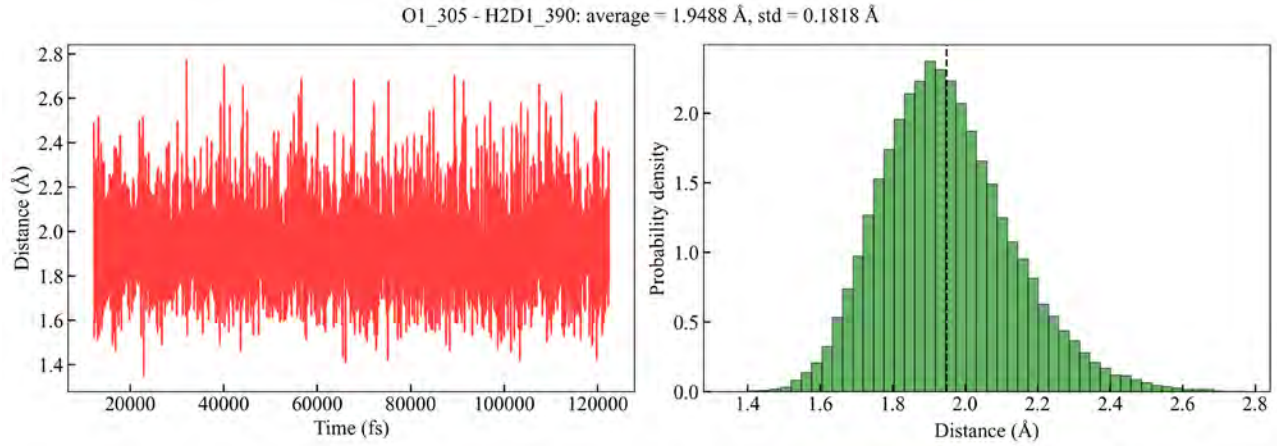
O1_160 - H2D1_243

Average distance = 1.9480 Å; standard deviation = 0.1906 Å; number of points = 110177



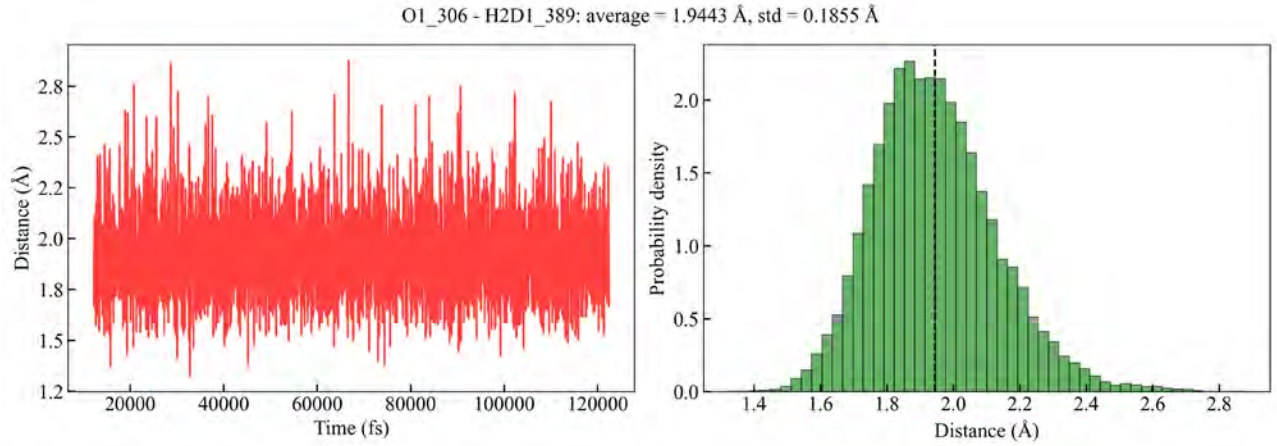
O1_305 - H2D1_390

Average distance = 1.9488 Å; standard deviation = 0.1818 Å; number of points = 110177



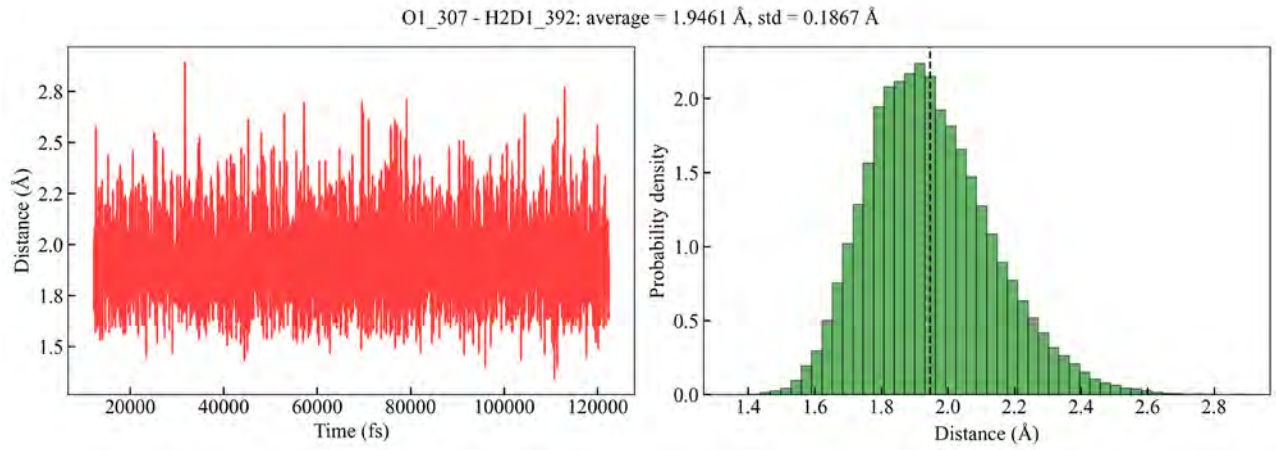
O1_306 - H2D1_389

Average distance = 1.9443 Å; standard deviation = 0.1855 Å; number of points = 110177



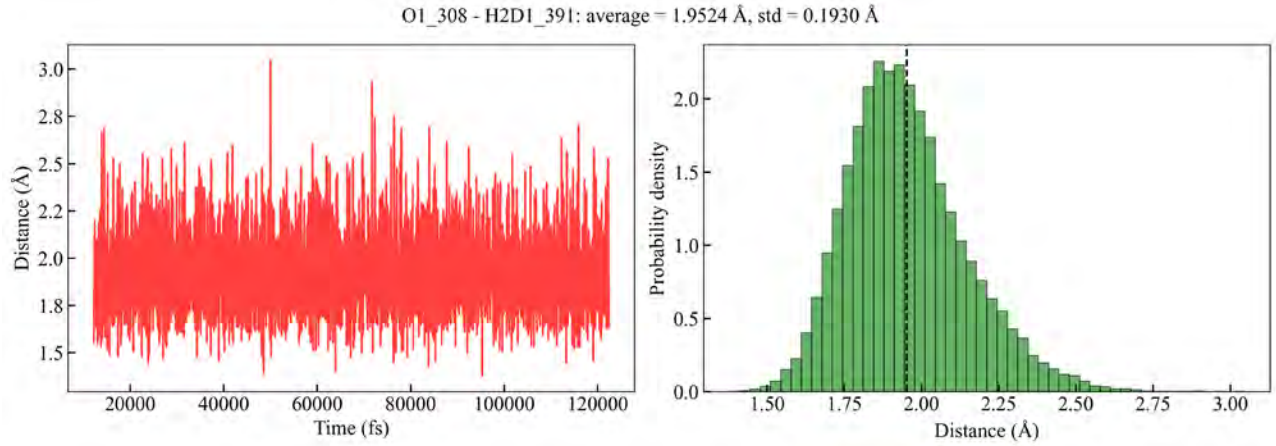
O1_307 - H2D1_392

Average distance = 1.9461 Å; standard deviation = 0.1867 Å; number of points = 110177



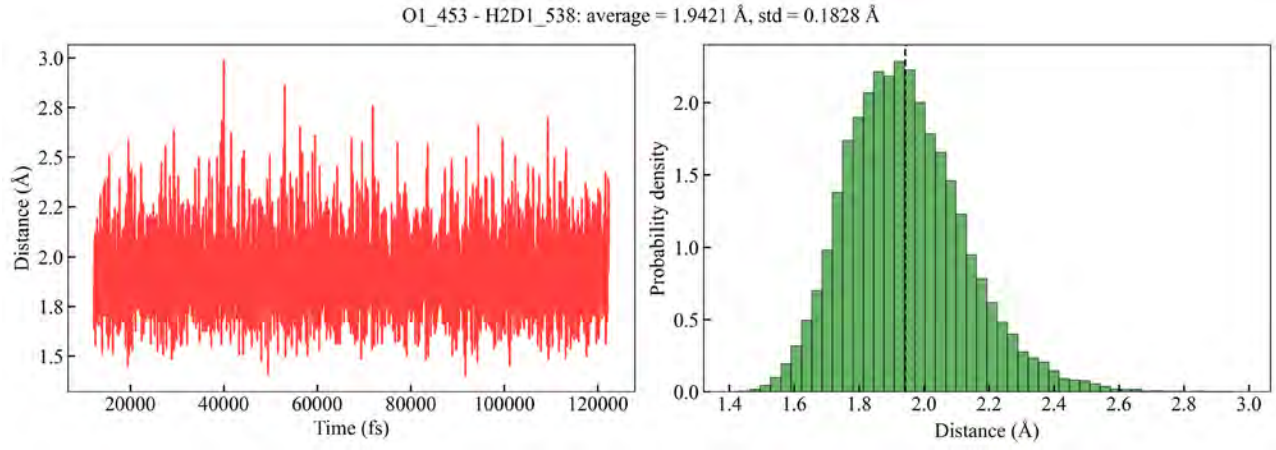
O1_308 - H2D1_391

Average distance = 1.9524 Å; standard deviation = 0.1930 Å; number of points = 110177



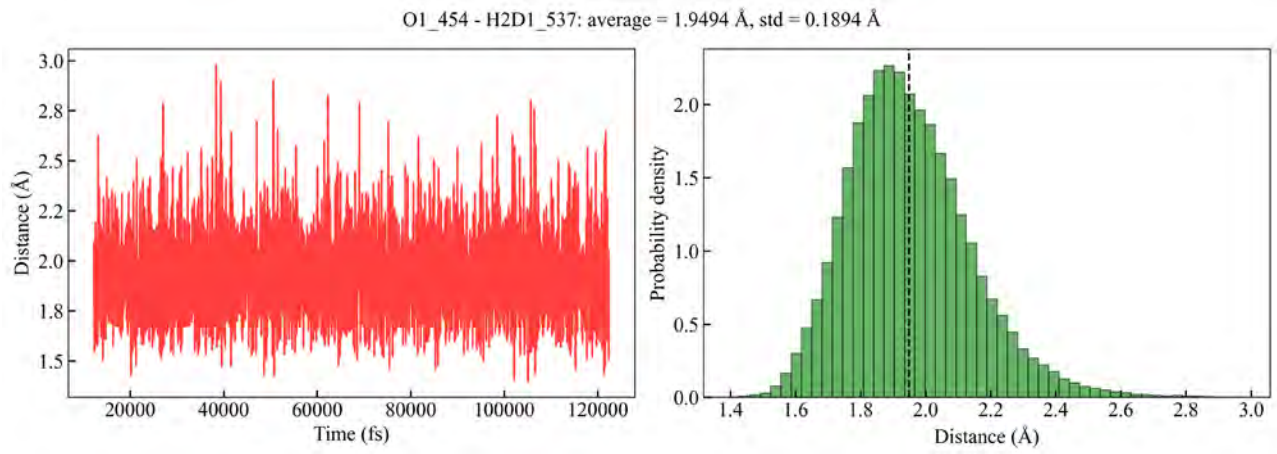
O1_453 - H2D1_538

Average distance = 1.9421 Å; standard deviation = 0.1828 Å; number of points = 110177



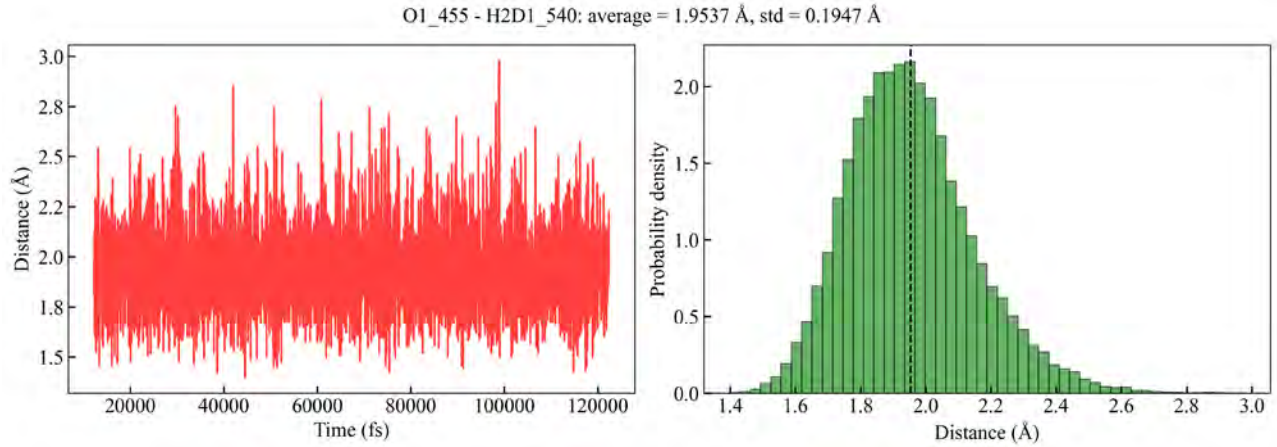
O1_454 - H2D1_537

Average distance = 1.9494 Å; standard deviation = 0.1894 Å; number of points = 110177



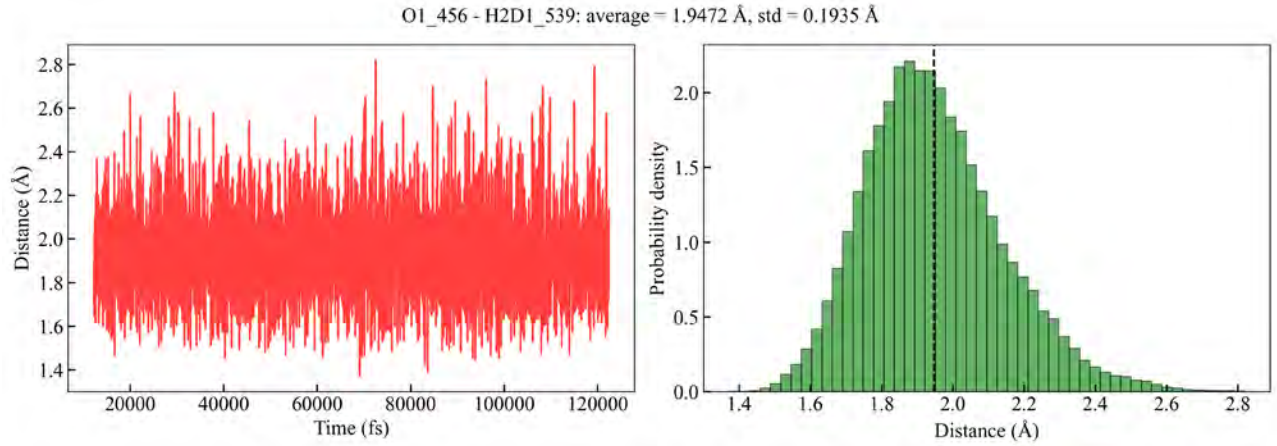
O1_455 - H2D1_540

Average distance = 1.9537 Å; standard deviation = 0.1947 Å; number of points = 110177



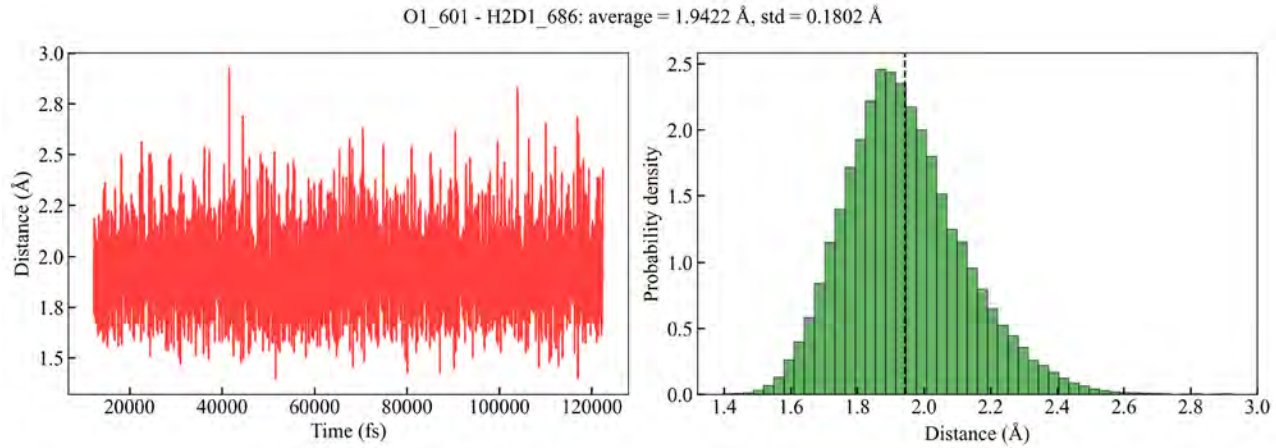
O1_456 - H2D1_539

Average distance = 1.9472 Å; standard deviation = 0.1935 Å; number of points = 110177



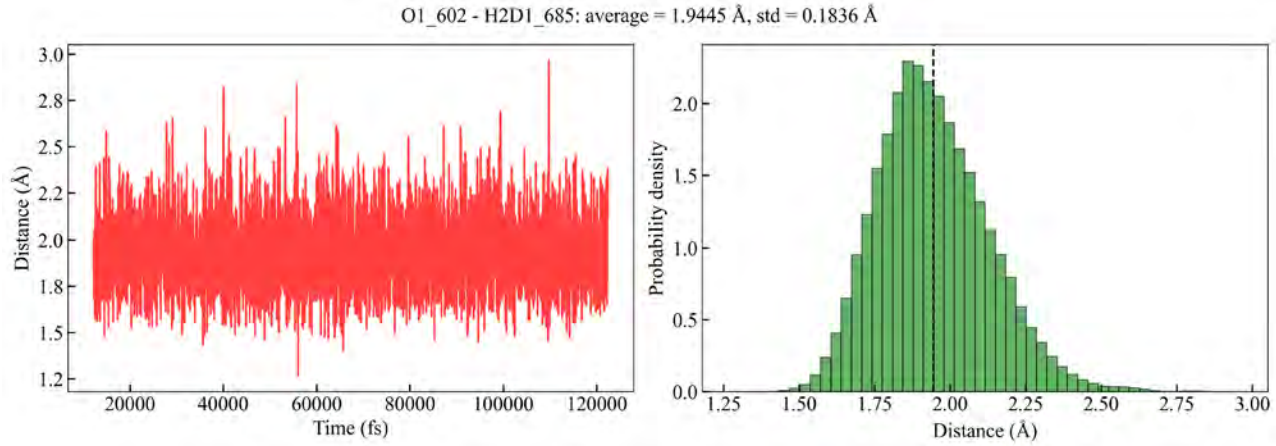
O1_601 - H2D1_686

Average distance = 1.9422 Å; standard deviation = 0.1802 Å; number of points = 110177



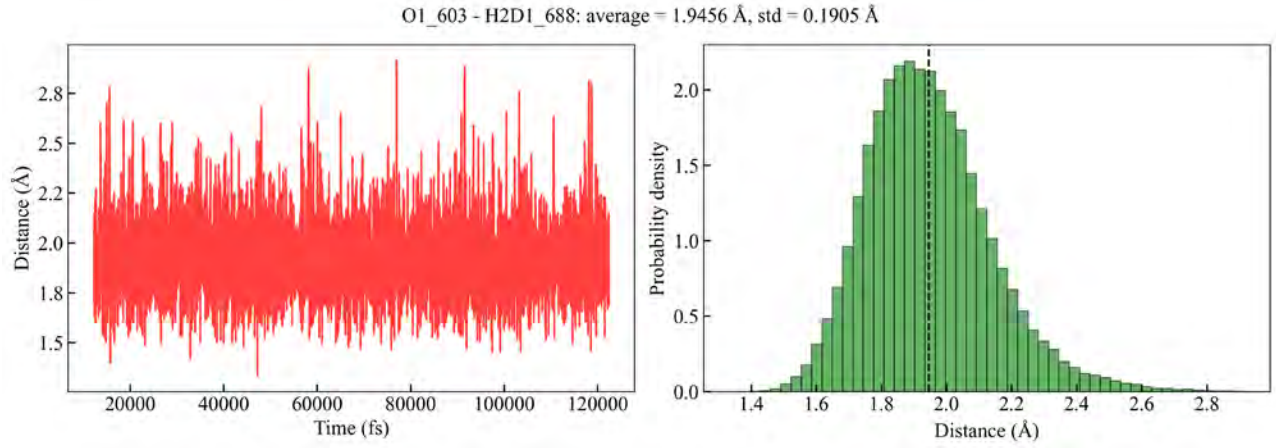
O1_602 - H2D1_685

Average distance = 1.9445 Å; standard deviation = 0.1836 Å; number of points = 110177



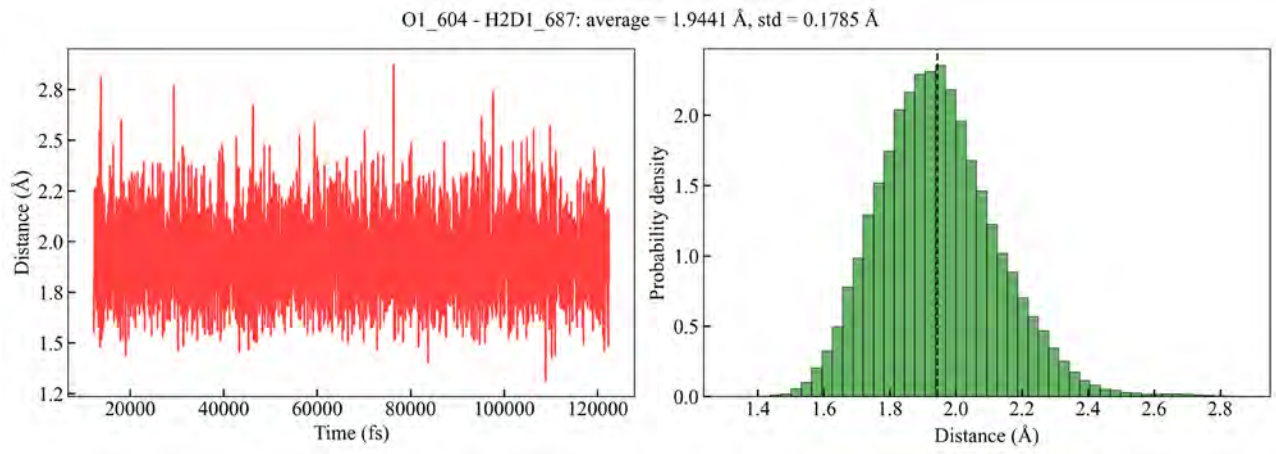
O1_603 - H2D1_688

Average distance = 1.9456 Å; standard deviation = 0.1905 Å; number of points = 110177



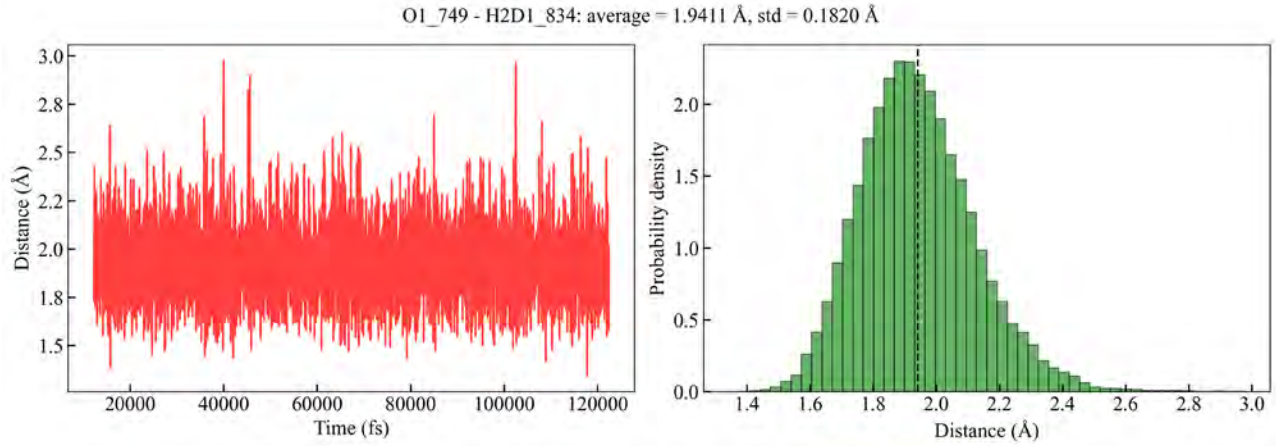
O1_604 - H2D1_687

Average distance = 1.9441 Å; standard deviation = 0.1785 Å; number of points = 110177



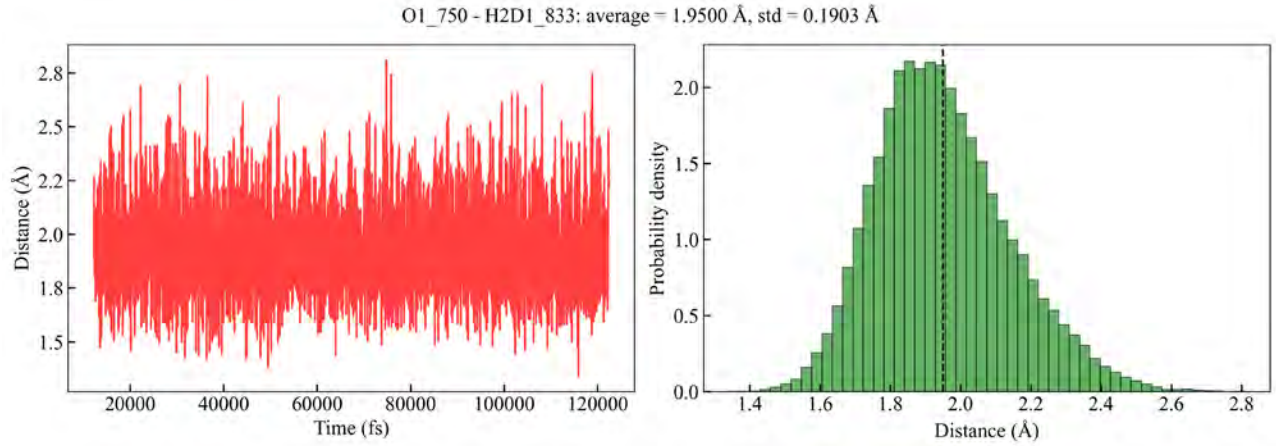
O1_749 - H2D1_834

Average distance = 1.9411 Å; standard deviation = 0.1820 Å; number of points = 110177



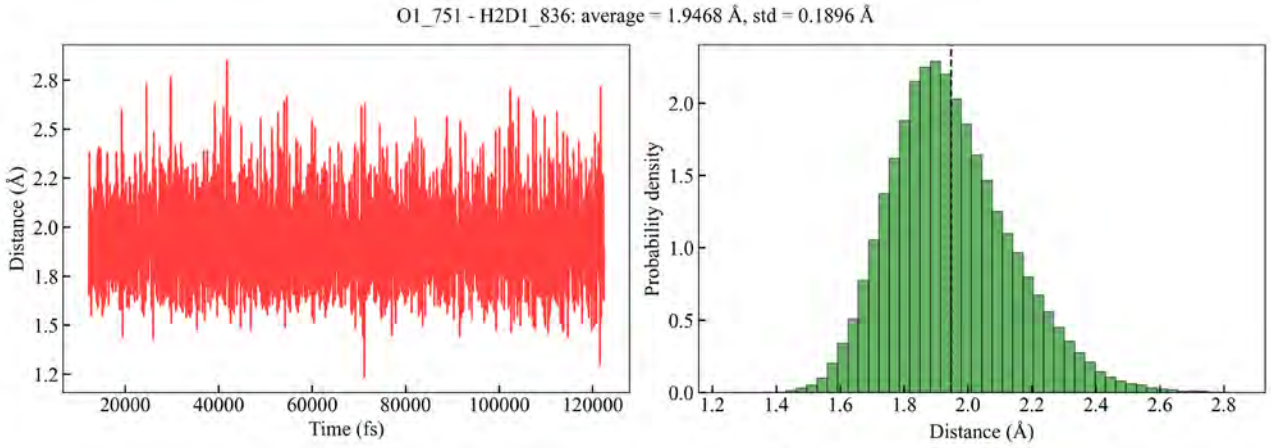
O1_750 - H2D1_833

Average distance = 1.9500 Å; standard deviation = 0.1903 Å; number of points = 110177



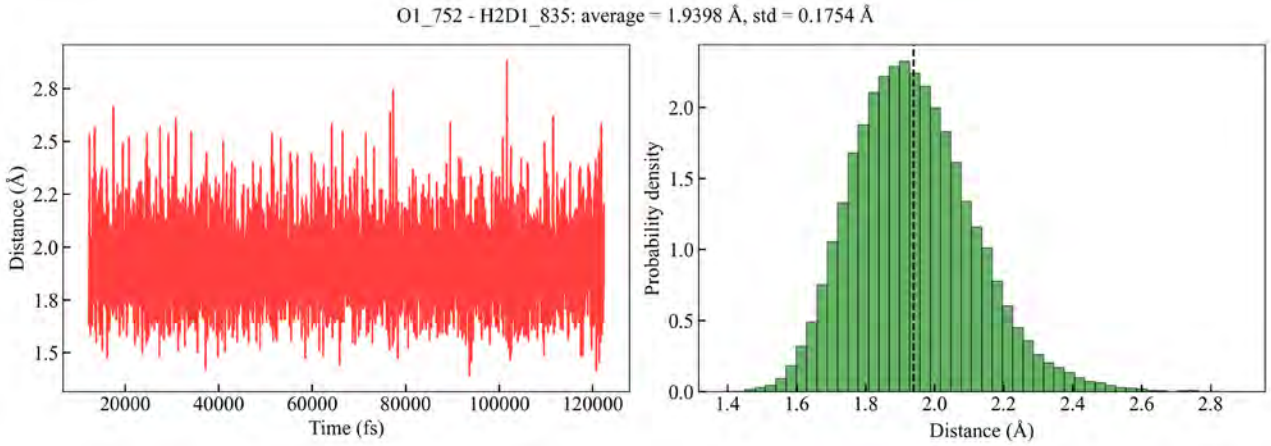
O1_751 - H2D1_836

Average distance = 1.9468 Å; standard deviation = 0.1896 Å; number of points = 110177



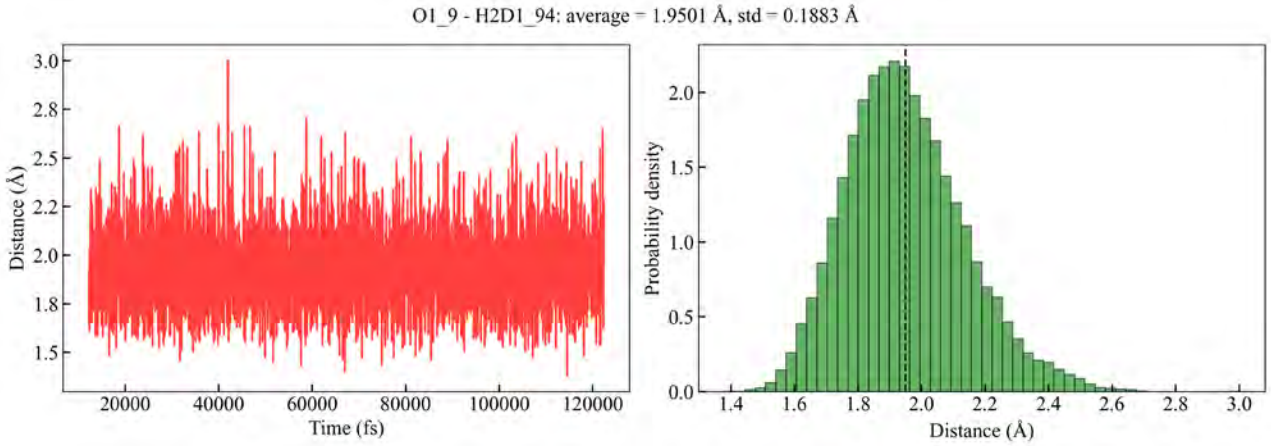
O1_752 - H2D1_835

Average distance = 1.9398 Å; standard deviation = 0.1754 Å; number of points = 110177



O1_9 - H2D1_94

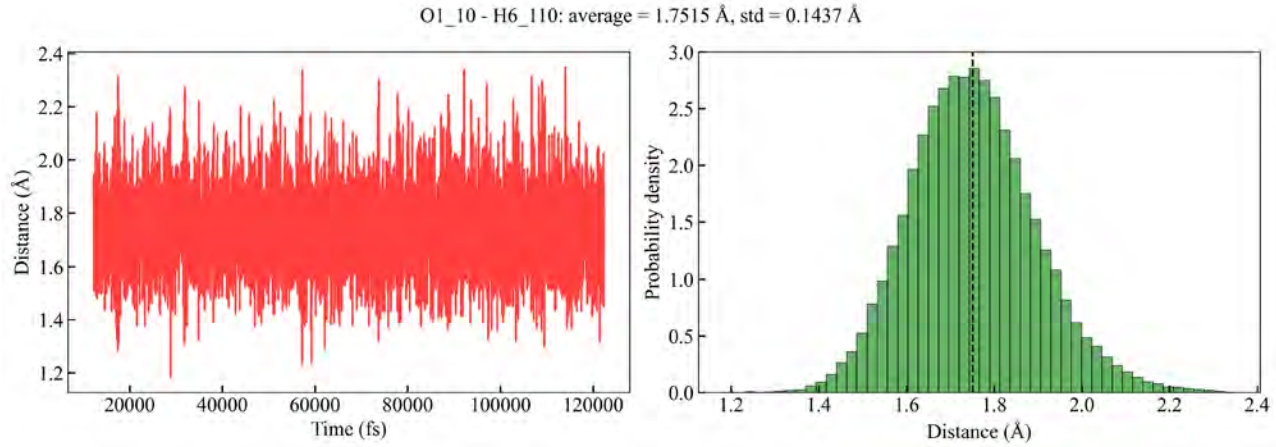
Average distance = 1.9501 Å; standard deviation = 0.1883 Å; number of points = 110177



O1 - H6

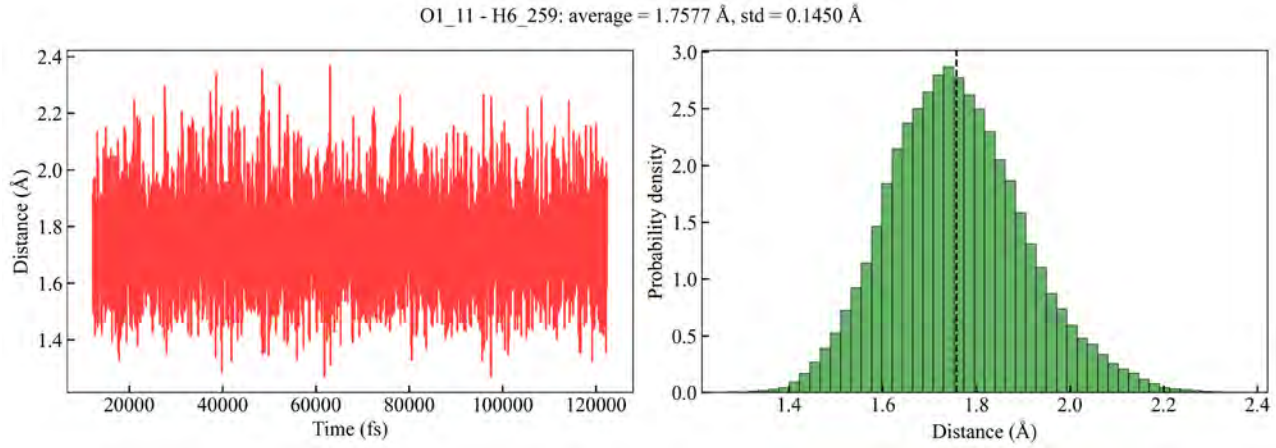
O1_10 - H6_110

Average distance = 1.7515 Å; standard deviation = 0.1437 Å; number of points = 110177



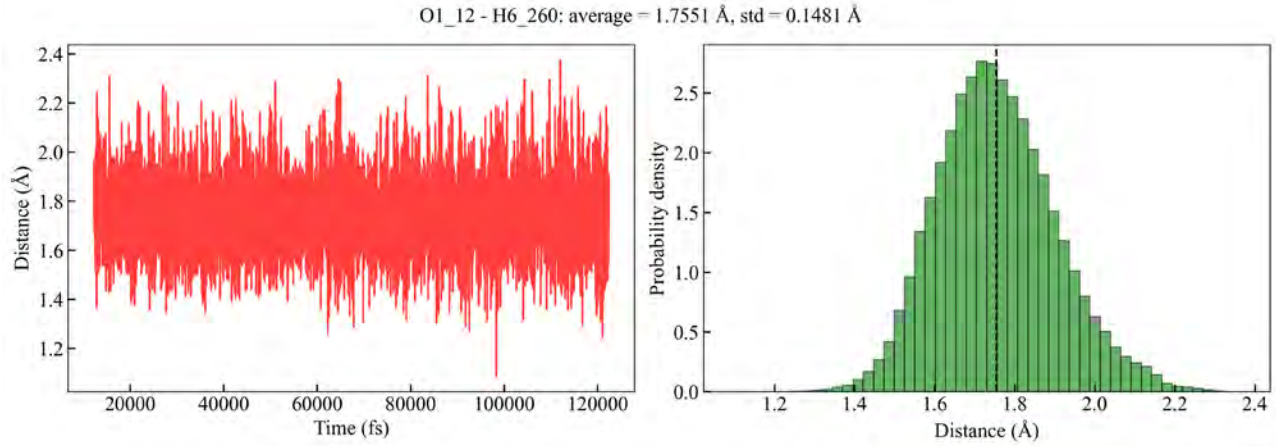
O1_11 - H6_259

Average distance = 1.7577 Å; standard deviation = 0.1450 Å; number of points = 110177



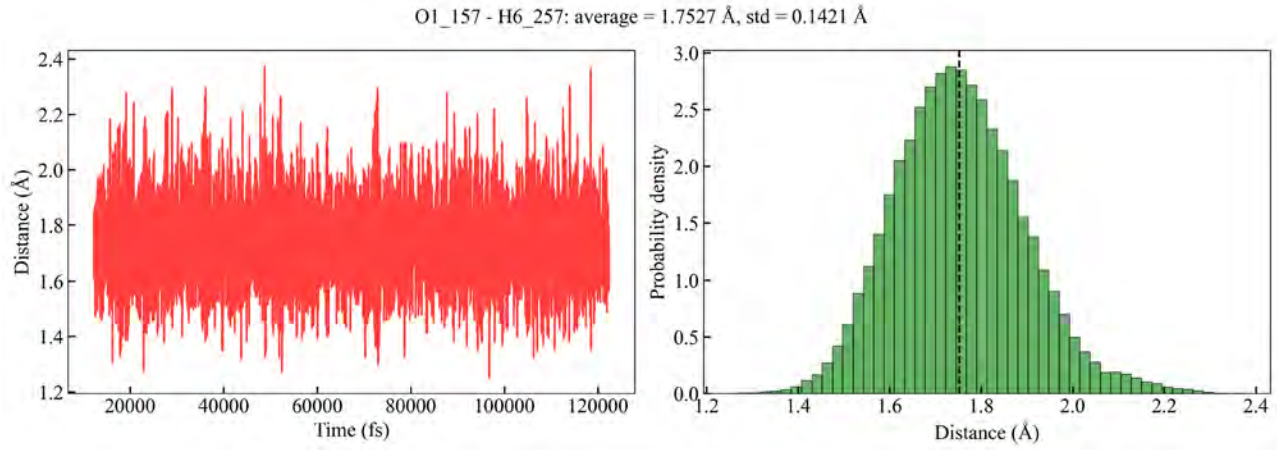
O1_12 - H6_260

Average distance = 1.7551 Å; standard deviation = 0.1481 Å; number of points = 110177



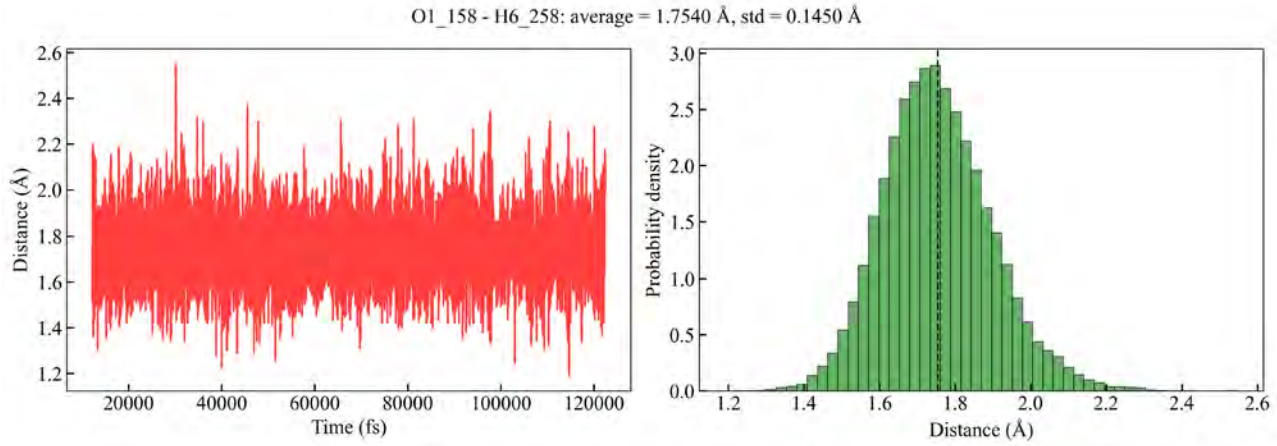
O1_157 - H6_257

Average distance = 1.7527 Å; standard deviation = 0.1421 Å; number of points = 110177



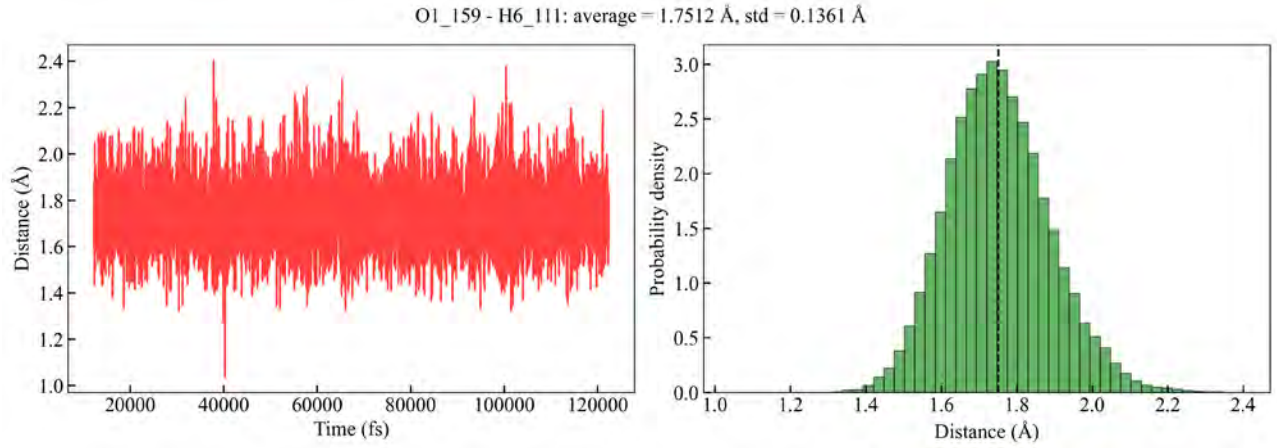
O1_158 - H6_258

Average distance = 1.7540 Å; standard deviation = 0.1450 Å; number of points = 110177



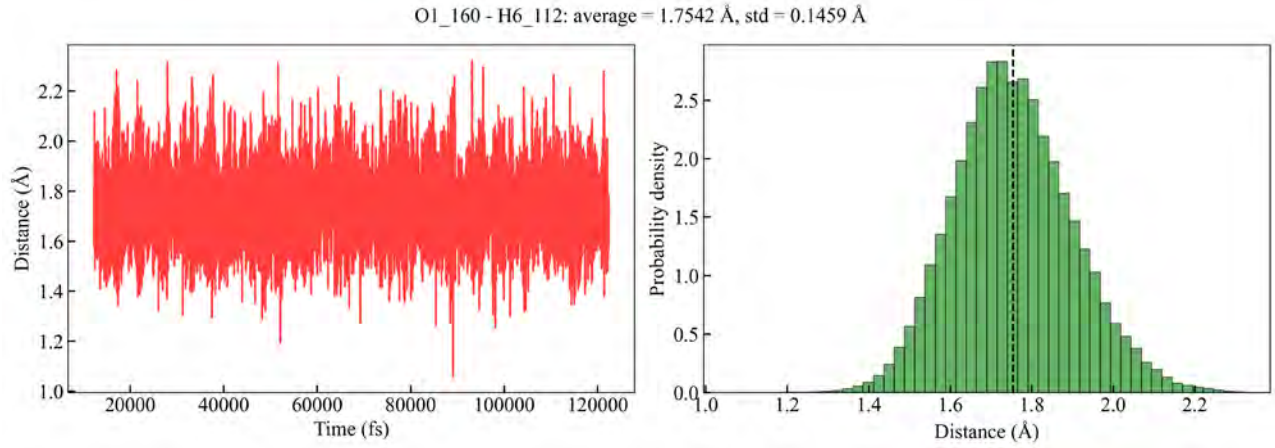
O1_159 - H6_111

Average distance = 1.7512 Å; standard deviation = 0.1361 Å; number of points = 110177



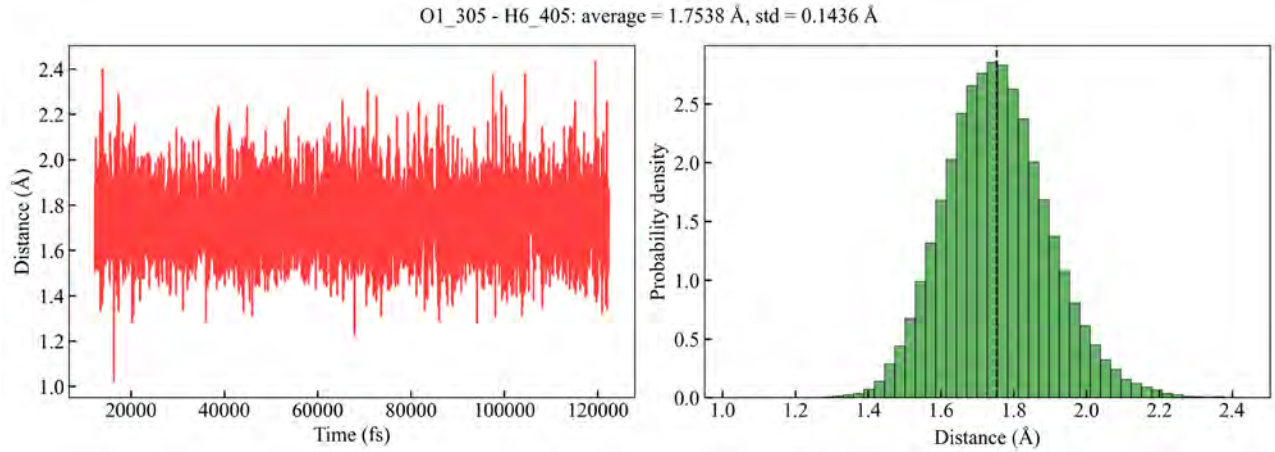
O1_160 - H6_112

Average distance = 1.7542 Å; standard deviation = 0.1459 Å; number of points = 110177



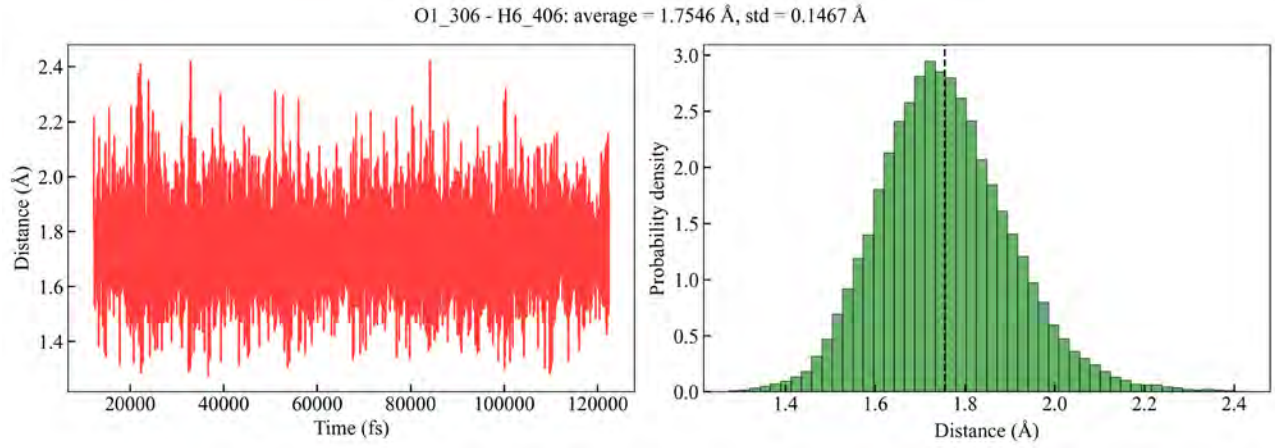
O1_305 - H6_405

Average distance = 1.7538 Å; standard deviation = 0.1436 Å; number of points = 110177



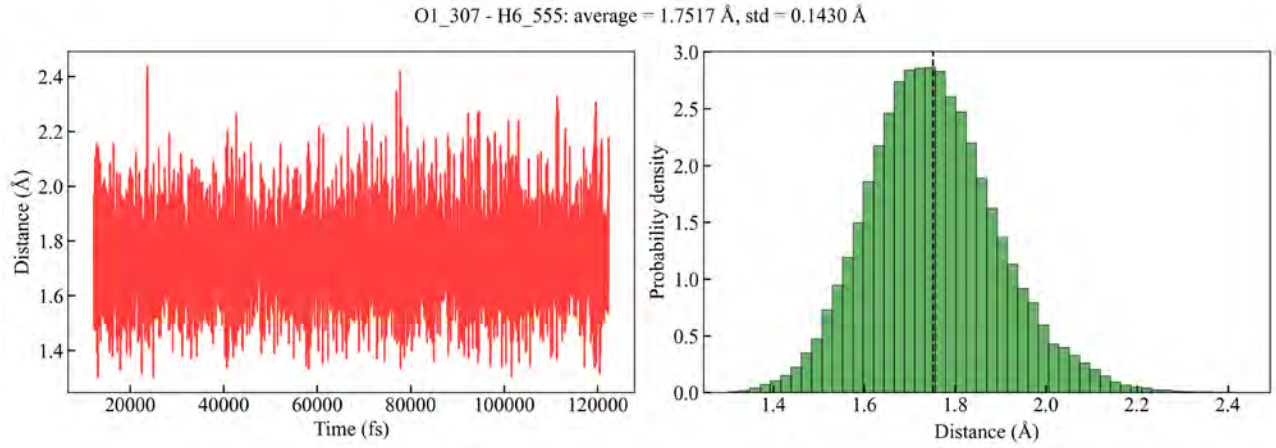
O1_306 - H6_406

Average distance = 1.7546 Å; standard deviation = 0.1467 Å; number of points = 110177



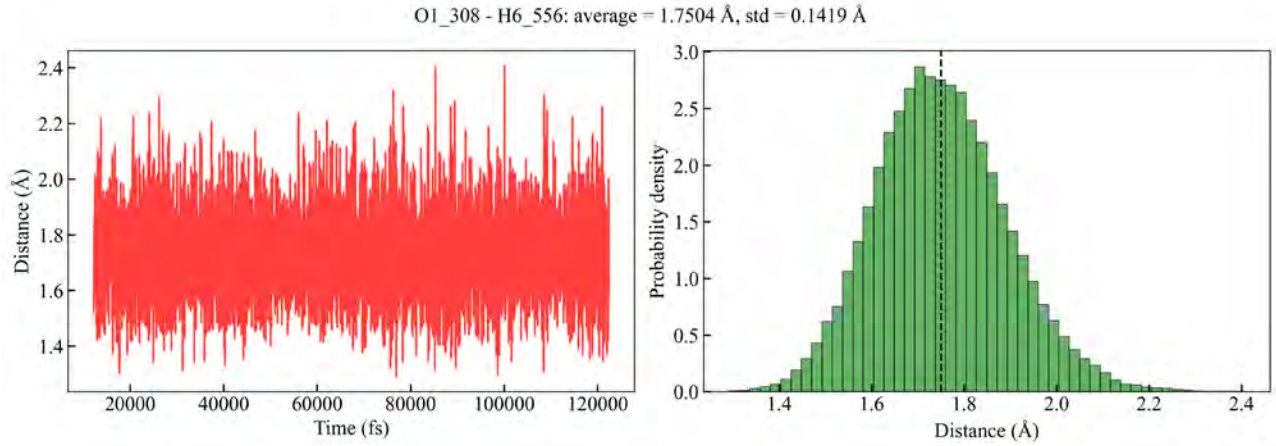
O1_307 - H6_555

Average distance = 1.7517 Å; standard deviation = 0.1430 Å; number of points = 110177



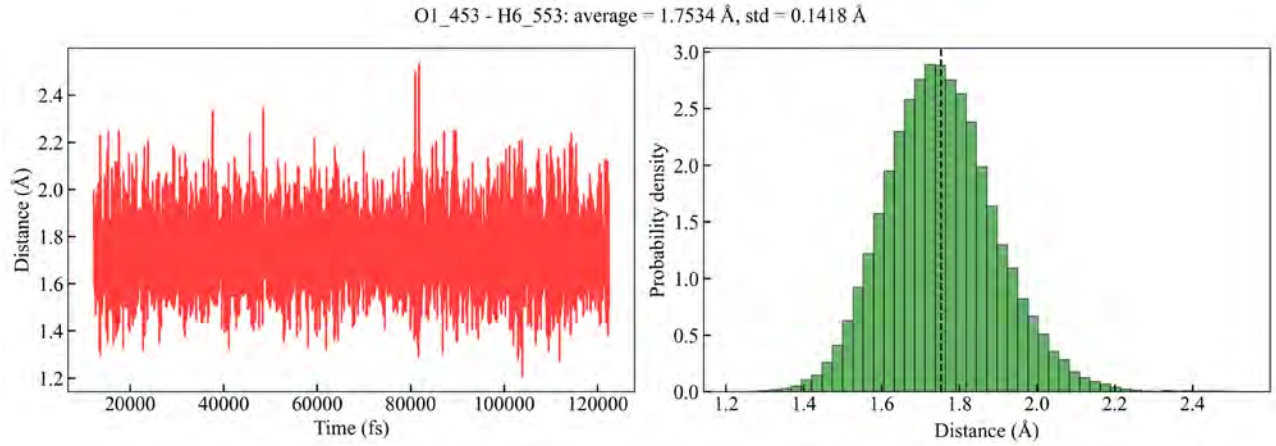
O1_308 - H6_556

Average distance = 1.7504 Å; standard deviation = 0.1419 Å; number of points = 110177



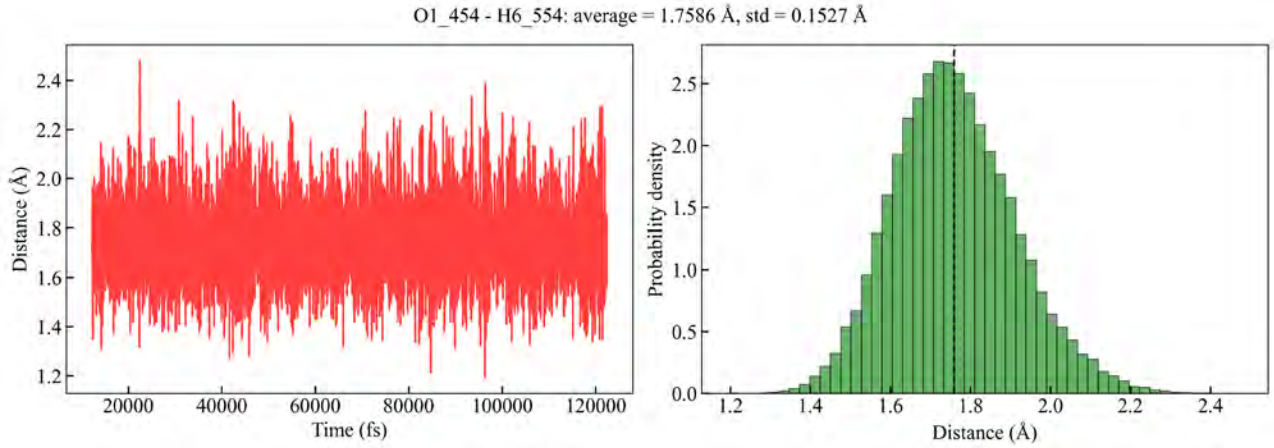
O1_453 - H6_553

Average distance = 1.7534 Å; standard deviation = 0.1418 Å; number of points = 110177



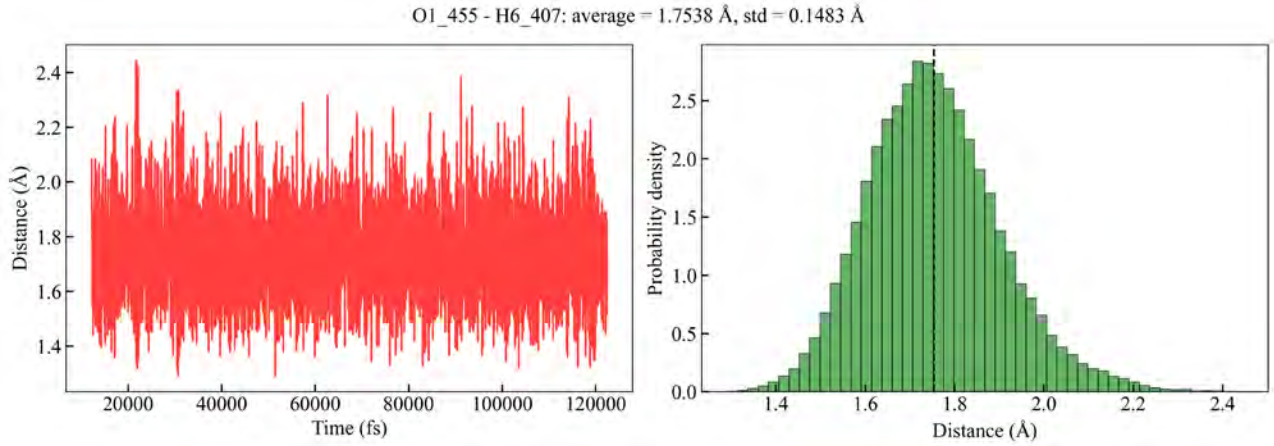
O1_454 - H6_554

Average distance = 1.7586 Å; standard deviation = 0.1527 Å; number of points = 110177



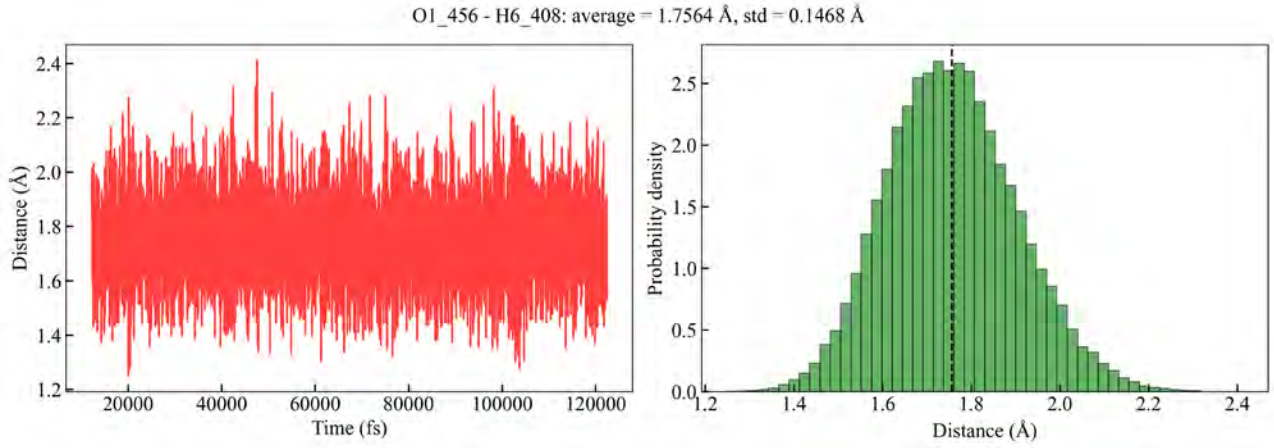
O1_455 - H6_407

Average distance = 1.7538 Å; standard deviation = 0.1483 Å; number of points = 110177



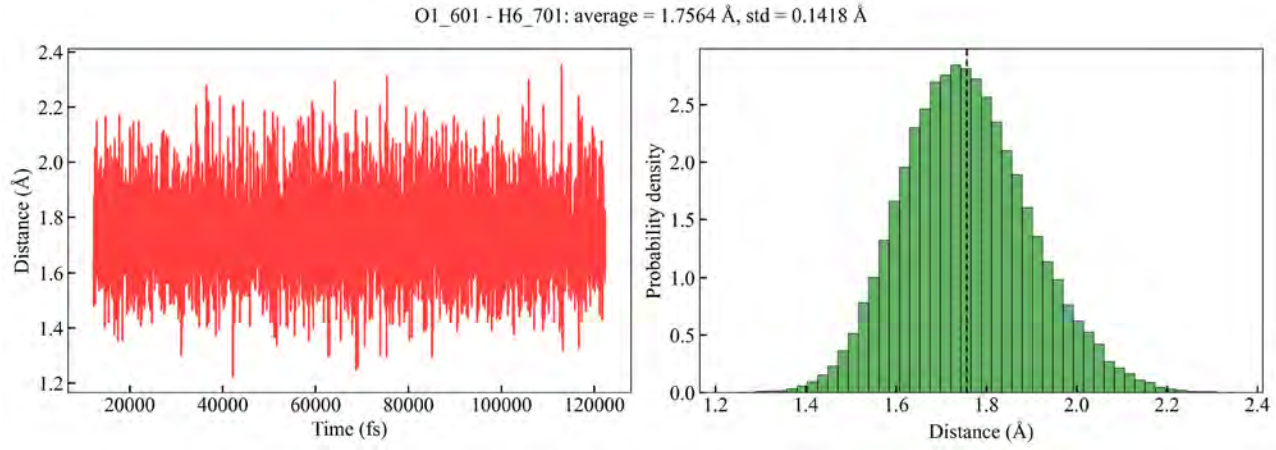
O1_456 - H6_408

Average distance = 1.7564 Å; standard deviation = 0.1468 Å; number of points = 110177



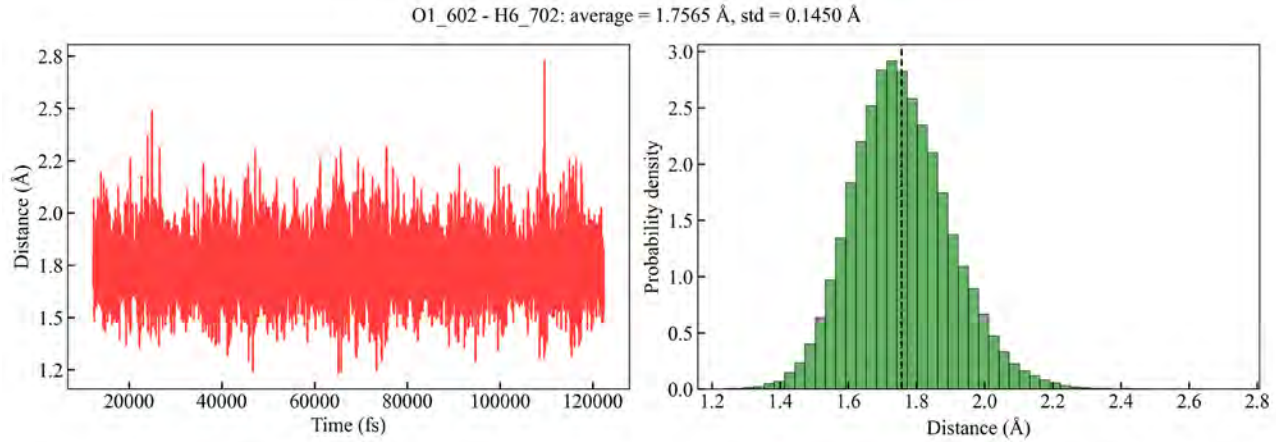
O1_601 - H6_701

Average distance = 1.7564 Å; standard deviation = 0.1418 Å; number of points = 110177



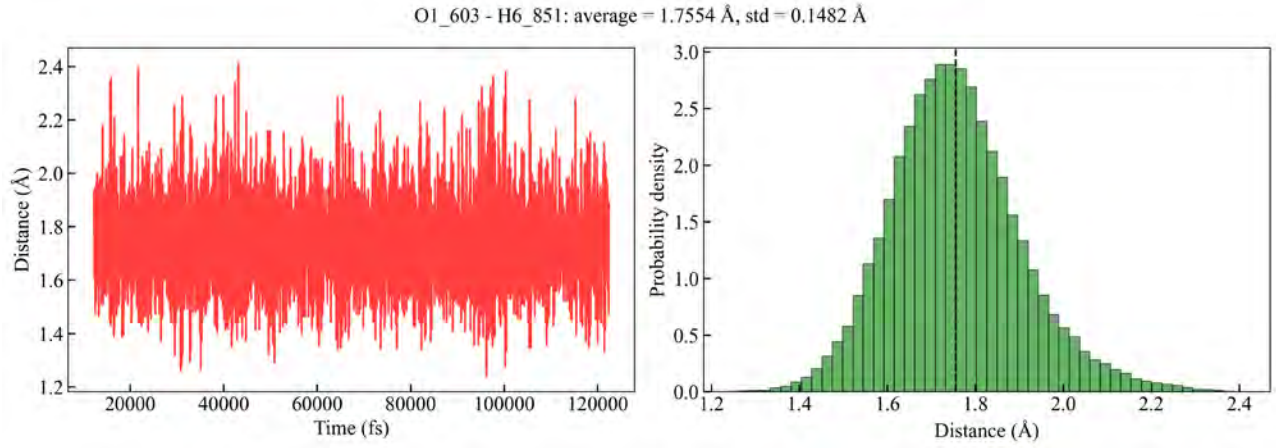
O1_602 - H6_702

Average distance = 1.7565 Å; standard deviation = 0.1450 Å; number of points = 110177



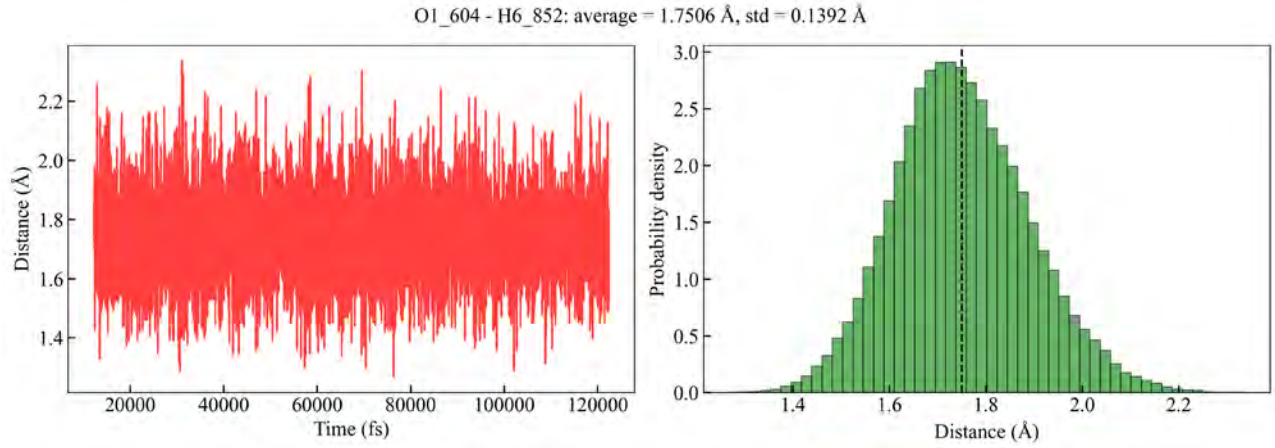
O1_603 - H6_851

Average distance = 1.7554 Å; standard deviation = 0.1482 Å; number of points = 110177



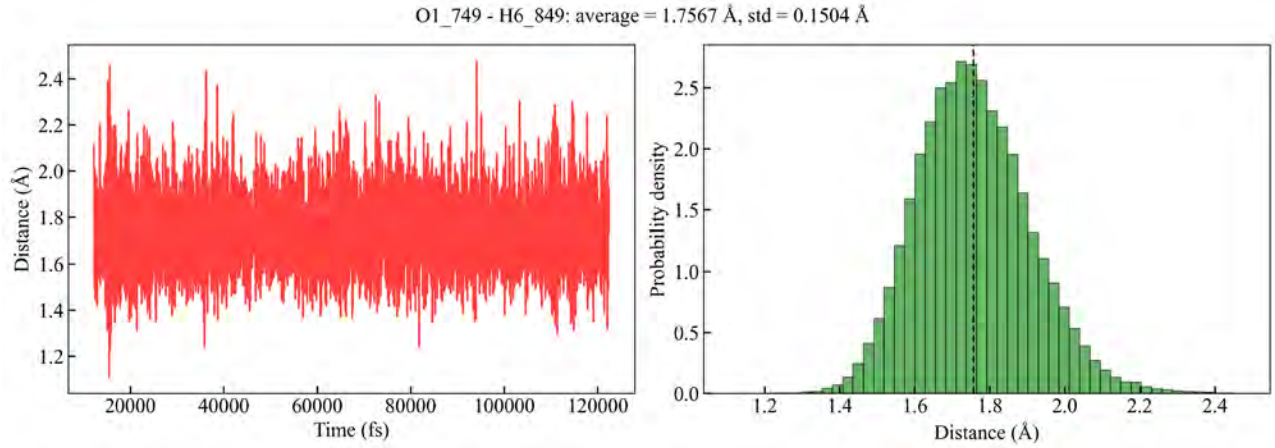
O1_604 - H6_852

Average distance = 1.7506 Å; standard deviation = 0.1392 Å; number of points = 110177



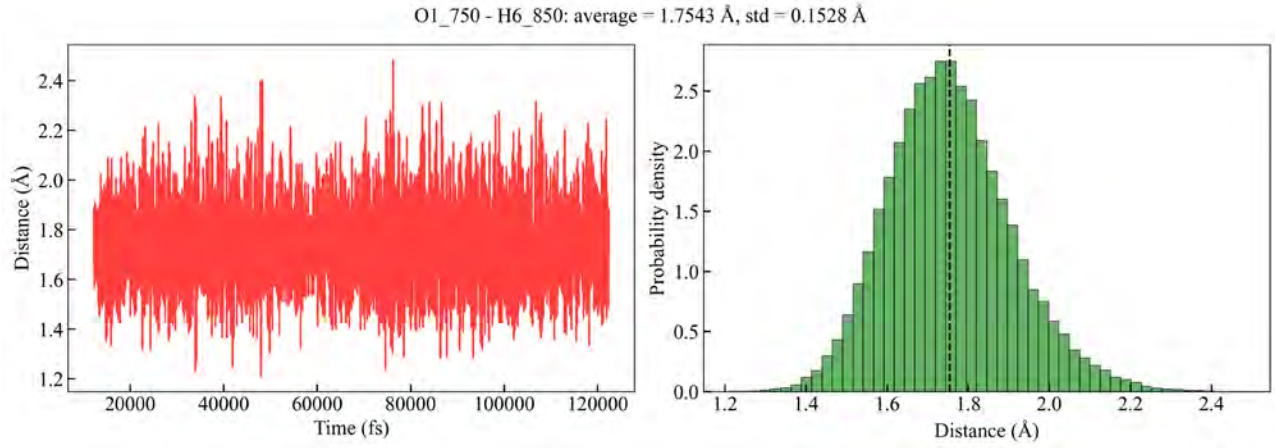
O1_749 - H6_849

Average distance = 1.7567 Å; standard deviation = 0.1504 Å; number of points = 110177



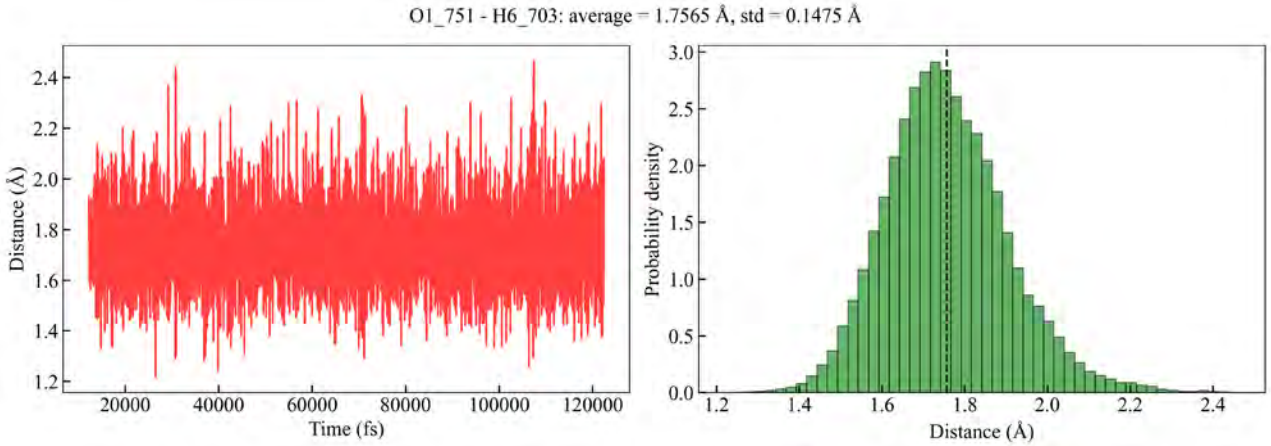
O1_750 - H6_850

Average distance = 1.7543 Å; standard deviation = 0.1528 Å; number of points = 110177



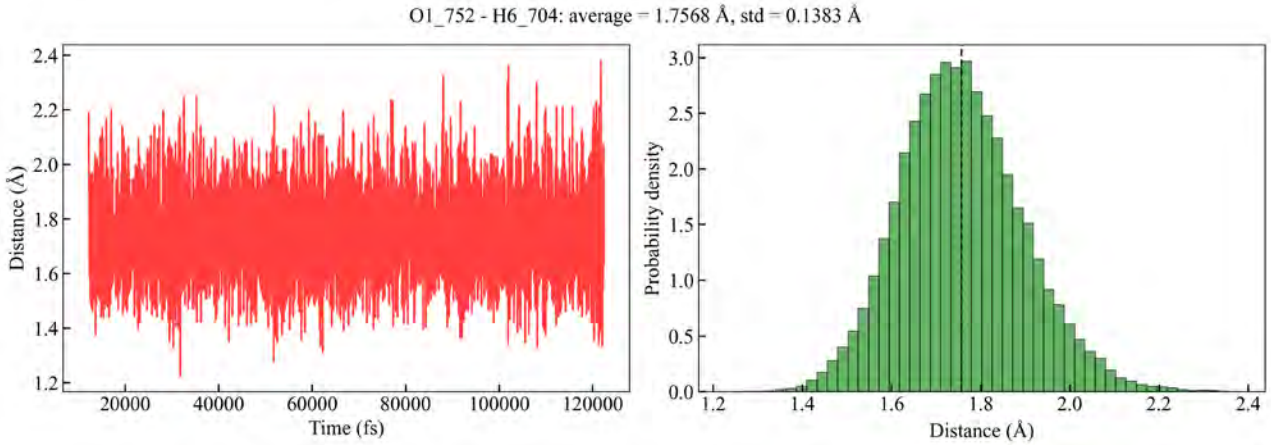
O1_751 - H6_703

Average distance = 1.7565 Å; standard deviation = 0.1475 Å; number of points = 110177



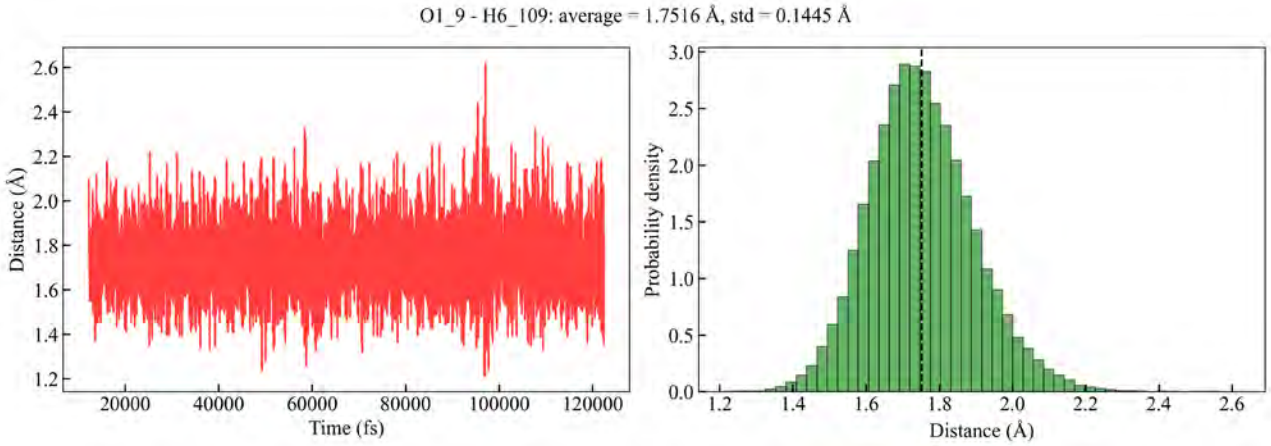
O1_752 - H6_704

Average distance = 1.7568 Å; standard deviation = 0.1383 Å; number of points = 110177



O1_9 - H6_109

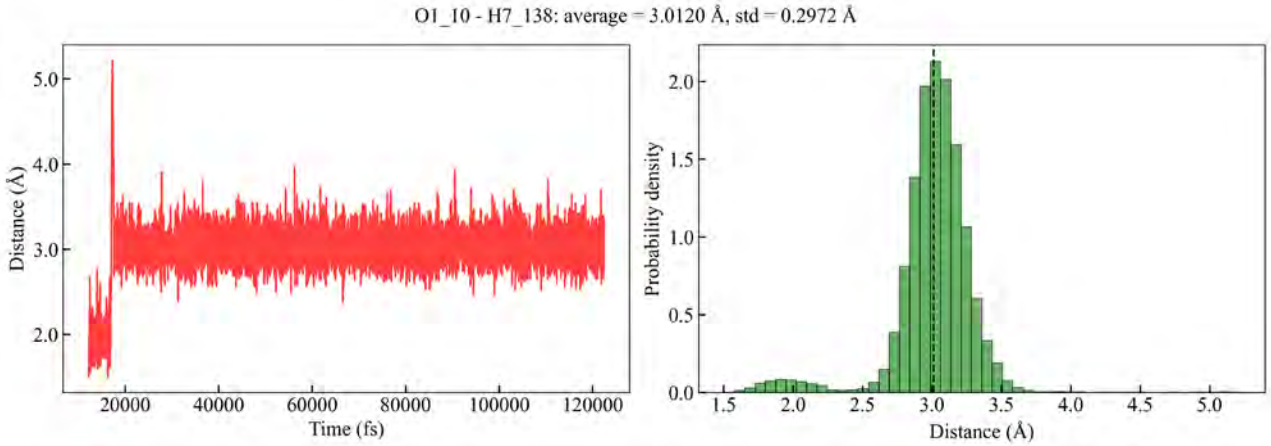
Average distance = 1.7516 Å; standard deviation = 0.1445 Å; number of points = 110177



O1 - H7

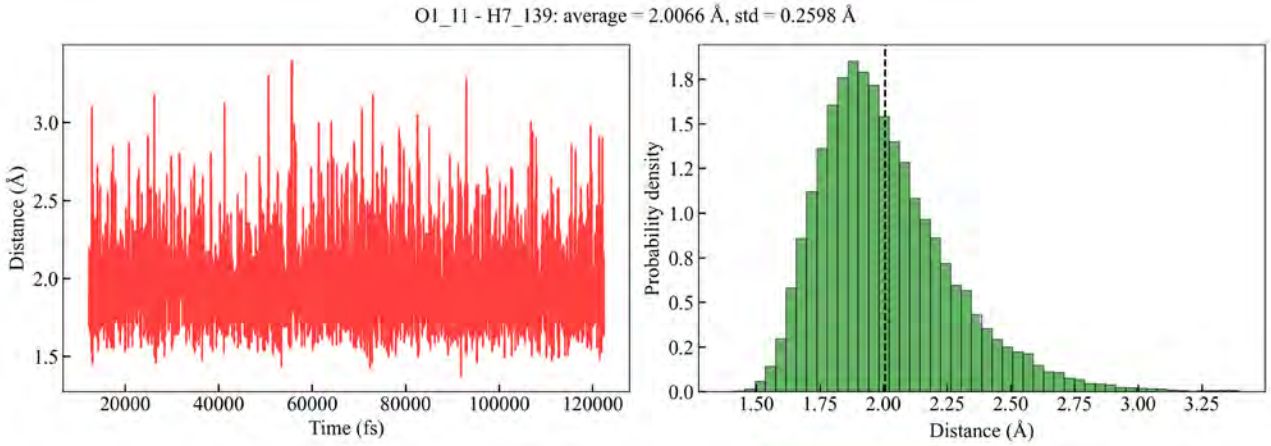
O1_10 - H7_138

Average distance = 3.0120 Å; standard deviation = 0.2972 Å; number of points = 110177



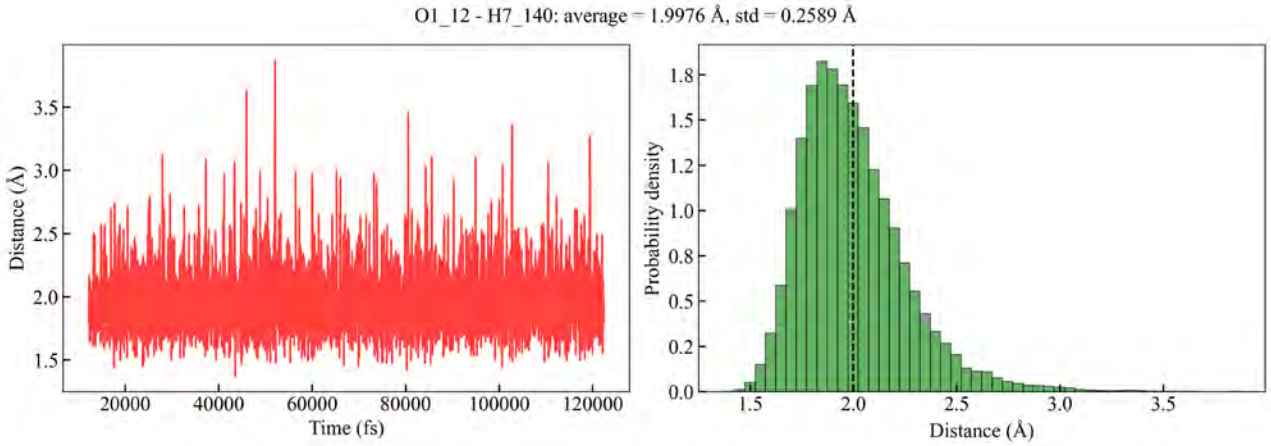
O1_11 - H7_139

Average distance = 2.0066 Å; standard deviation = 0.2598 Å; number of points = 110177



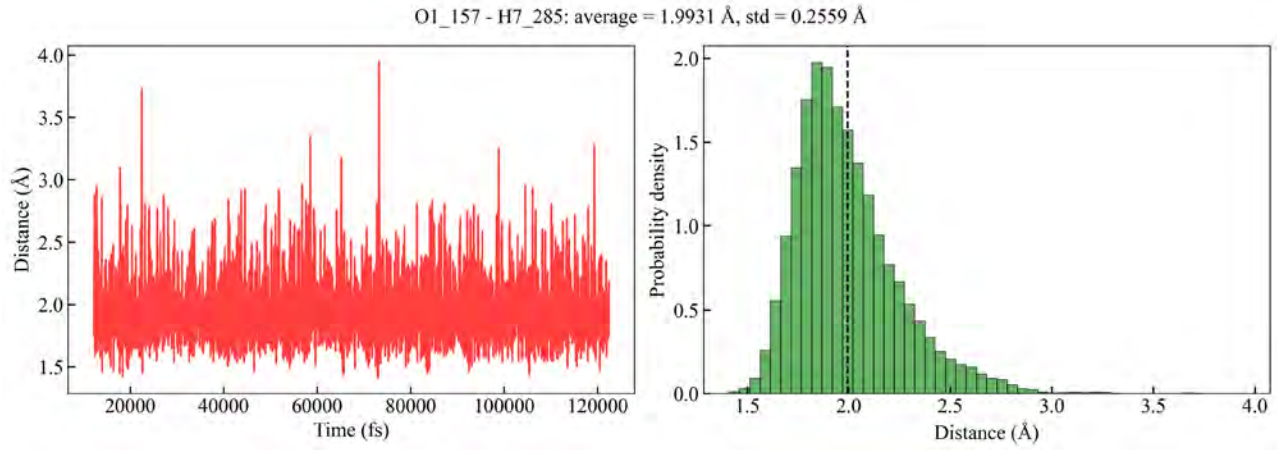
O1_12 - H7_140

Average distance = 1.9976 Å; standard deviation = 0.2589 Å; number of points = 110177



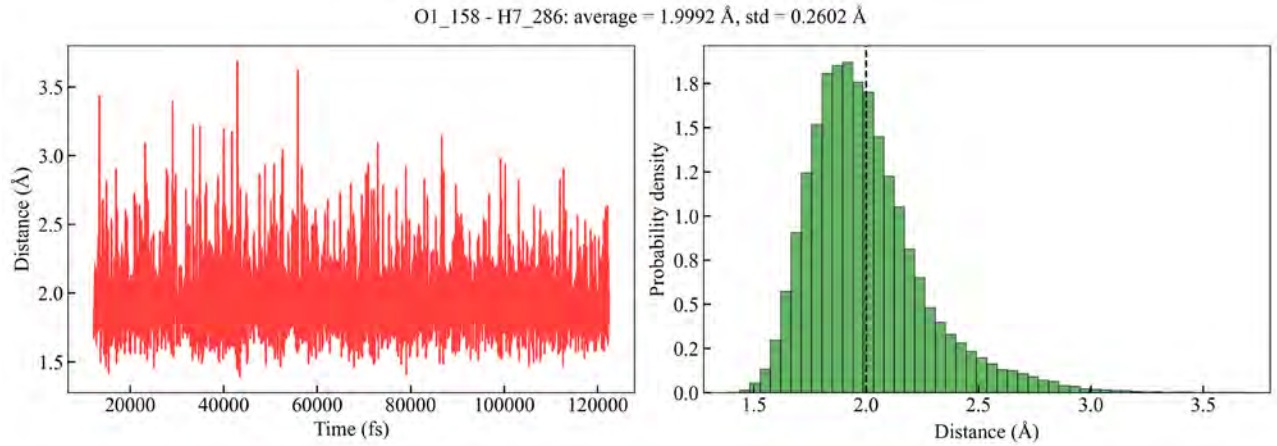
O1_157 - H7_285

Average distance = 1.9931 Å; standard deviation = 0.2559 Å; number of points = 110177



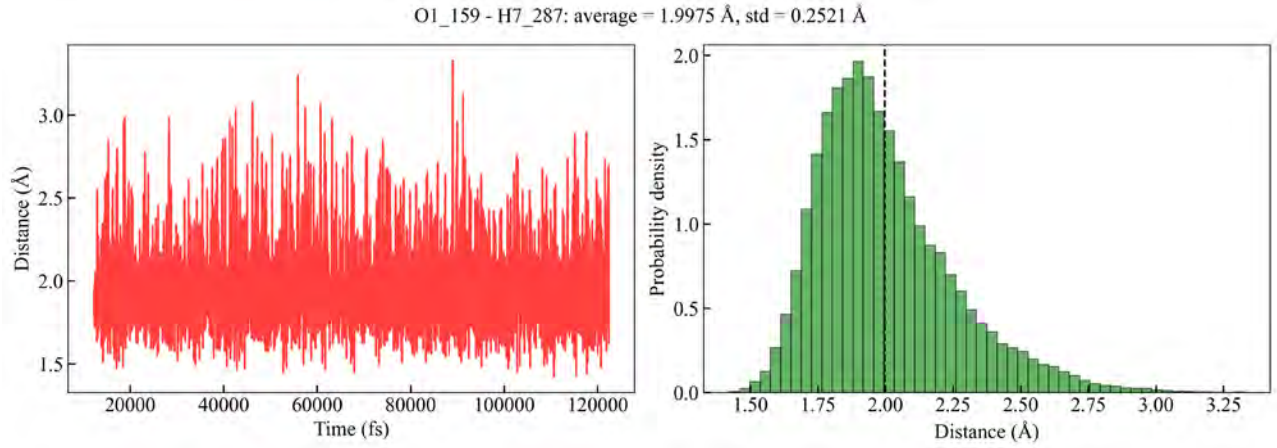
O1_158 - H7_286

Average distance = 1.9992 Å; standard deviation = 0.2602 Å; number of points = 110177



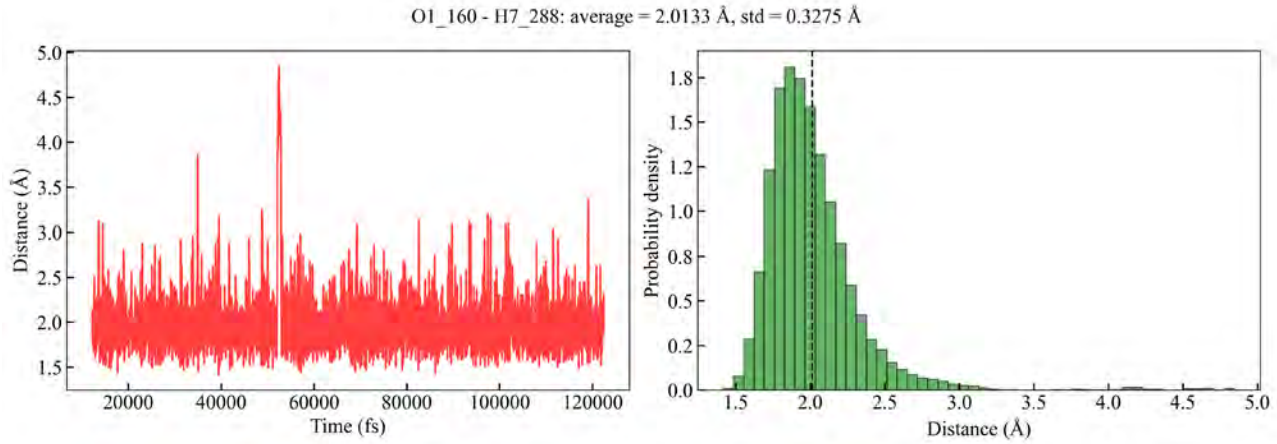
O1_159 - H7_287

Average distance = 1.9975 Å; standard deviation = 0.2521 Å; number of points = 110177



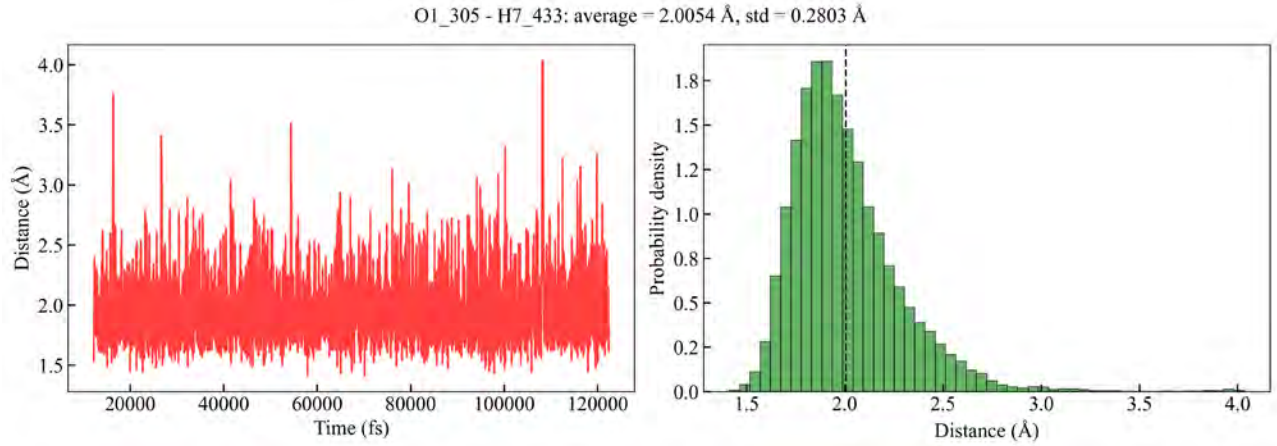
O1_160 - H7_288

Average distance = 2.0133 Å; standard deviation = 0.3275 Å; number of points = 110177



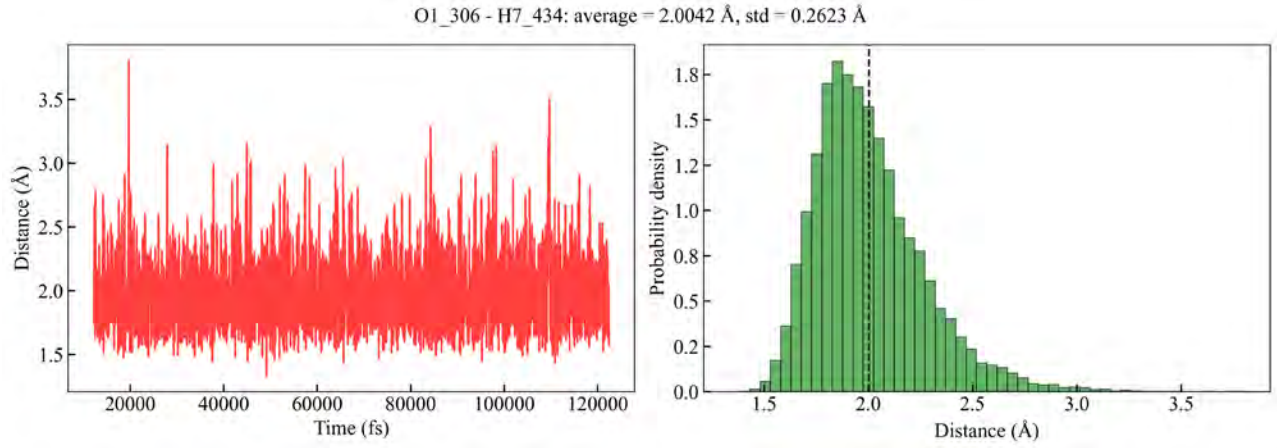
O1_305 - H7_433

Average distance = 2.0054 Å; standard deviation = 0.2803 Å; number of points = 110177



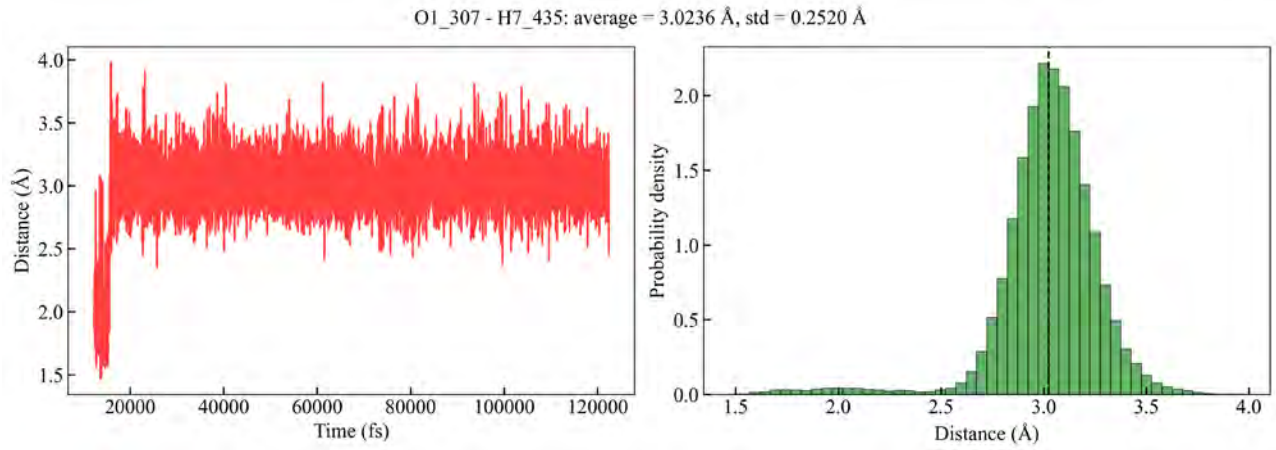
O1_306 - H7_434

Average distance = 2.0042 Å; standard deviation = 0.2623 Å; number of points = 110177



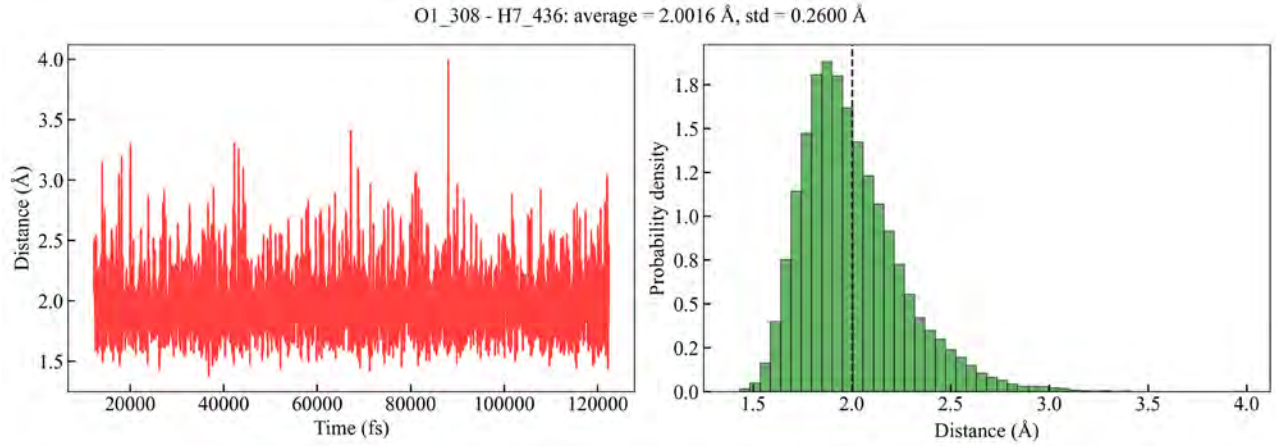
O1_307 - H7_435

Average distance = 3.0236 Å; standard deviation = 0.2520 Å; number of points = 110177



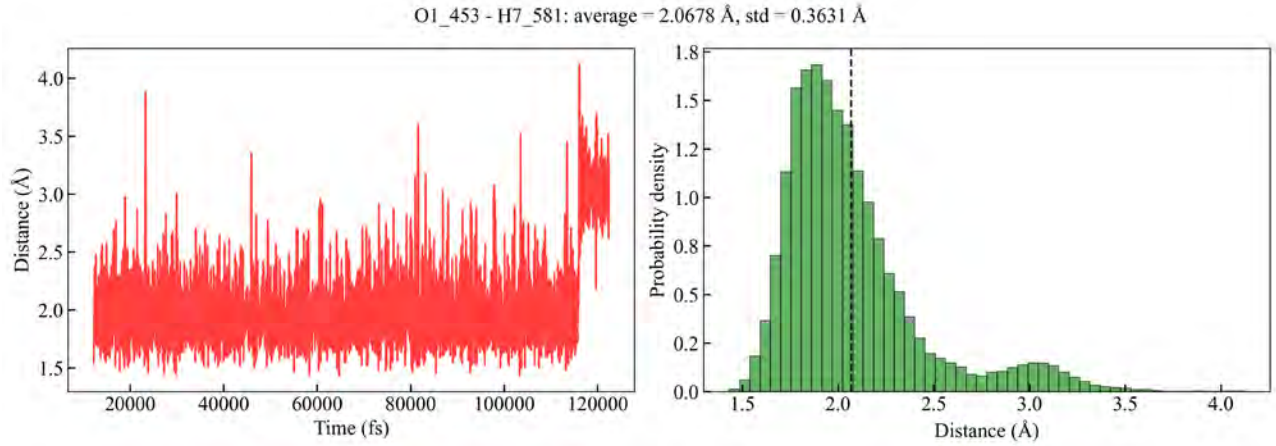
O1_308 - H7_436

Average distance = 2.0016 Å; standard deviation = 0.2600 Å; number of points = 110177



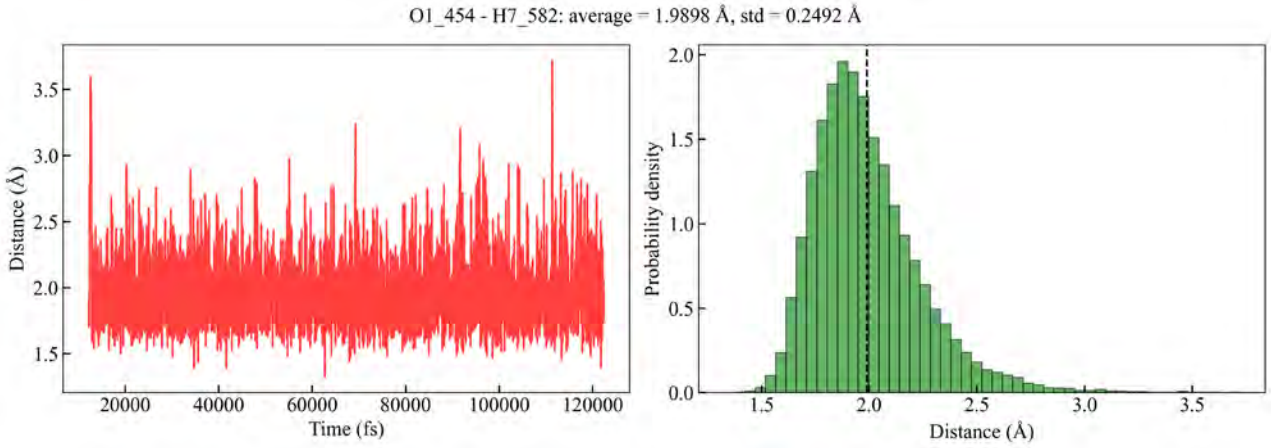
O1_453 - H7_581

Average distance = 2.0678 Å; standard deviation = 0.3631 Å; number of points = 110177



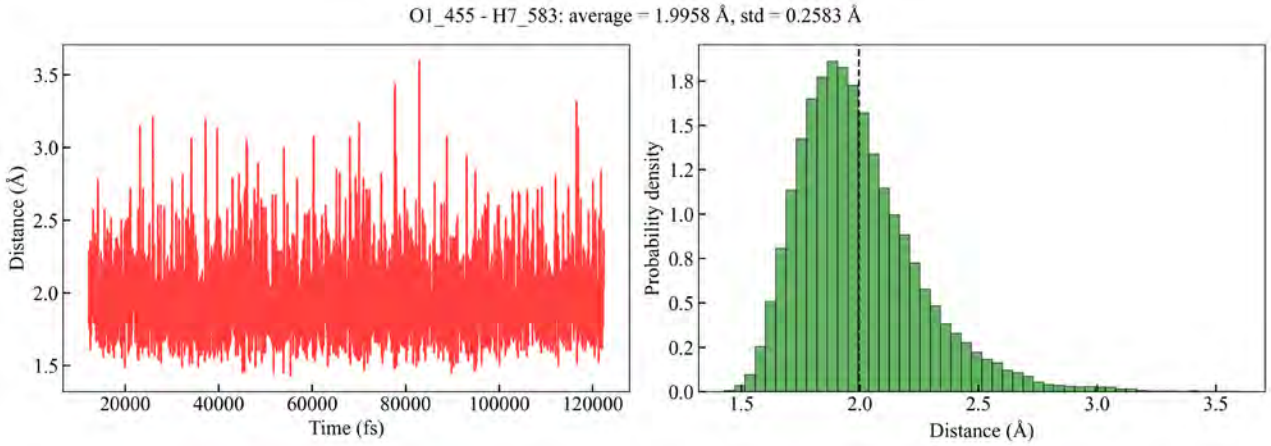
O1_454 - H7_582

Average distance = 1.9898 Å; standard deviation = 0.2492 Å; number of points = 110177



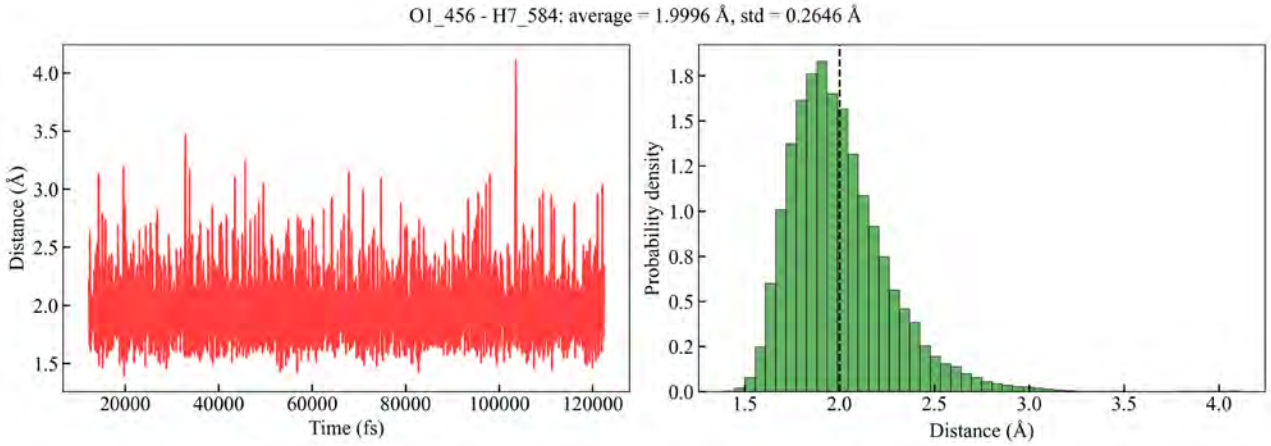
O1_455 - H7_583

Average distance = 1.9958 Å; standard deviation = 0.2583 Å; number of points = 110177



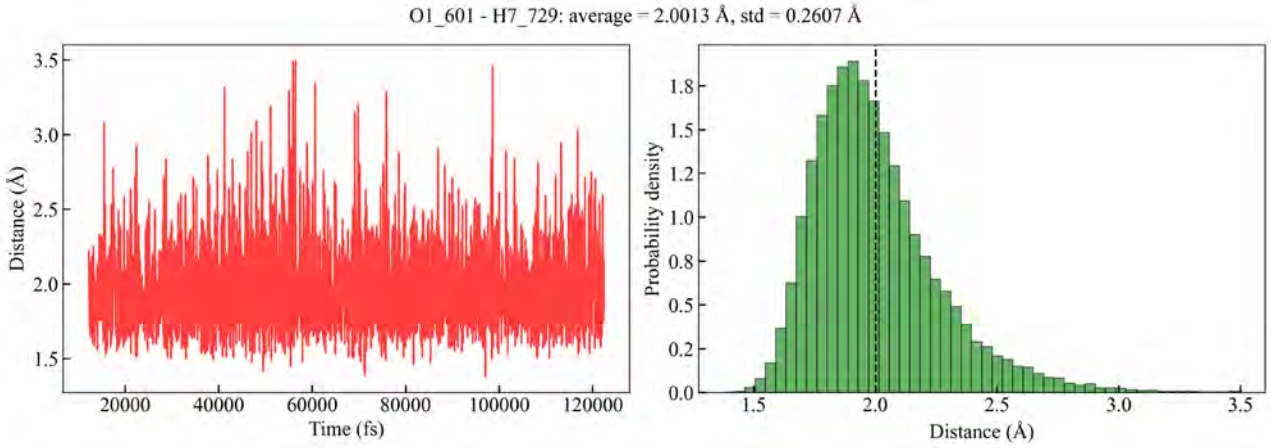
O1_456 - H7_584

Average distance = 1.9996 Å; standard deviation = 0.2646 Å; number of points = 110177



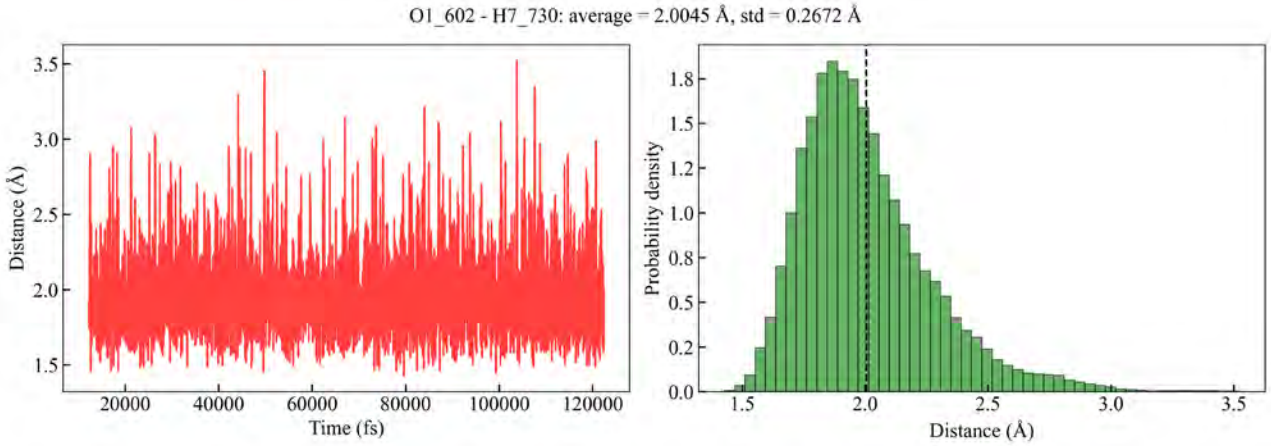
O1_601 - H7_729

Average distance = 2.0013 Å; standard deviation = 0.2607 Å; number of points = 110177



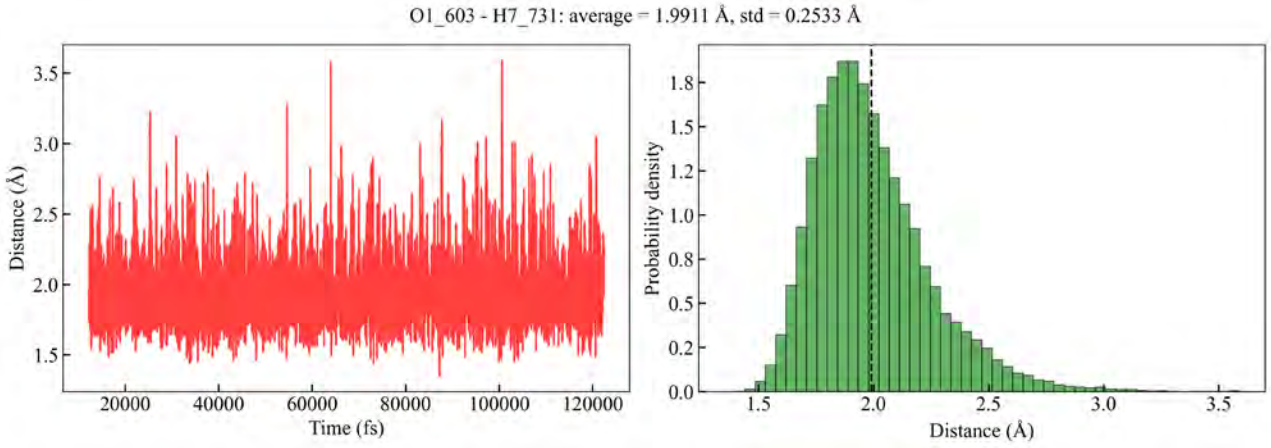
O1_602 - H7_730

Average distance = 2.0045 Å; standard deviation = 0.2672 Å; number of points = 110177



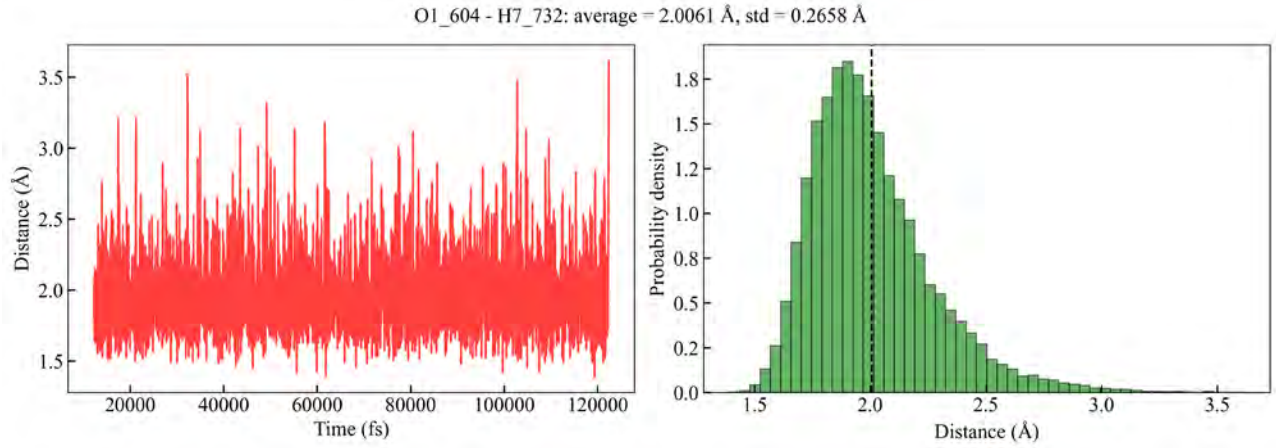
O1_603 - H7_731

Average distance = 1.9911 Å; standard deviation = 0.2533 Å; number of points = 110177



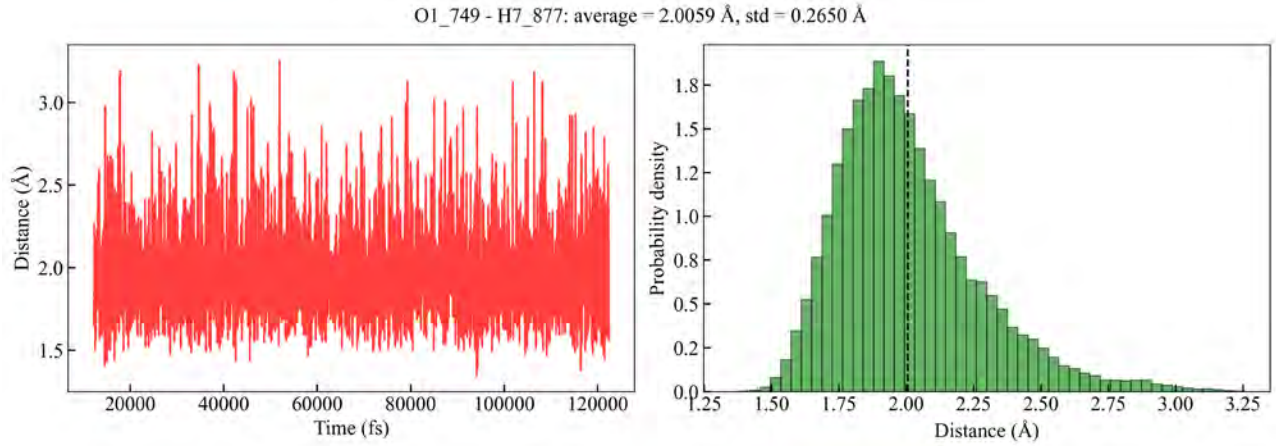
O1_604 - H7_732

Average distance = 2.0061 Å; standard deviation = 0.2658 Å; number of points = 110177



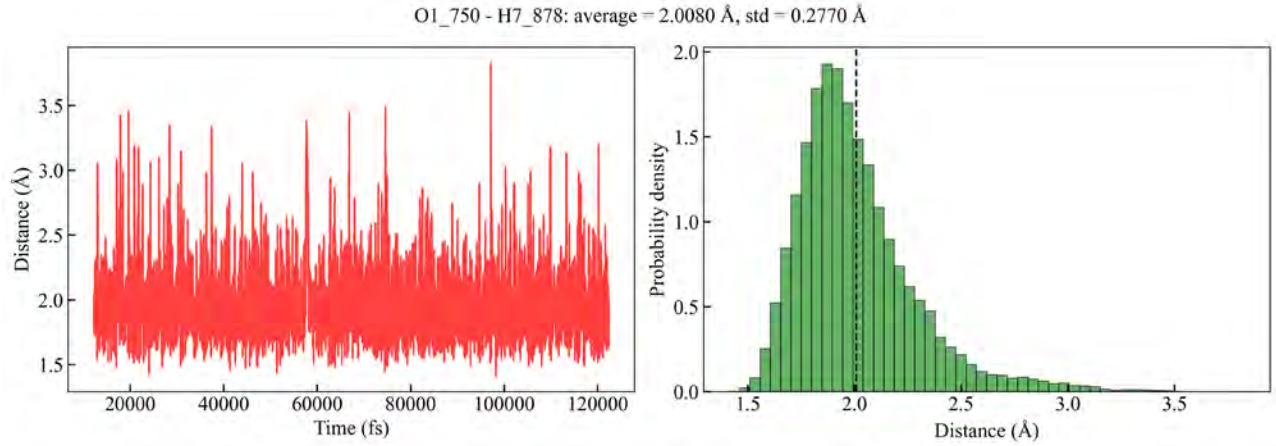
O1_749 - H7_877

Average distance = 2.0059 Å; standard deviation = 0.2650 Å; number of points = 110177



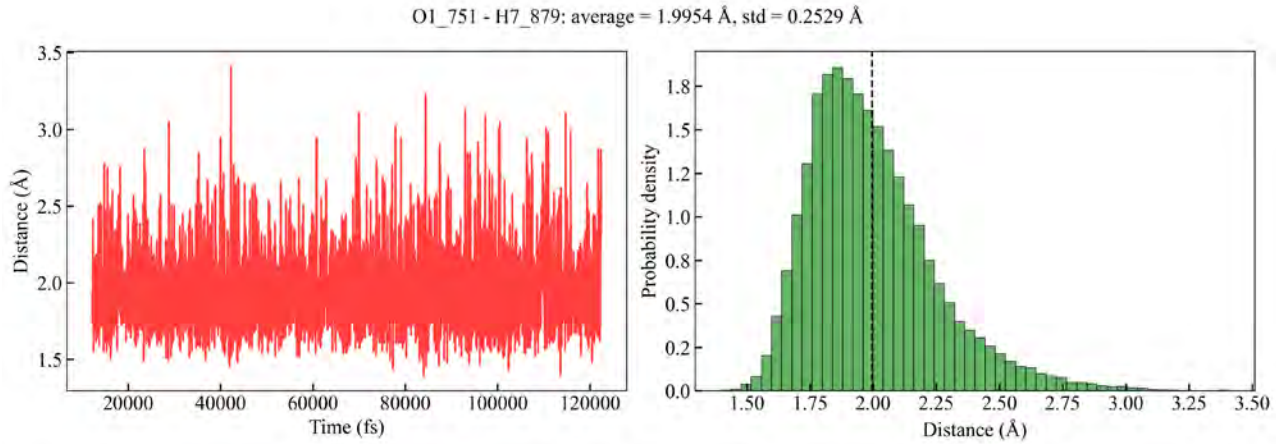
O1_750 - H7_878

Average distance = 2.0080 Å; standard deviation = 0.2770 Å; number of points = 110177



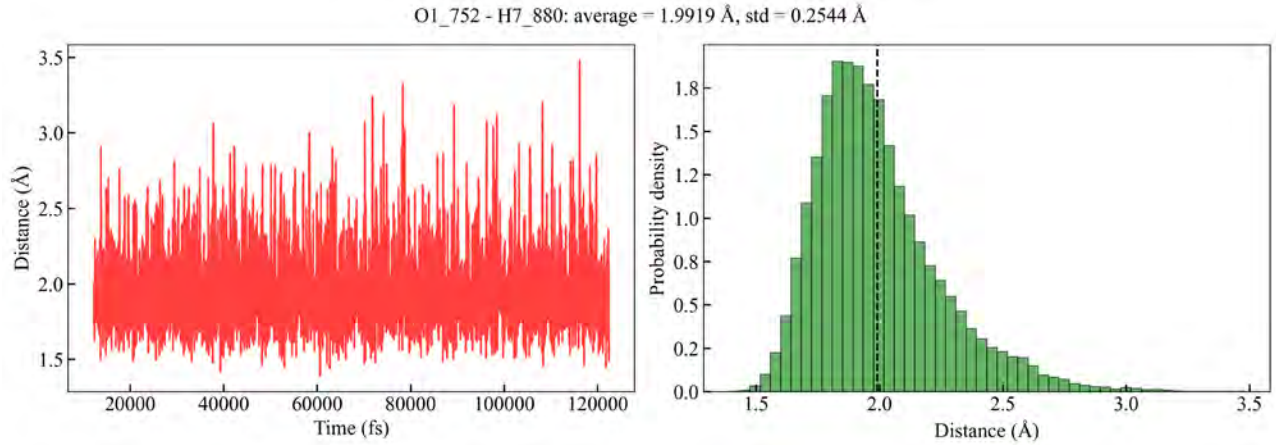
O1_751 - H7_879

Average distance = 1.9954 Å; standard deviation = 0.2529 Å; number of points = 110177



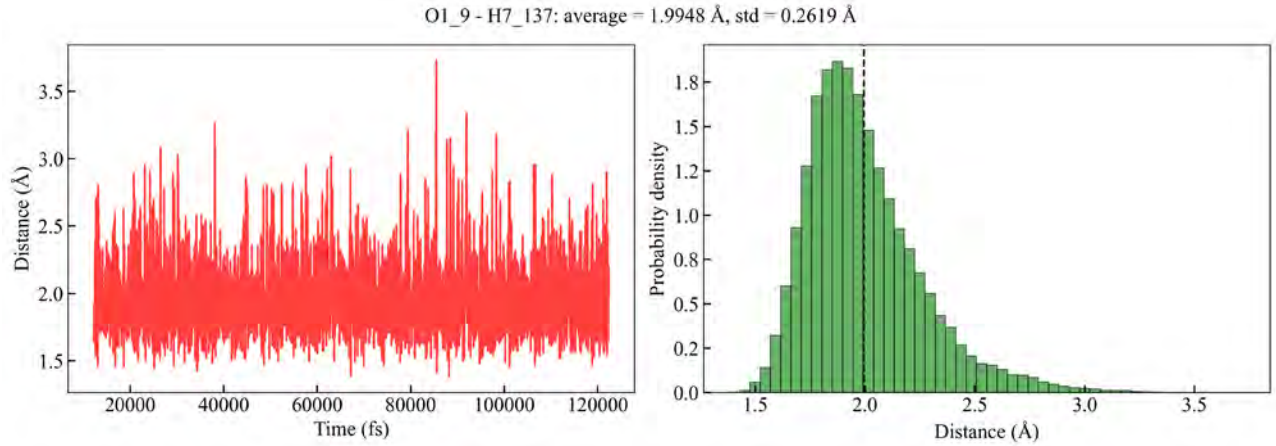
O1_752 - H7_880

Average distance = 1.9919 Å; standard deviation = 0.2544 Å; number of points = 110177



O1_9 - H7_137

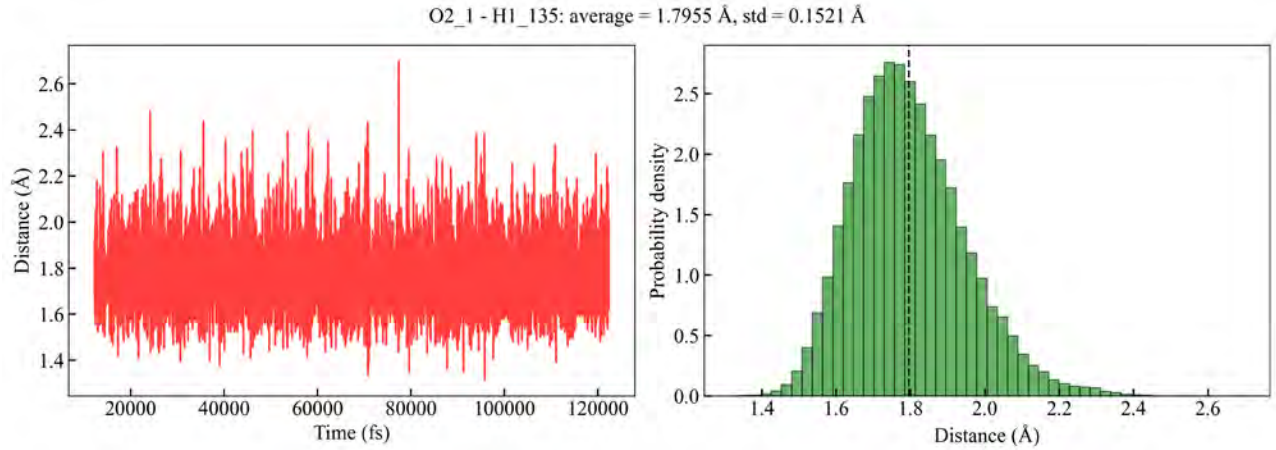
Average distance = 1.9948 Å; standard deviation = 0.2619 Å; number of points = 110177



O2 - H1

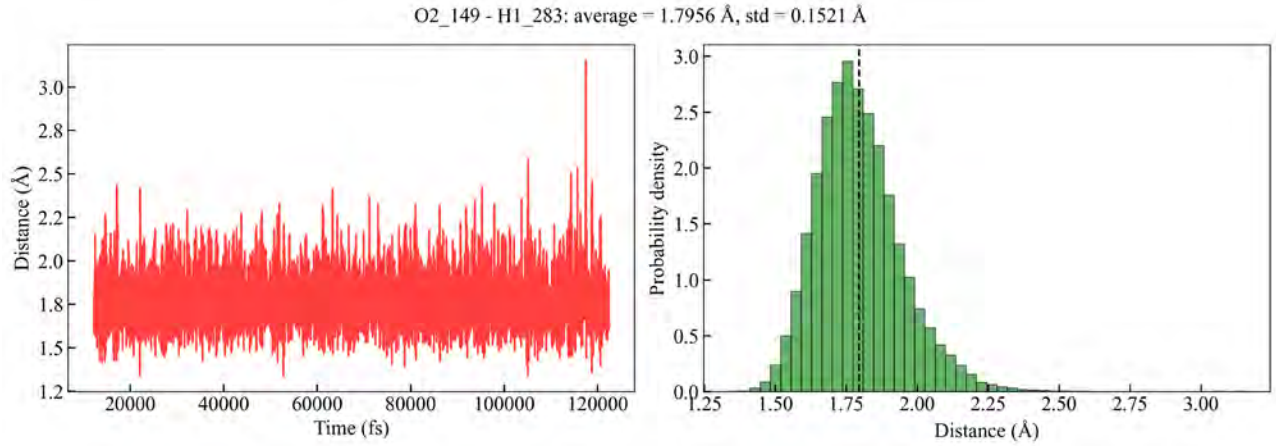
O2_1 - H1_135

Average distance = 1.7955 Å; standard deviation = 0.1521 Å; number of points = 110177



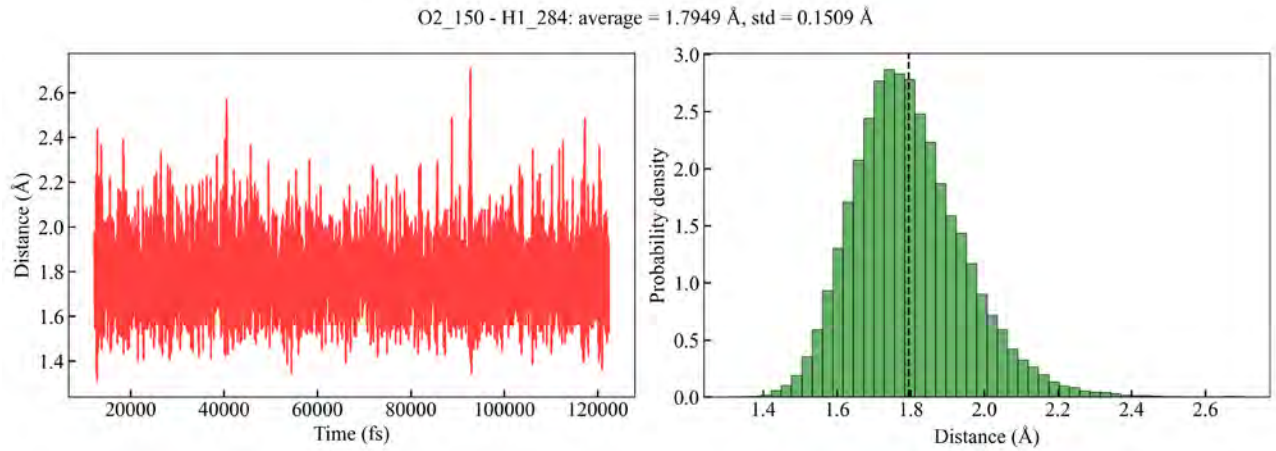
O2_149 - H1_283

Average distance = 1.7956 Å; standard deviation = 0.1521 Å; number of points = 110177



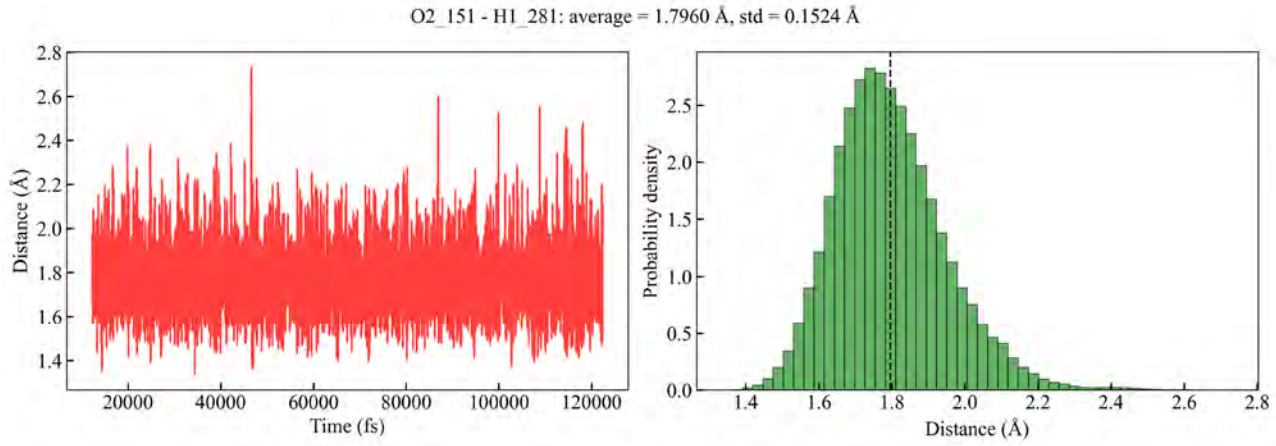
O2_150 - H1_284

Average distance = 1.7949 Å; standard deviation = 0.1509 Å; number of points = 110177



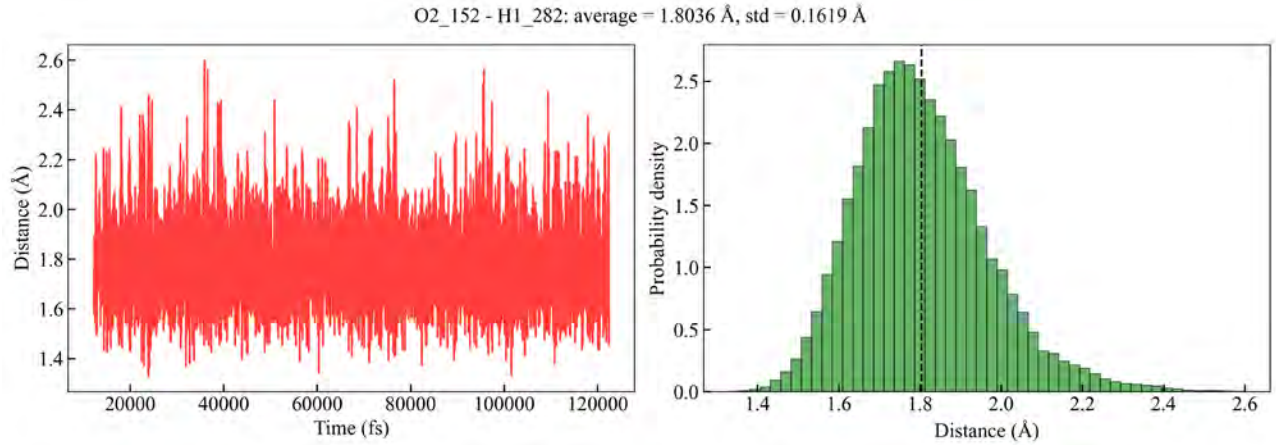
O2_151 - H1_281

Average distance = 1.7960 Å; standard deviation = 0.1524 Å; number of points = 110177



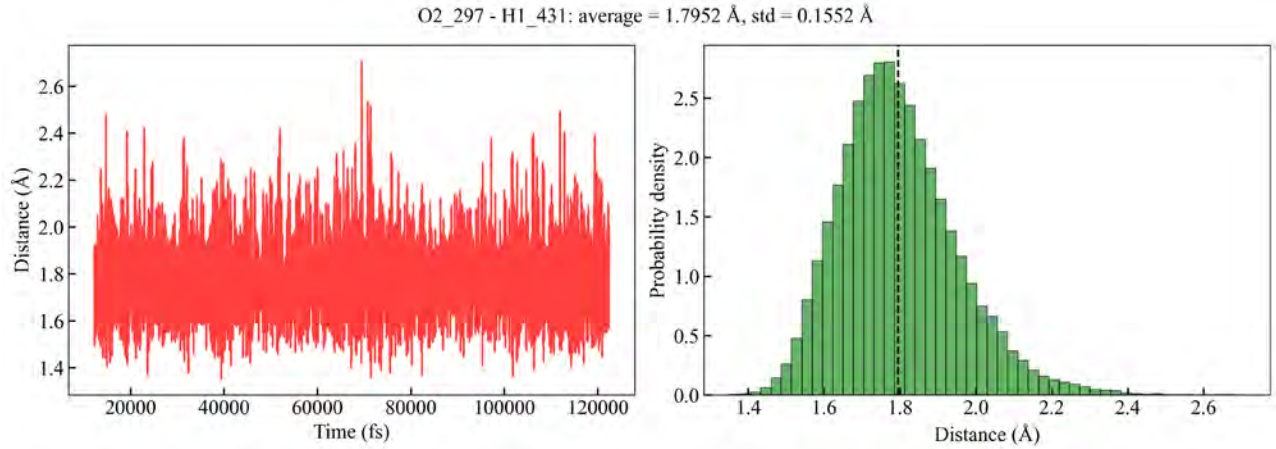
O2_152 - H1_282

Average distance = 1.8036 Å; standard deviation = 0.1619 Å; number of points = 110177



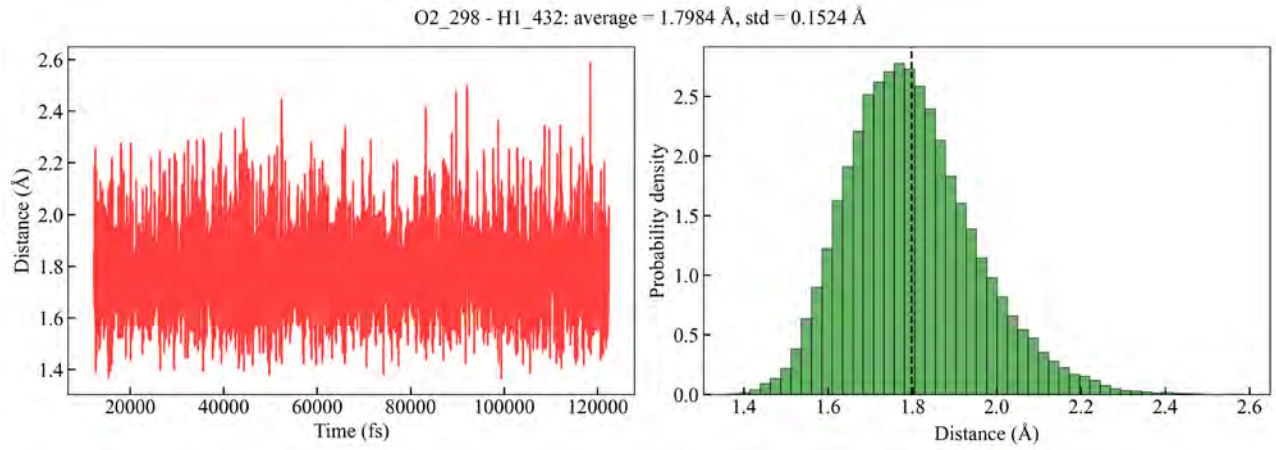
O2_297 - H1_431

Average distance = 1.7952 Å; standard deviation = 0.1552 Å; number of points = 110177



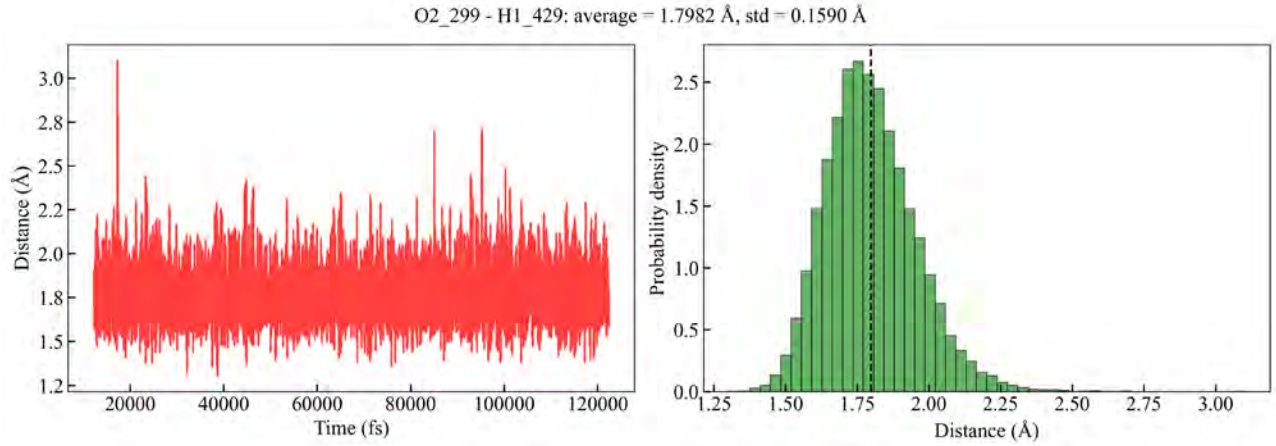
O2_298 - H1_432

Average distance = 1.7984 Å; standard deviation = 0.1524 Å; number of points = 110177



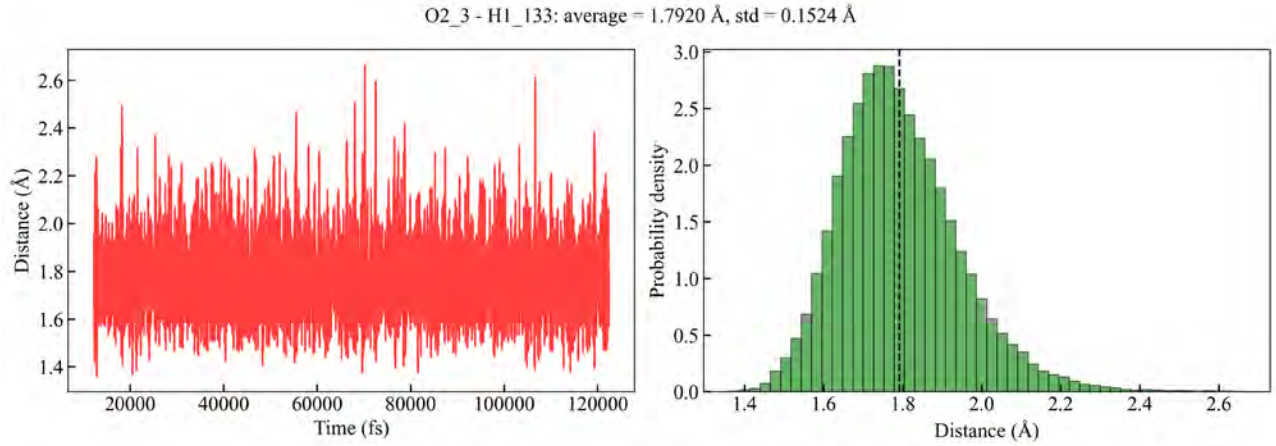
O2_299 - H1_429

Average distance = 1.7982 Å; standard deviation = 0.1590 Å; number of points = 110177



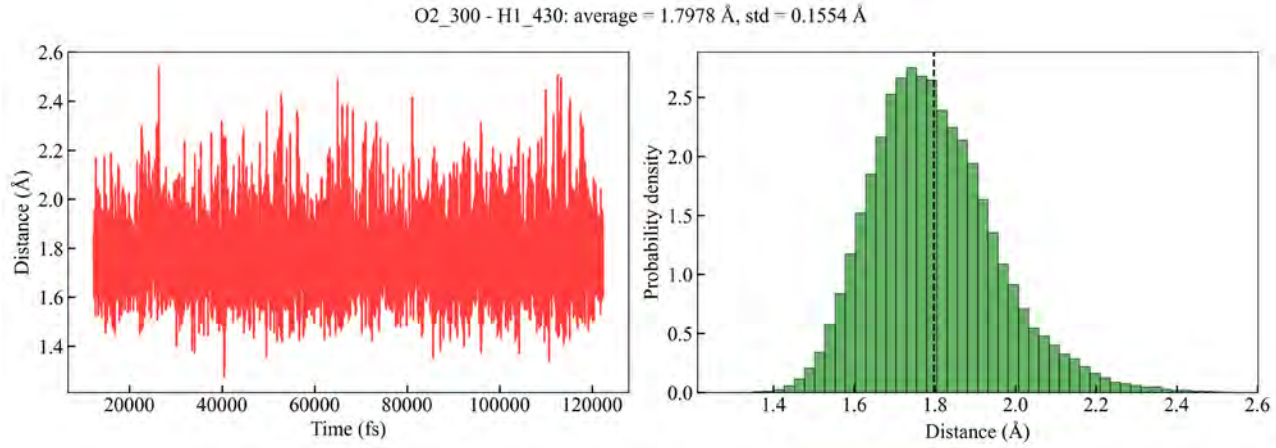
O2_3 - H1_133

Average distance = 1.7920 Å; standard deviation = 0.1524 Å; number of points = 110177



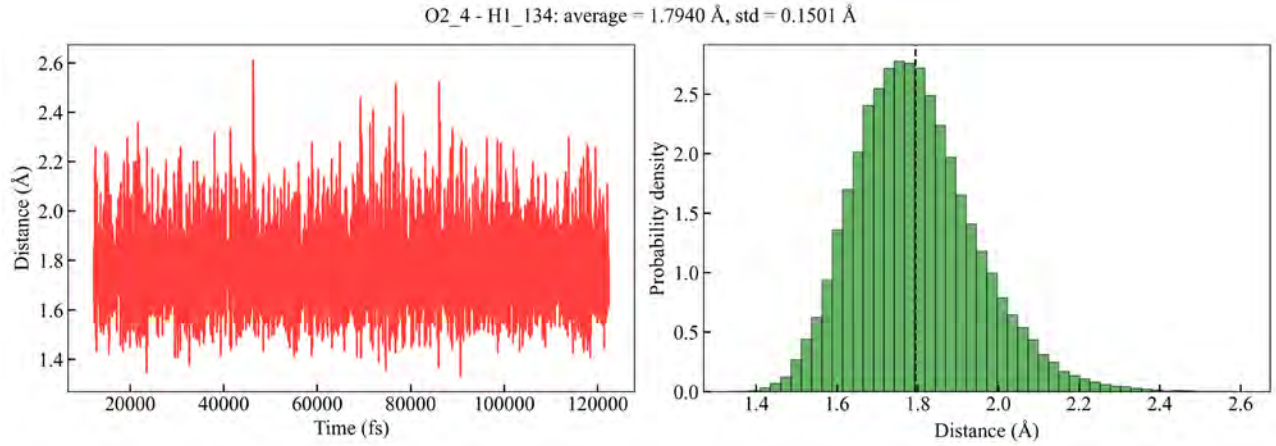
O2_300 - H1_430

Average distance = 1.7978 Å; standard deviation = 0.1554 Å; number of points = 110177



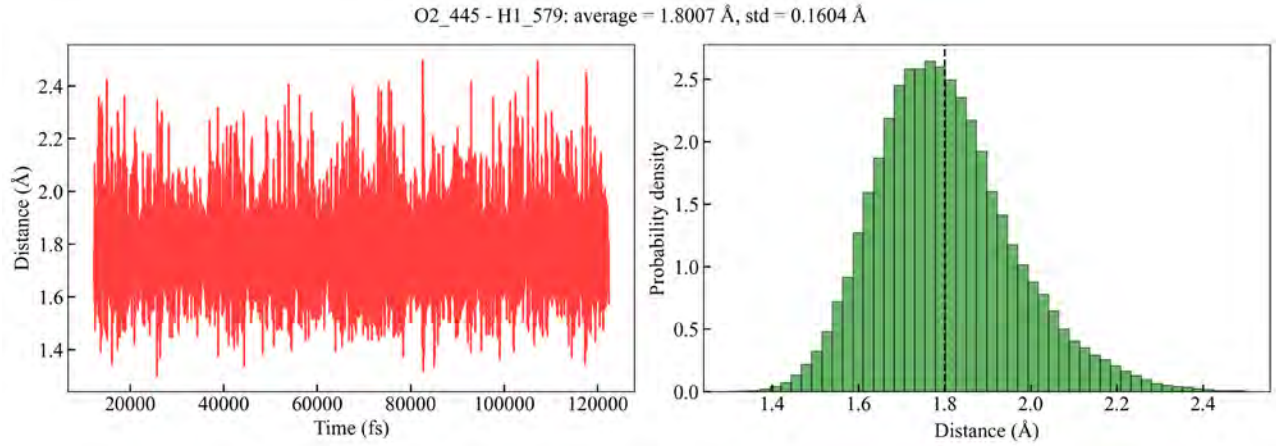
O2_4 - H1_134

Average distance = 1.7940 Å; standard deviation = 0.1501 Å; number of points = 110177



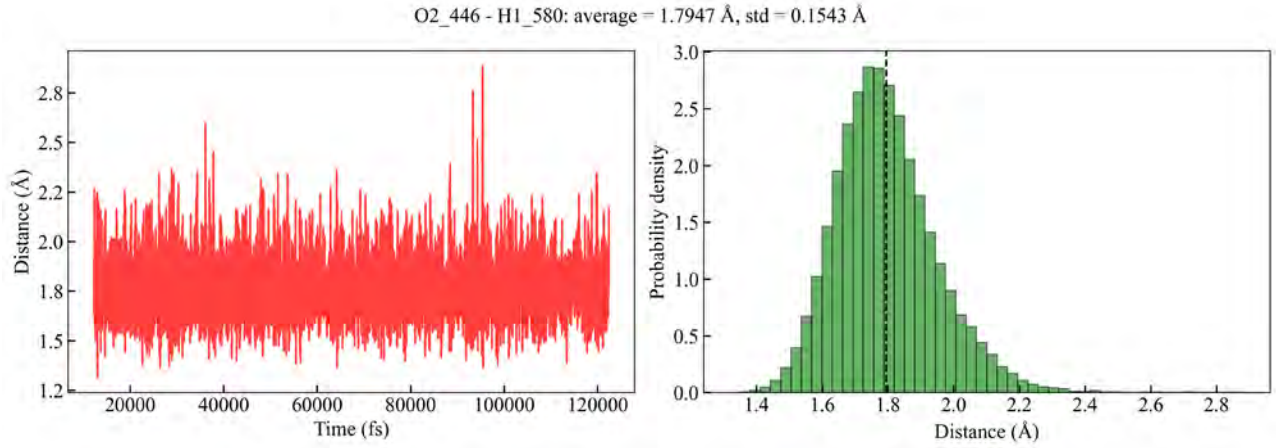
O2_445 - H1_579

Average distance = 1.8007 Å; standard deviation = 0.1604 Å; number of points = 110177



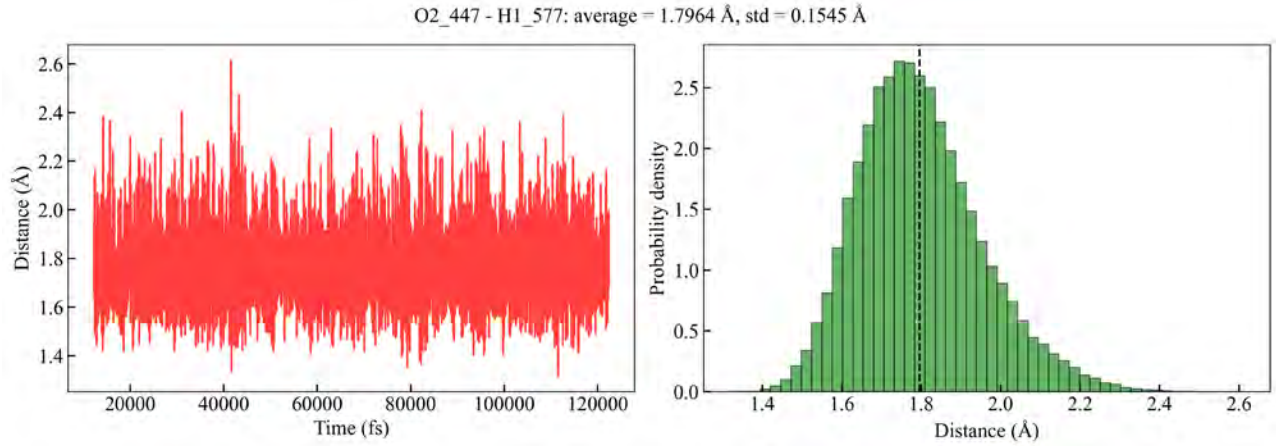
O2_446 - H1_580

Average distance = 1.7947 Å; standard deviation = 0.1543 Å; number of points = 110177



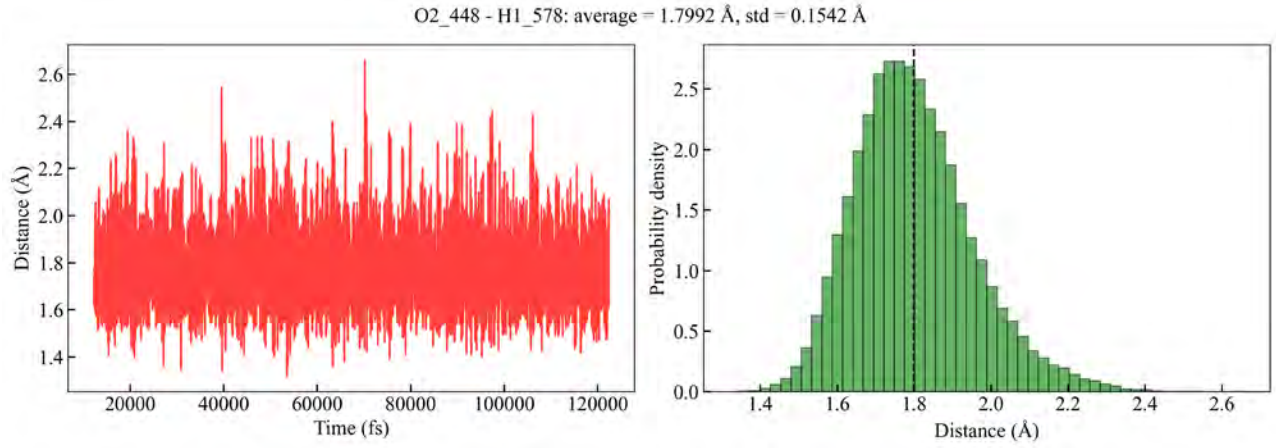
O2_447 - H1_577

Average distance = 1.7964 Å; standard deviation = 0.1545 Å; number of points = 110177



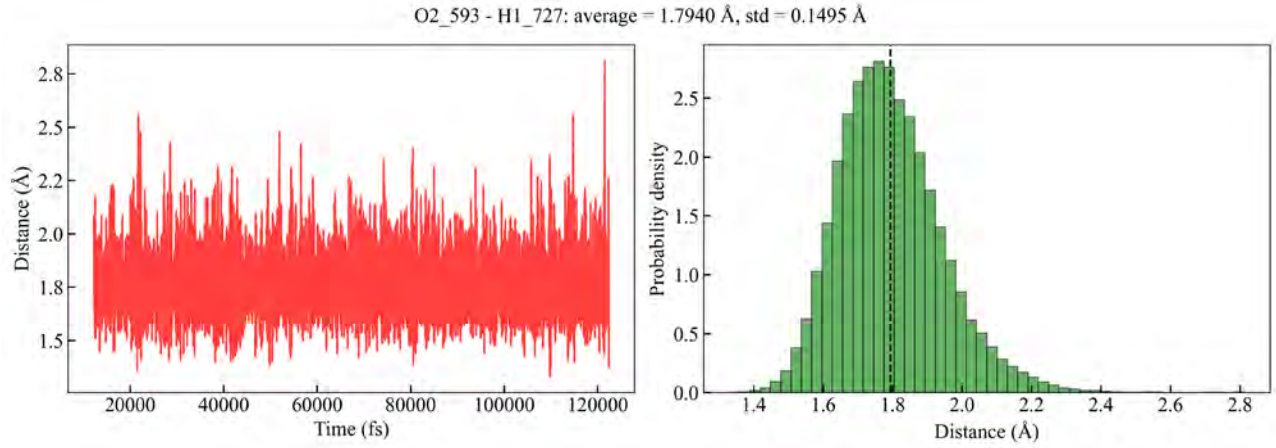
O2_448 - H1_578

Average distance = 1.7992 Å; standard deviation = 0.1542 Å; number of points = 110177



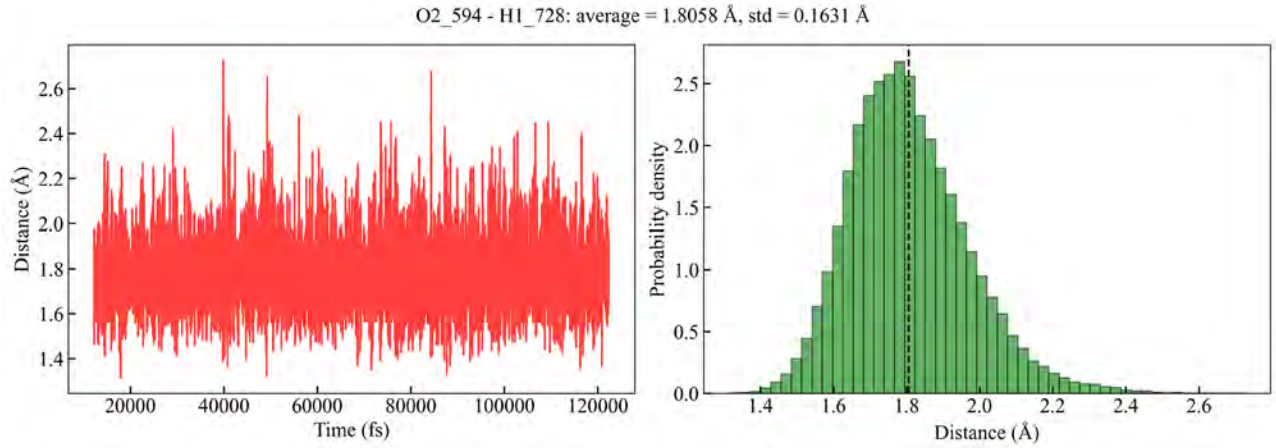
O2_593 - H1_727

Average distance = 1.7940 Å; standard deviation = 0.1495 Å; number of points = 110177



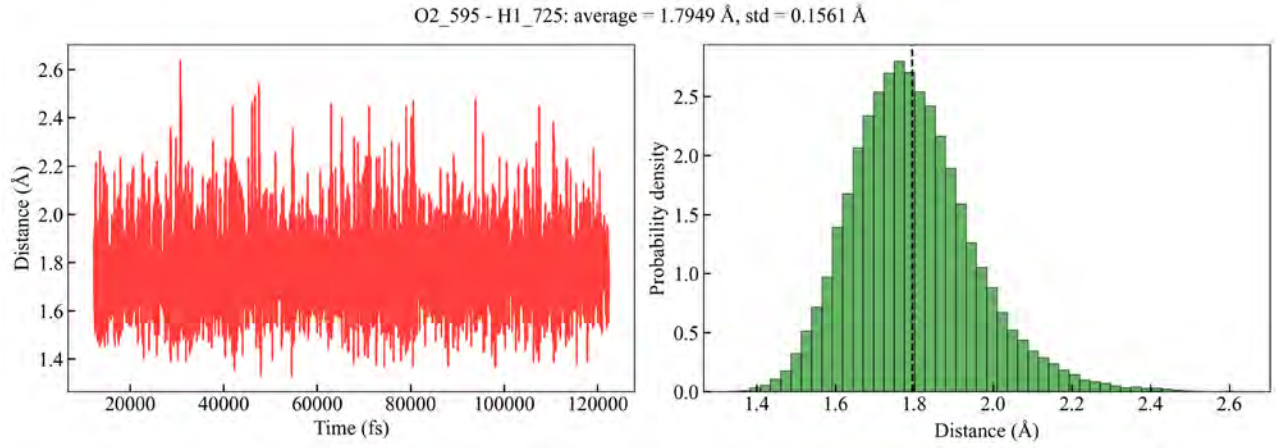
O2_594 - H1_728

Average distance = 1.8058 Å; standard deviation = 0.1631 Å; number of points = 110177



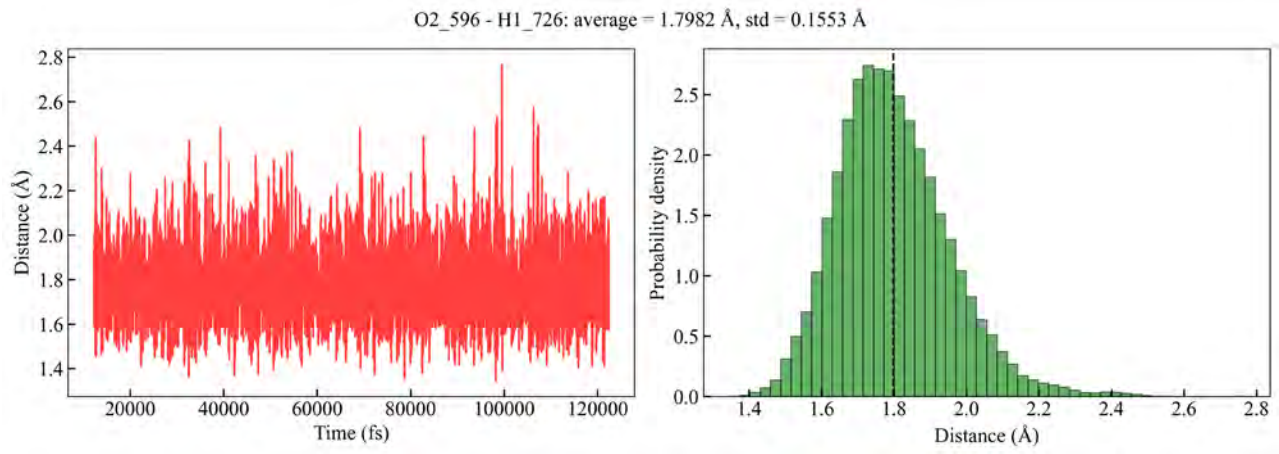
O2_595 - H1_725

Average distance = 1.7949 Å; standard deviation = 0.1561 Å; number of points = 110177



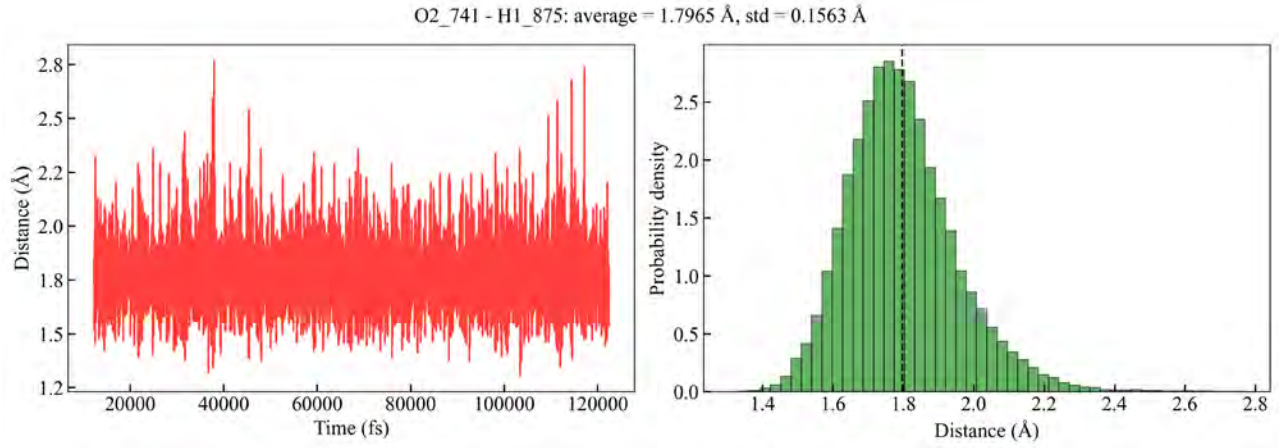
O2_596 - H1_726

Average distance = 1.7982 Å; standard deviation = 0.1553 Å; number of points = 110177



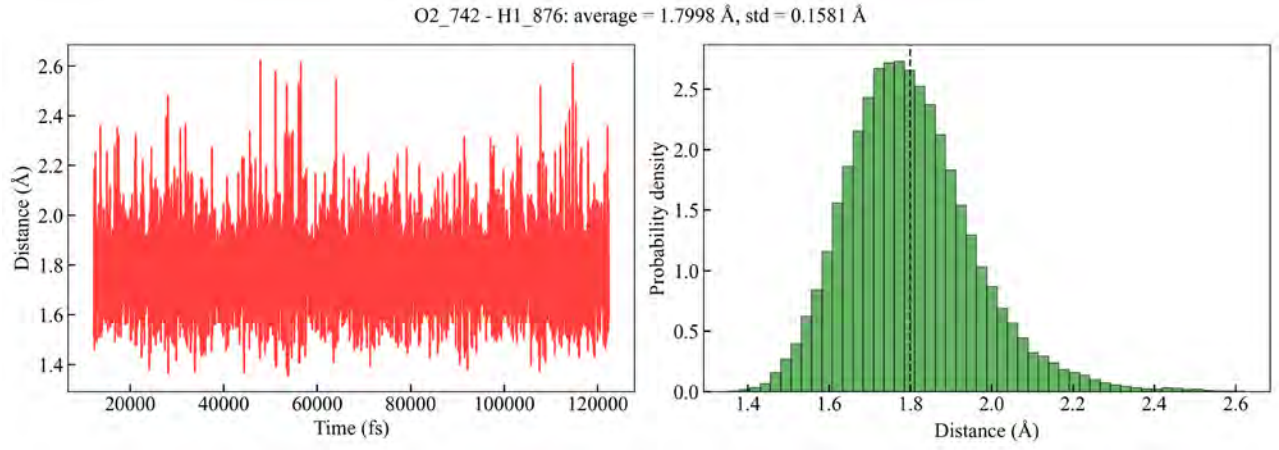
O2_741 - H1_875

Average distance = 1.7965 Å; standard deviation = 0.1563 Å; number of points = 110177



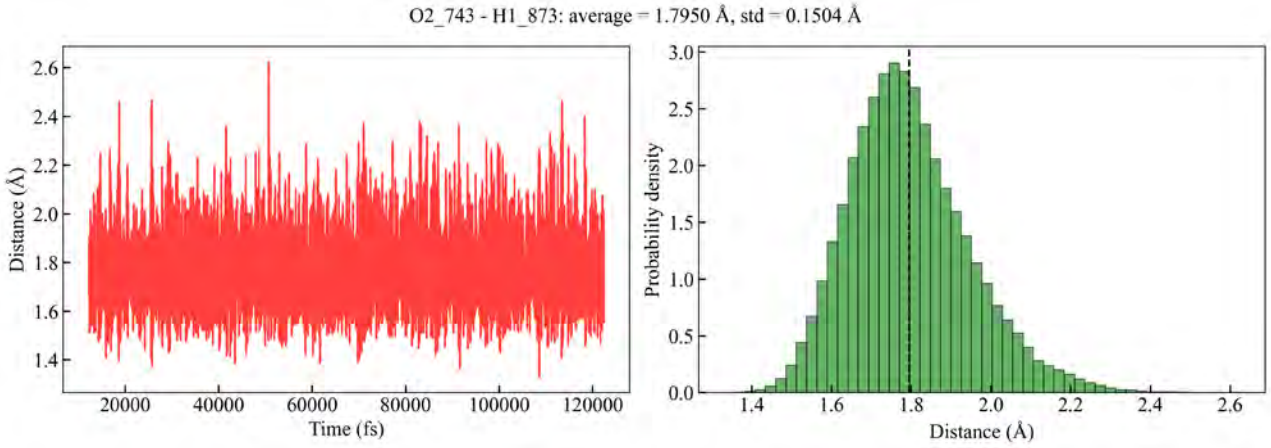
O2_742 - H1_876

Average distance = 1.7998 Å; standard deviation = 0.1581 Å; number of points = 110177



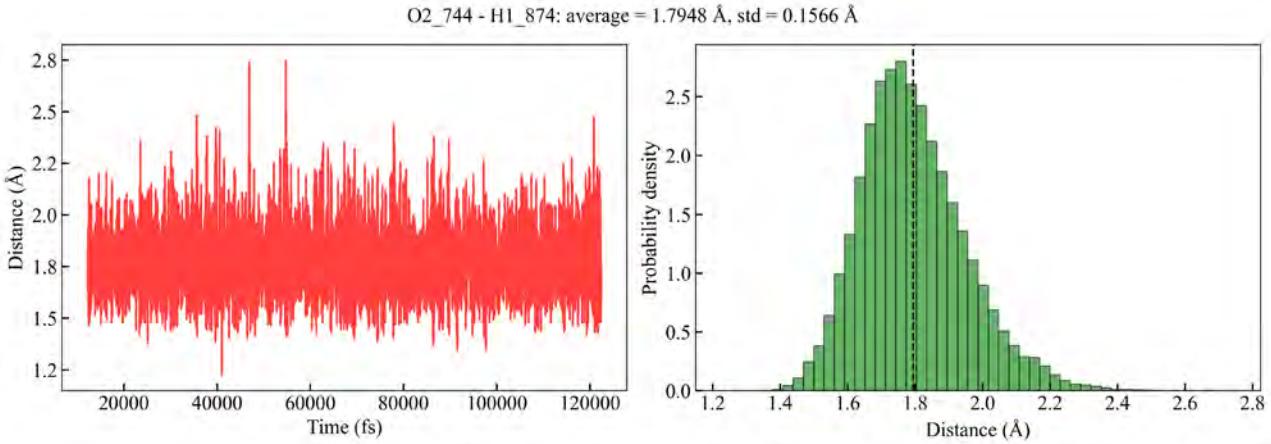
O2_743 - H1_873

Average distance = 1.7950 Å; standard deviation = 0.1504 Å; number of points = 110177



O2_744 - H1_874

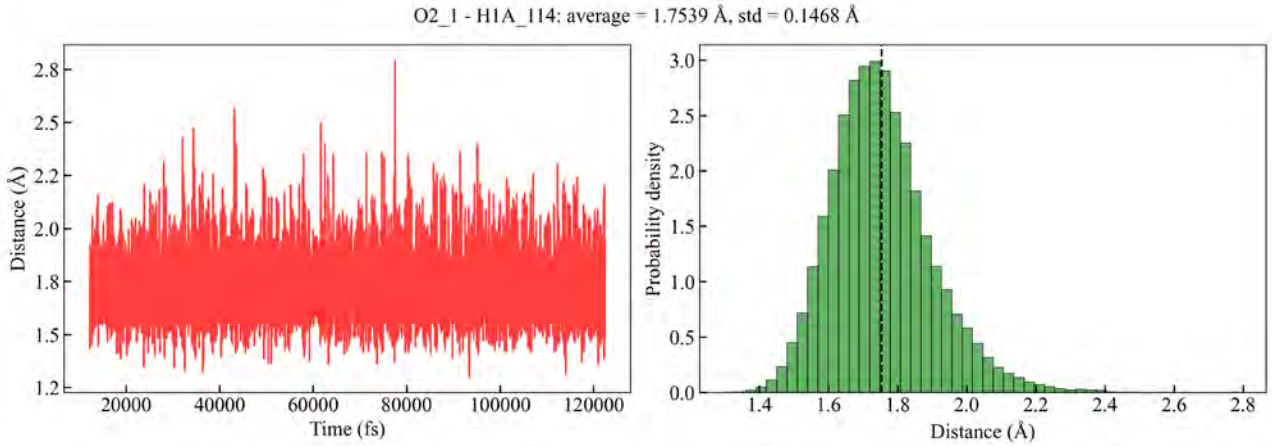
Average distance = 1.7948 Å; standard deviation = 0.1566 Å; number of points = 110177



O2 - H1A

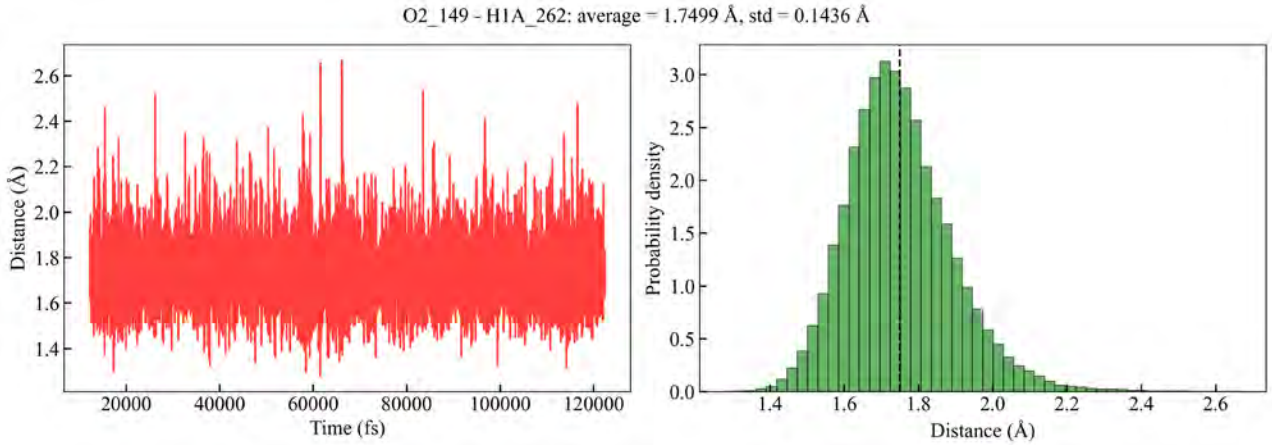
O2_1 - H1A_114

Average distance = 1.7539 Å; standard deviation = 0.1468 Å; number of points = 110177



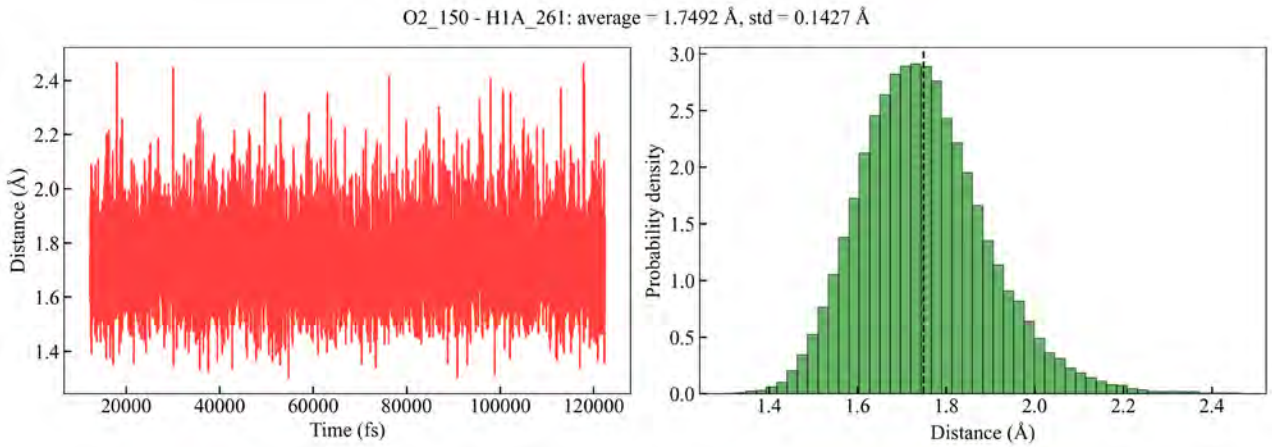
O2_149 - H1A_262

Average distance = 1.7499 Å; standard deviation = 0.1436 Å; number of points = 110177



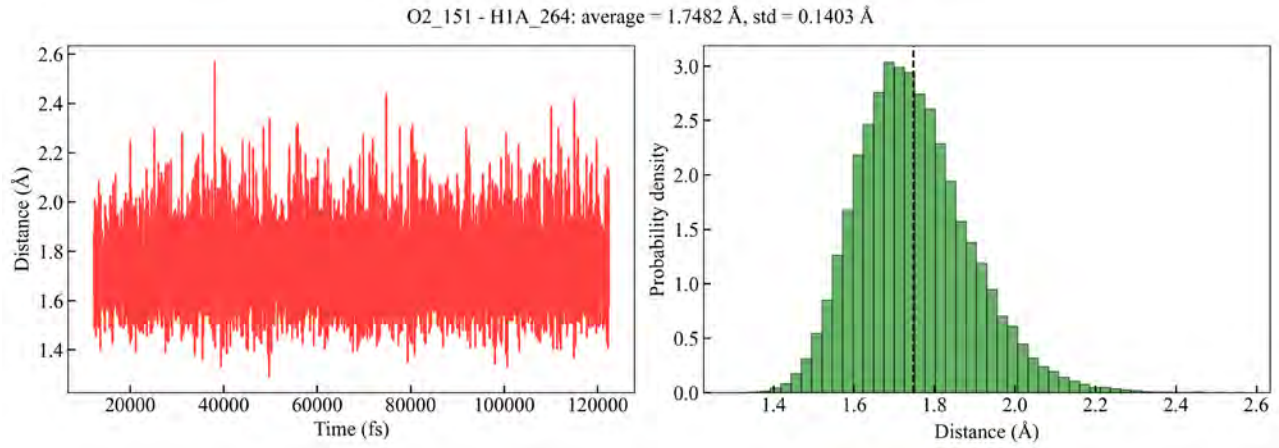
O2_150 - H1A_261

Average distance = 1.7492 Å; standard deviation = 0.1427 Å; number of points = 110177



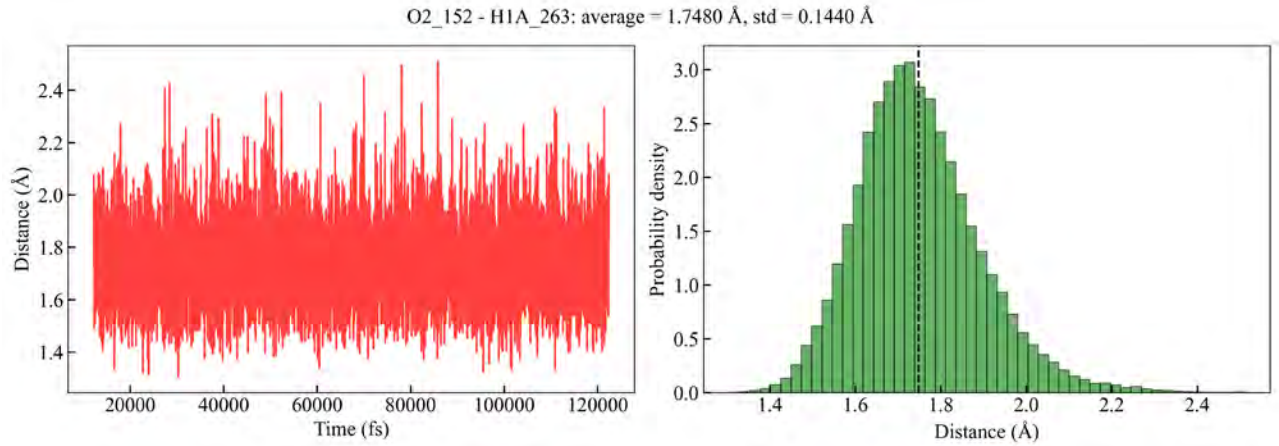
O2_151 - H1A_264

Average distance = 1.7482 Å; standard deviation = 0.1403 Å; number of points = 110177



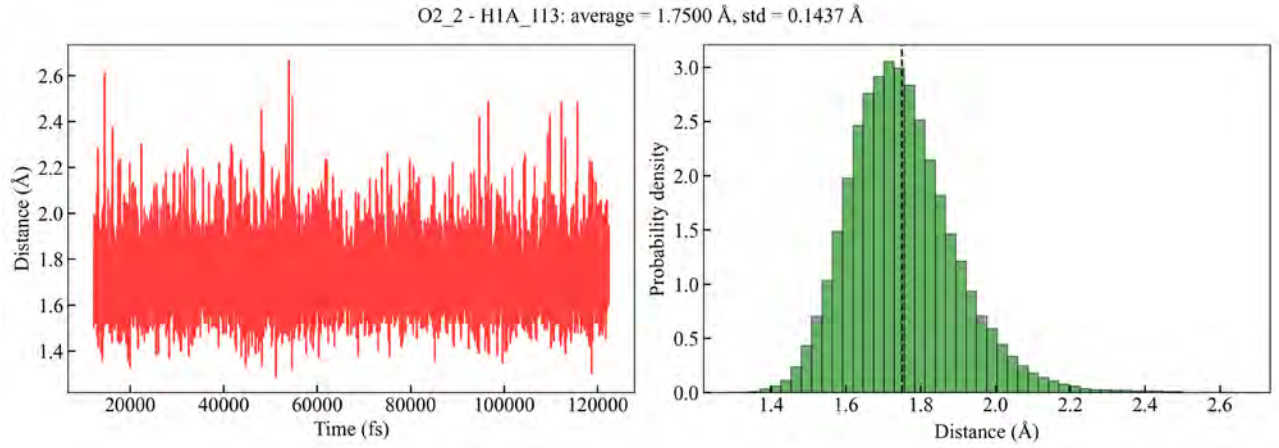
O2_152 - H1A_263

Average distance = 1.7480 Å; standard deviation = 0.1440 Å; number of points = 110177



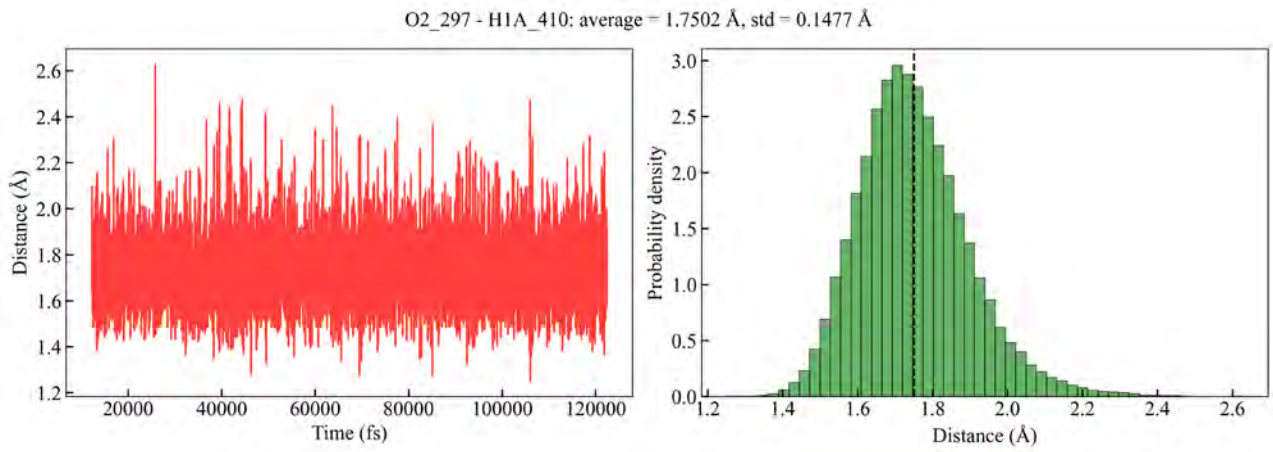
O2_2 - H1A_113

Average distance = 1.7500 Å; standard deviation = 0.1437 Å; number of points = 110177



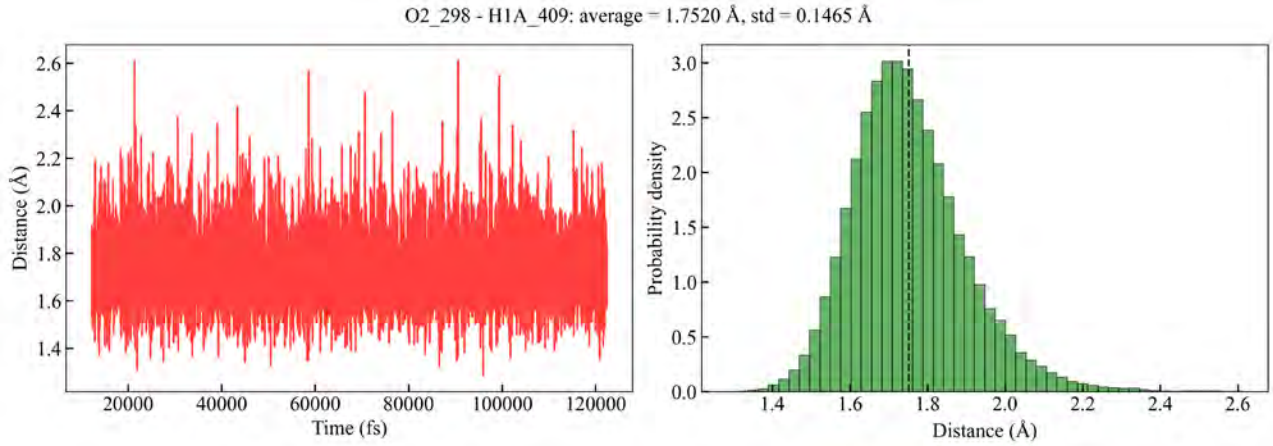
O2_297 - H1A_410

Average distance = 1.7502 Å; standard deviation = 0.1477 Å; number of points = 110177



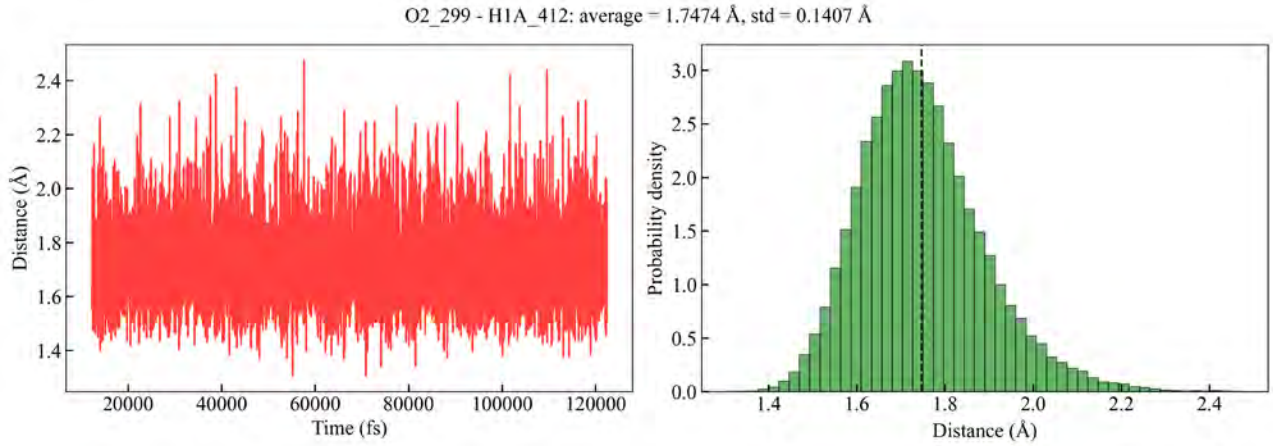
O2_298 - H1A_409

Average distance = 1.7520 Å; standard deviation = 0.1465 Å; number of points = 110177



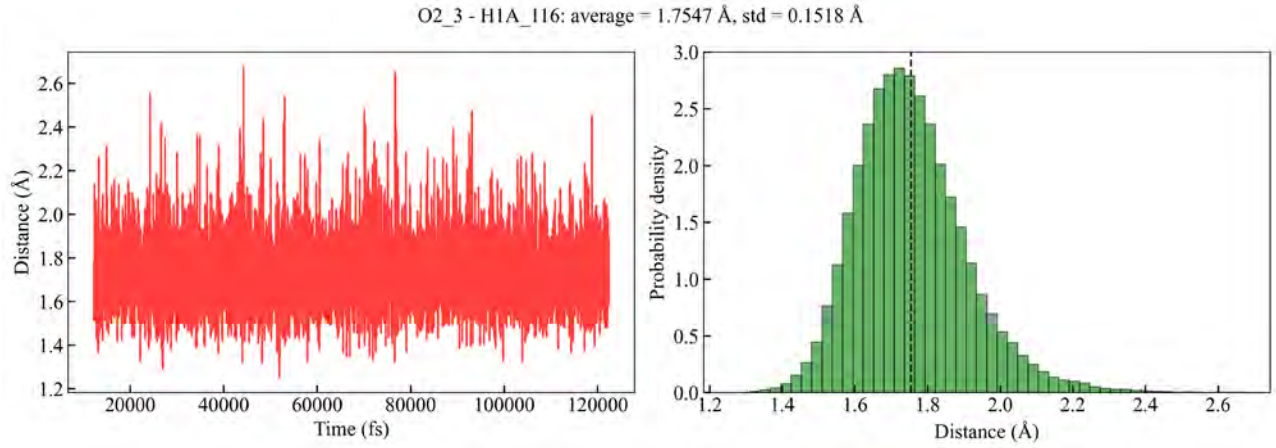
O2_299 - H1A_412

Average distance = 1.7474 Å; standard deviation = 0.1407 Å; number of points = 110177



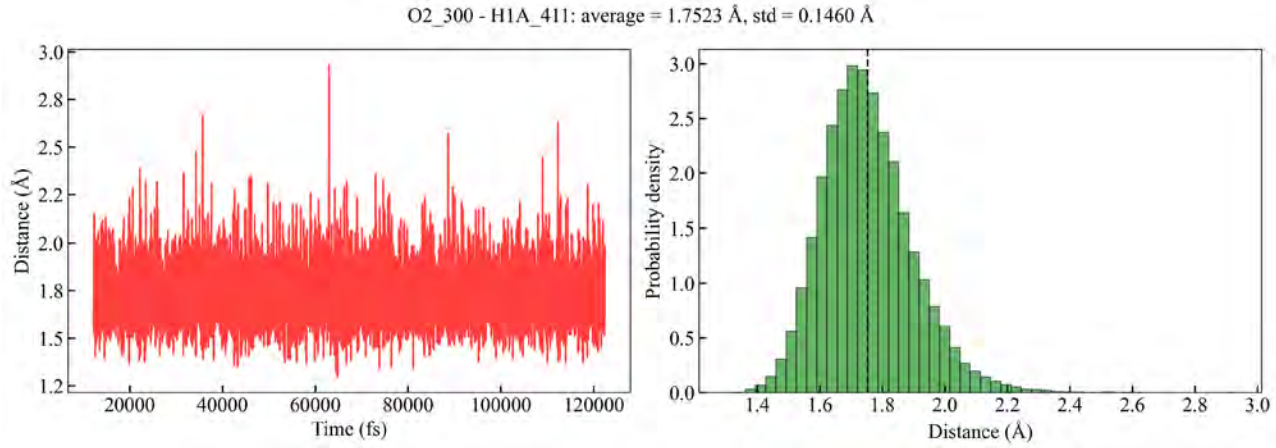
O2_3 - H1A_116

Average distance = 1.7547 Å; standard deviation = 0.1518 Å; number of points = 110177



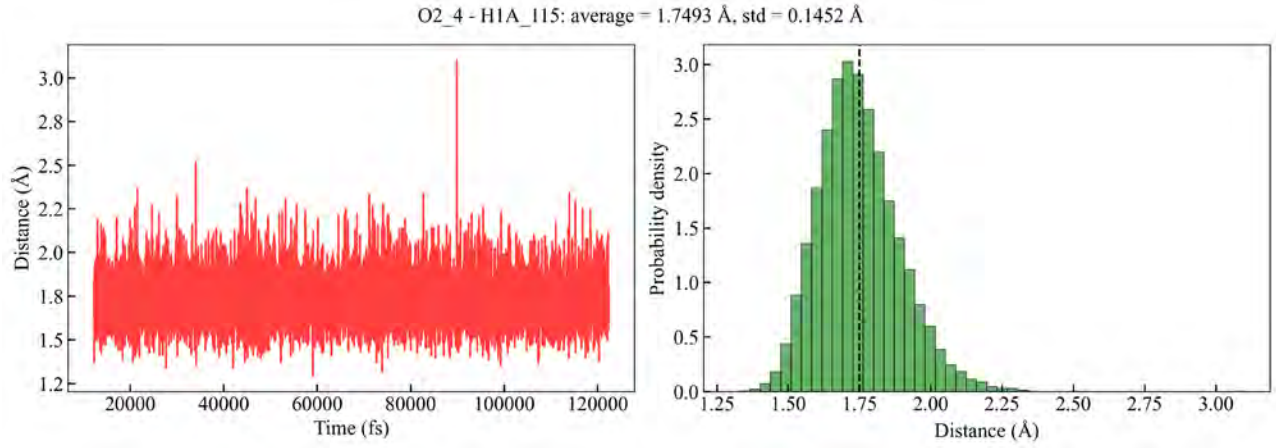
O2_300 - H1A_411

Average distance = 1.7523 Å; standard deviation = 0.1460 Å; number of points = 110177



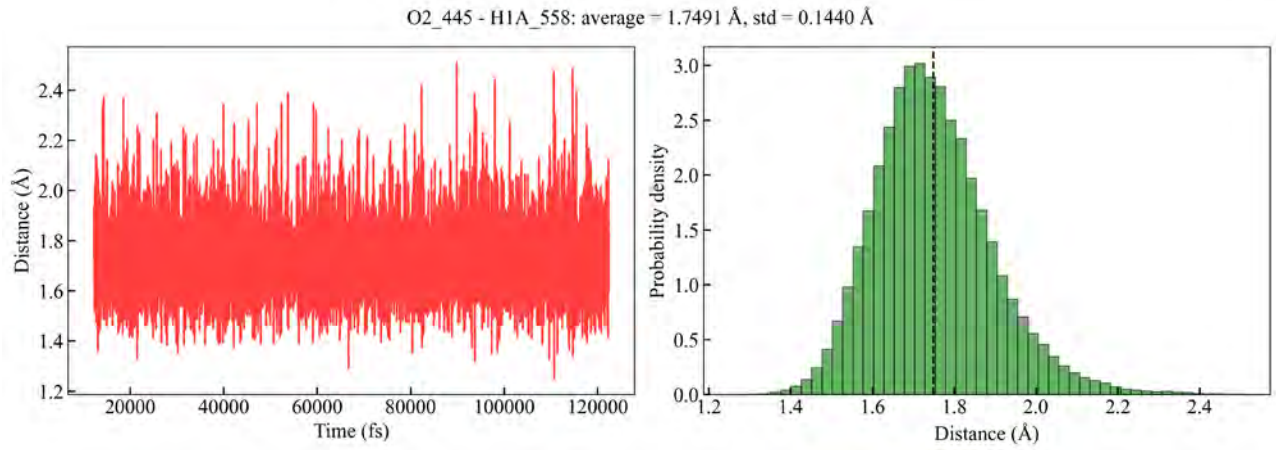
O2_4 - H1A_115

Average distance = 1.7493 Å; standard deviation = 0.1452 Å; number of points = 110177



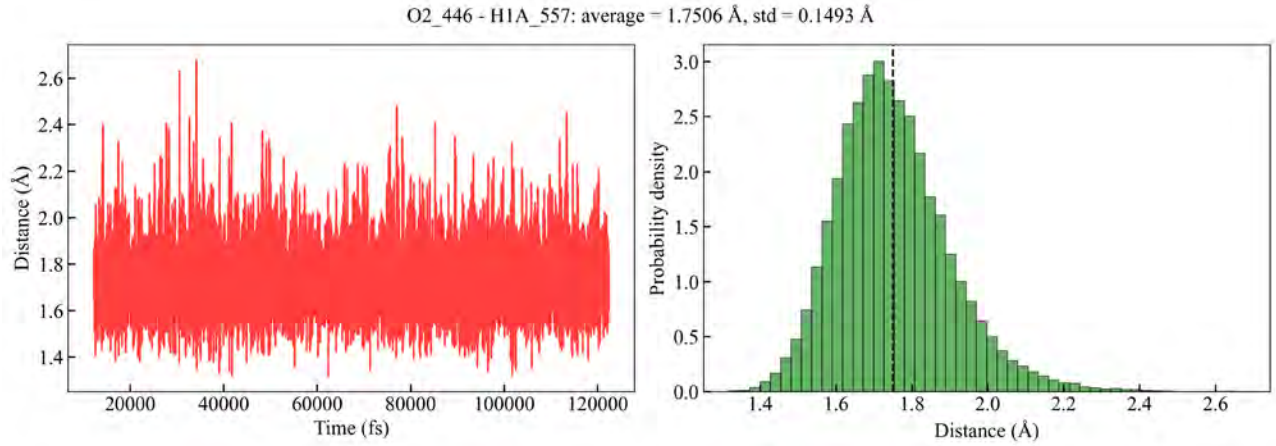
O2_445 - H1A_558

Average distance = 1.7491 Å; standard deviation = 0.1440 Å; number of points = 110177



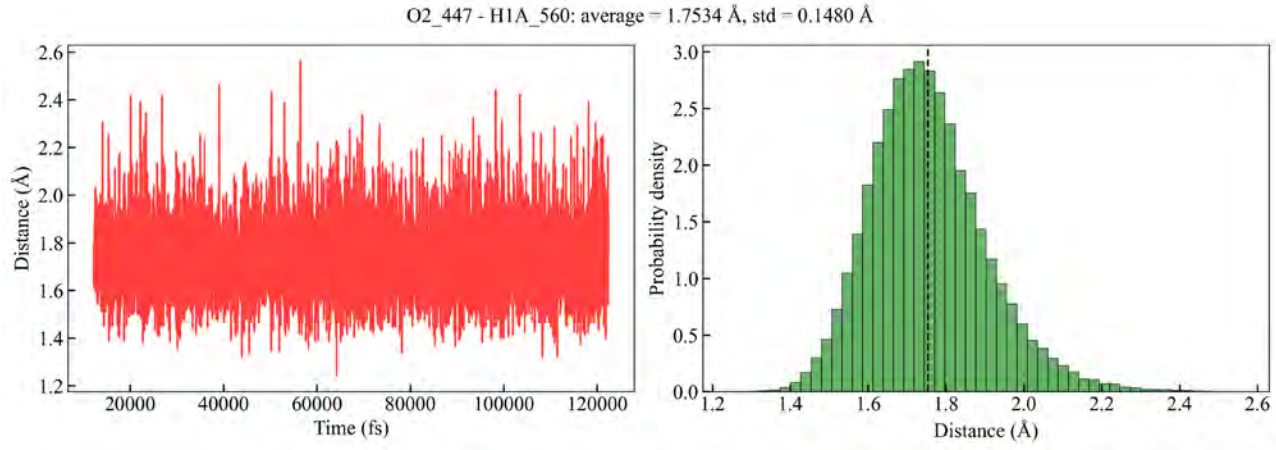
O2_446 - H1A_557

Average distance = 1.7506 Å; standard deviation = 0.1493 Å; number of points = 110177



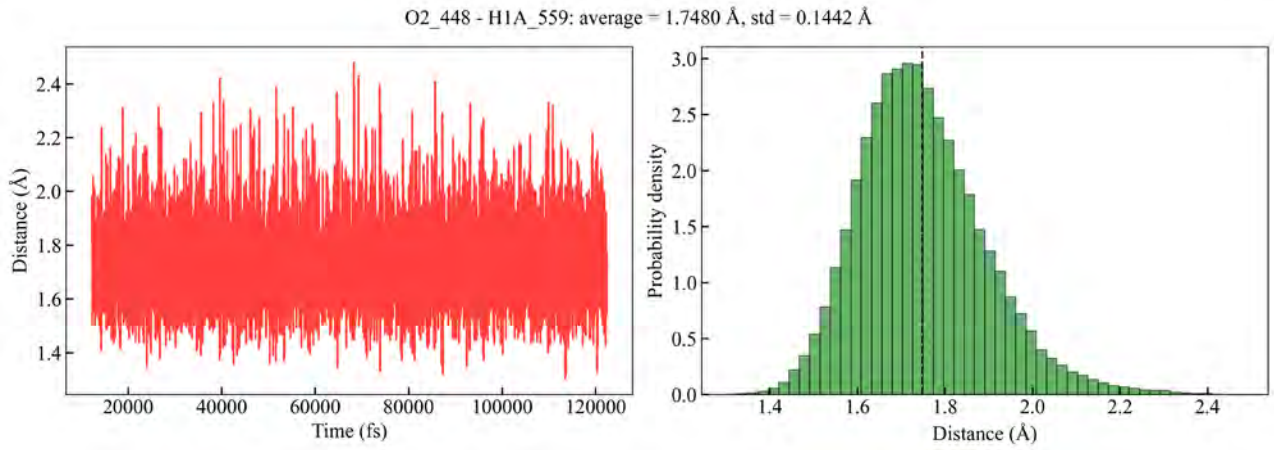
O2_447 - H1A_560

Average distance = 1.7534 Å; standard deviation = 0.1480 Å; number of points = 110177



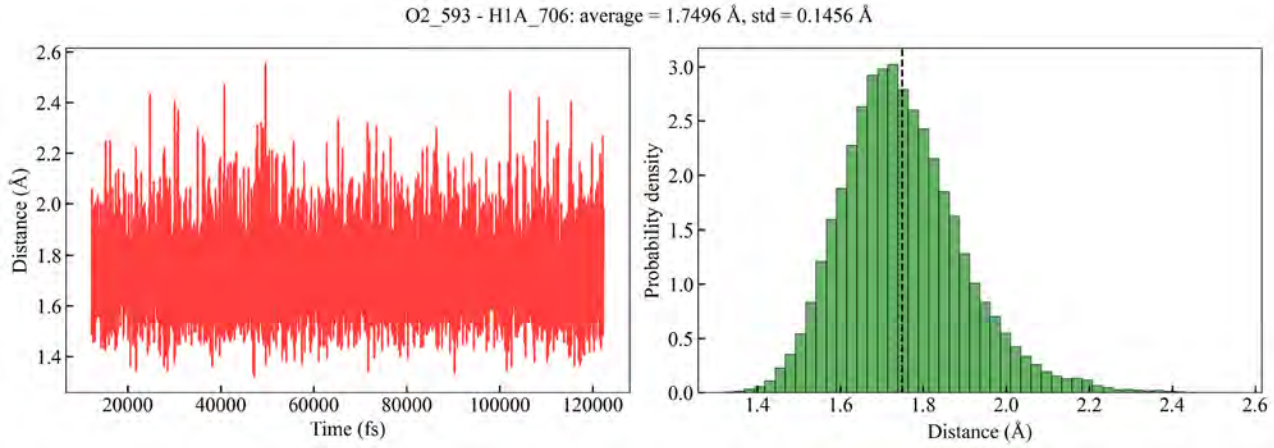
O2_448 - H1A_559

Average distance = 1.7480 Å; standard deviation = 0.1442 Å; number of points = 110177



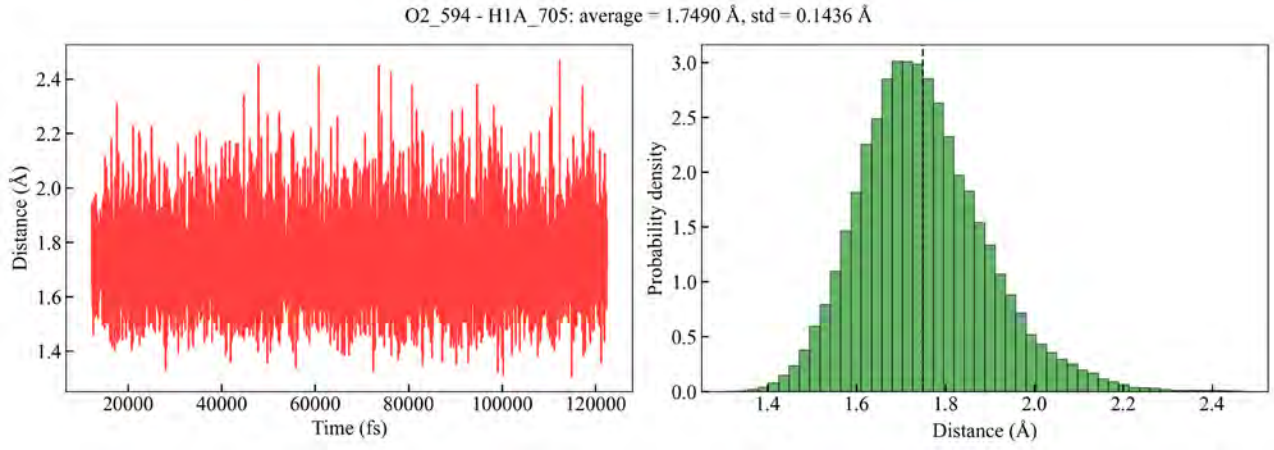
O2_593 - H1A_706

Average distance = 1.7496 Å; standard deviation = 0.1456 Å; number of points = 110177



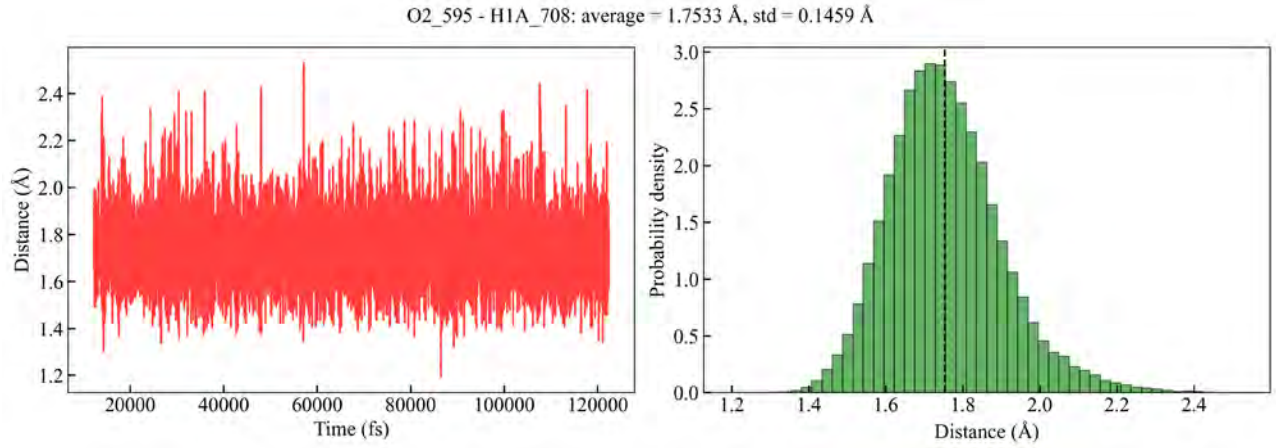
O2_594 - H1A_705

Average distance = 1.7490 Å; standard deviation = 0.1436 Å; number of points = 110177



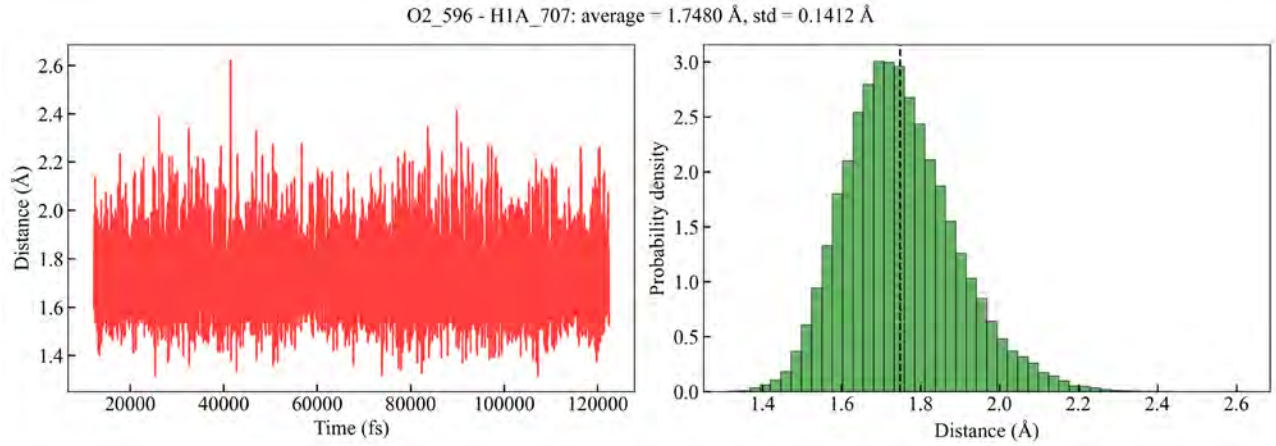
O2_595 - H1A_708

Average distance = 1.7533 Å; standard deviation = 0.1459 Å; number of points = 110177



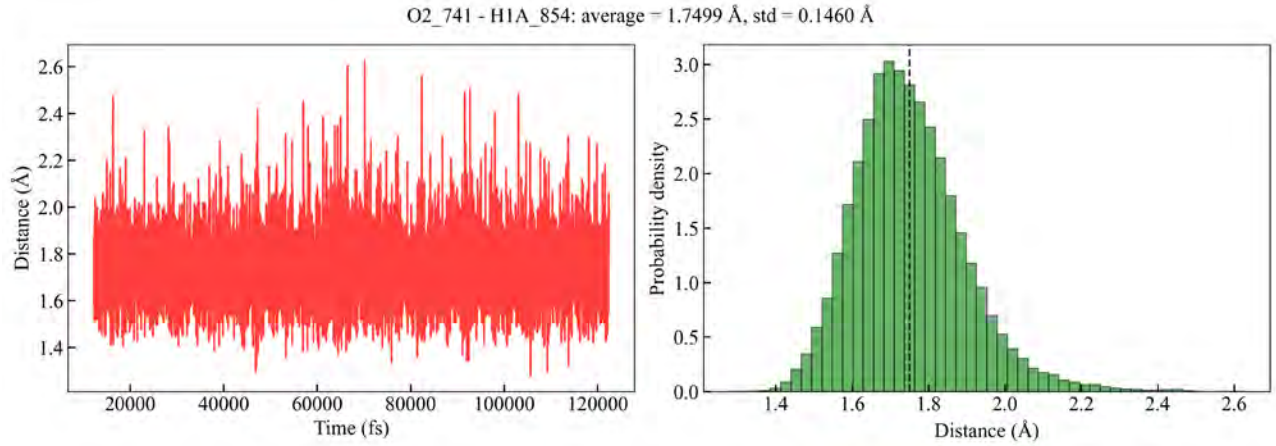
O2_596 - H1A_707

Average distance = 1.7480 Å; standard deviation = 0.1412 Å; number of points = 110177



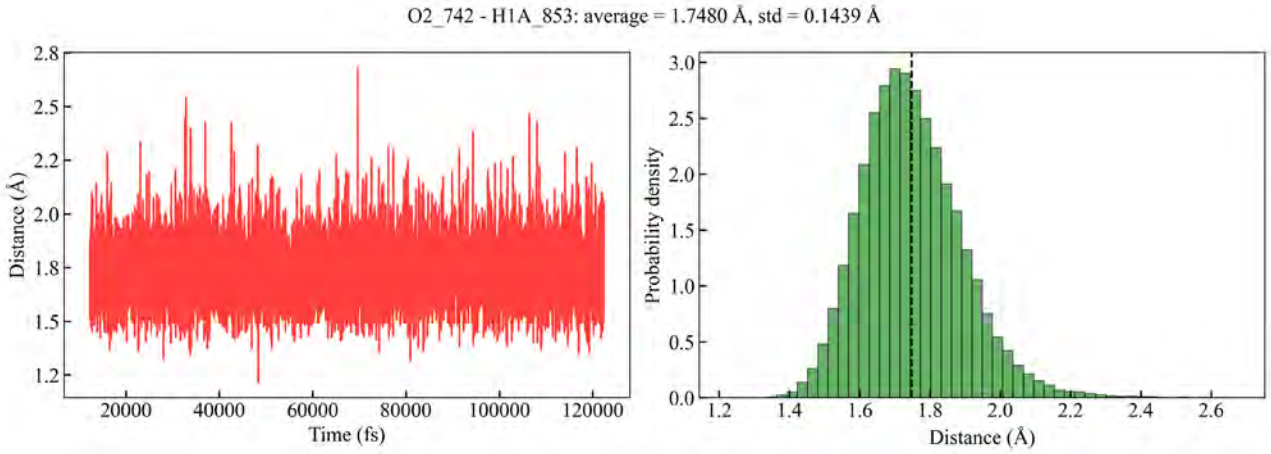
O2_741 - H1A_854

Average distance = 1.7499 Å; standard deviation = 0.1460 Å; number of points = 110177



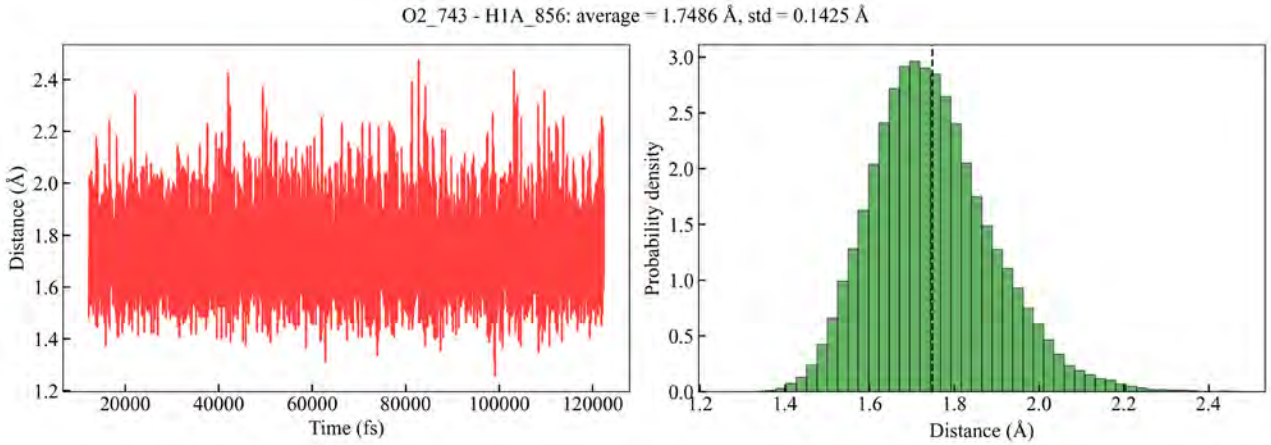
O2_742 - H1A_853

Average distance = 1.7480 Å; standard deviation = 0.1439 Å; number of points = 110177



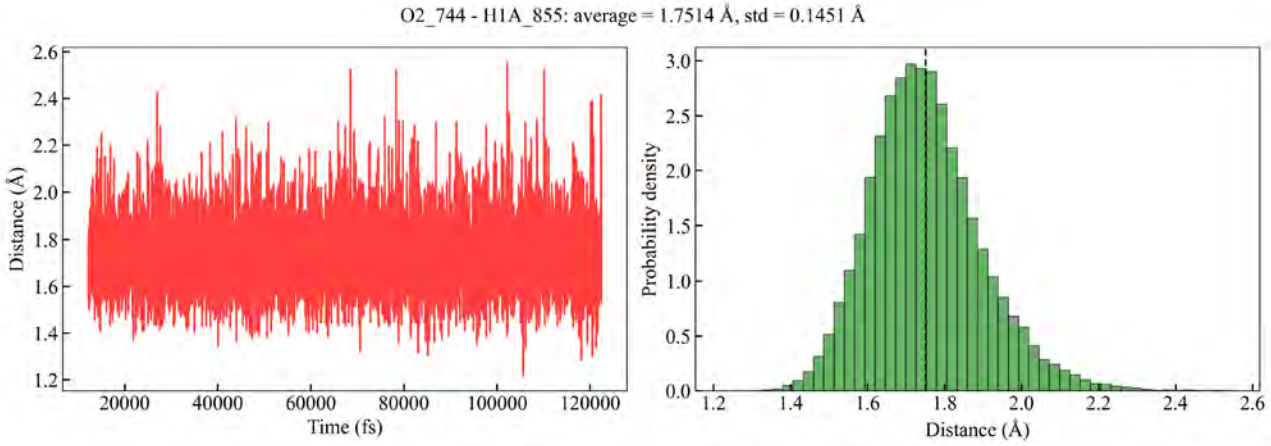
O2_743 - H1A_856

Average distance = 1.7486 Å; standard deviation = 0.1425 Å; number of points = 110177



O2_744 - H1A_855

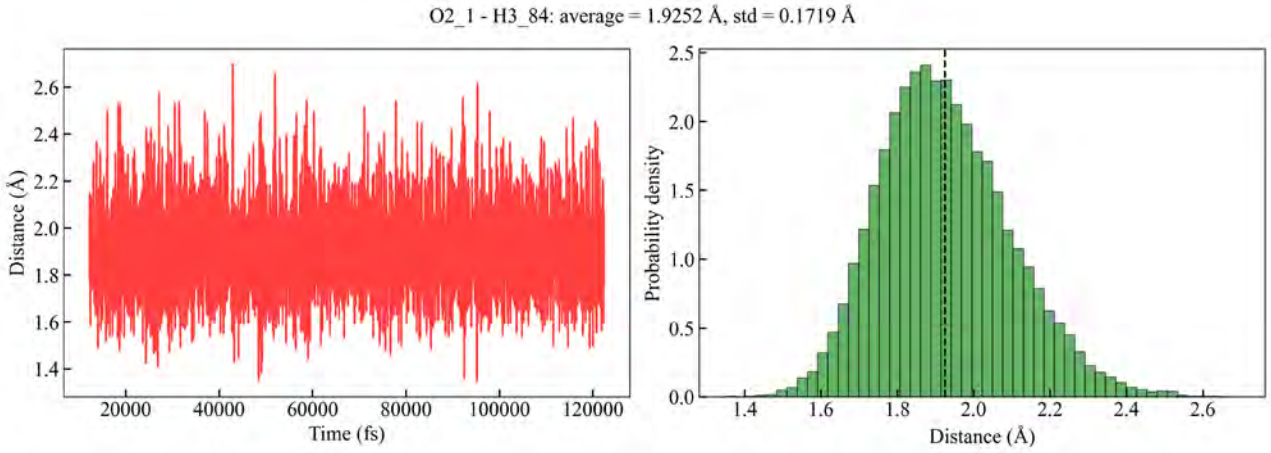
Average distance = 1.7514 Å; standard deviation = 0.1451 Å; number of points = 110177



O2 - H3

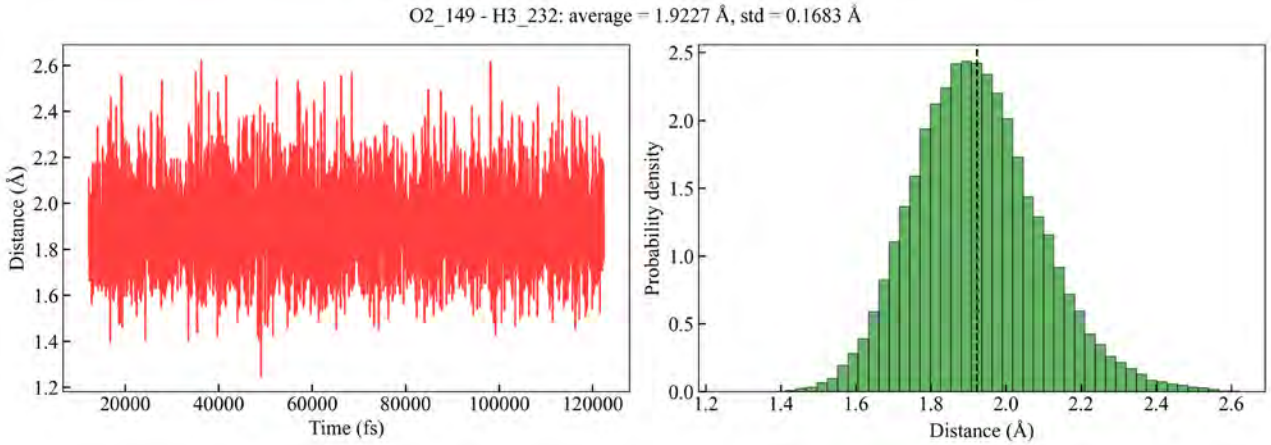
O2_1 - H3_84

Average distance = 1.9252 Å; standard deviation = 0.1719 Å; number of points = 110177



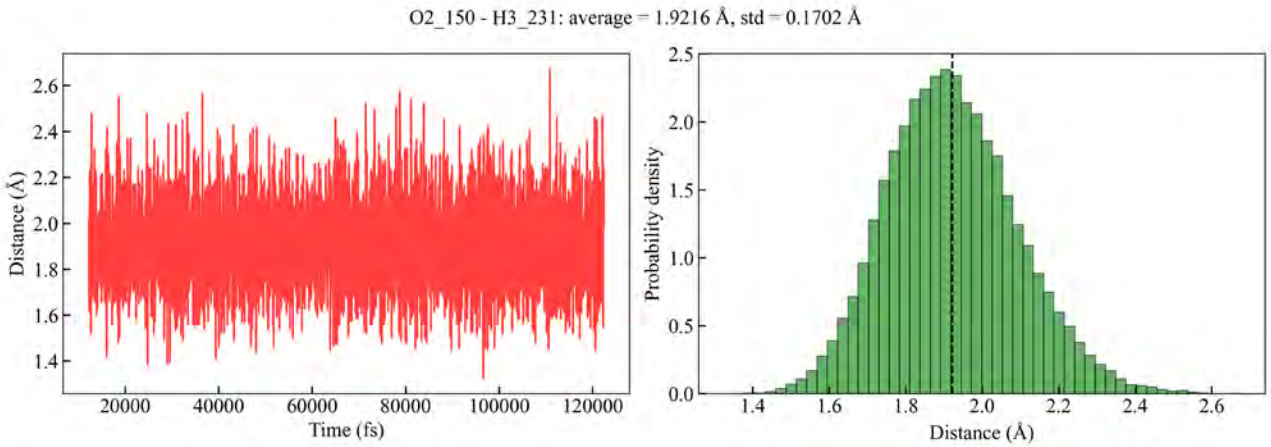
O2_149 - H3_232

Average distance = 1.9227 Å; standard deviation = 0.1683 Å; number of points = 110177



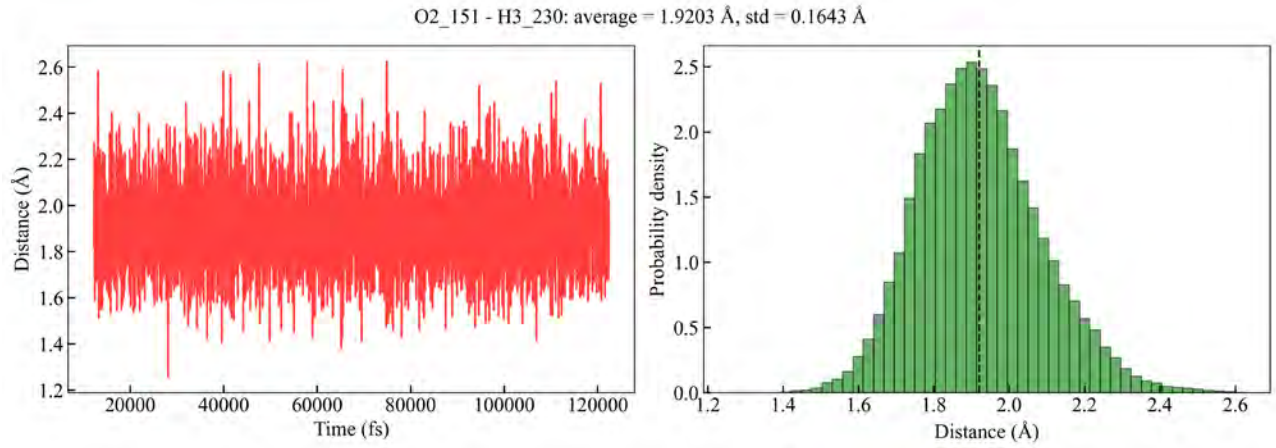
O2_150 - H3_231

Average distance = 1.9216 Å; standard deviation = 0.1702 Å; number of points = 110177



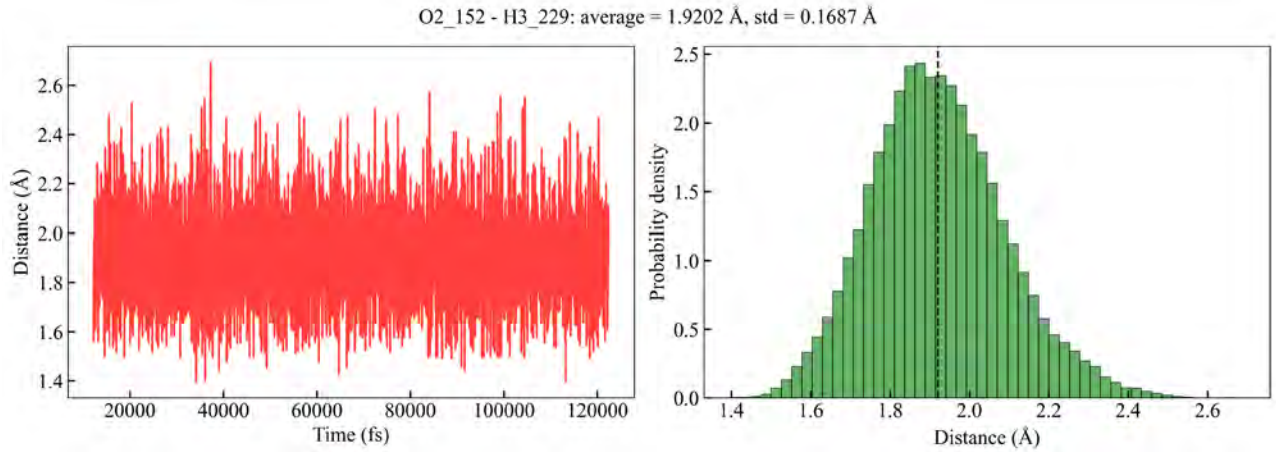
O2_151 - H3_230

Average distance = 1.9203 Å; standard deviation = 0.1643 Å; number of points = 110177



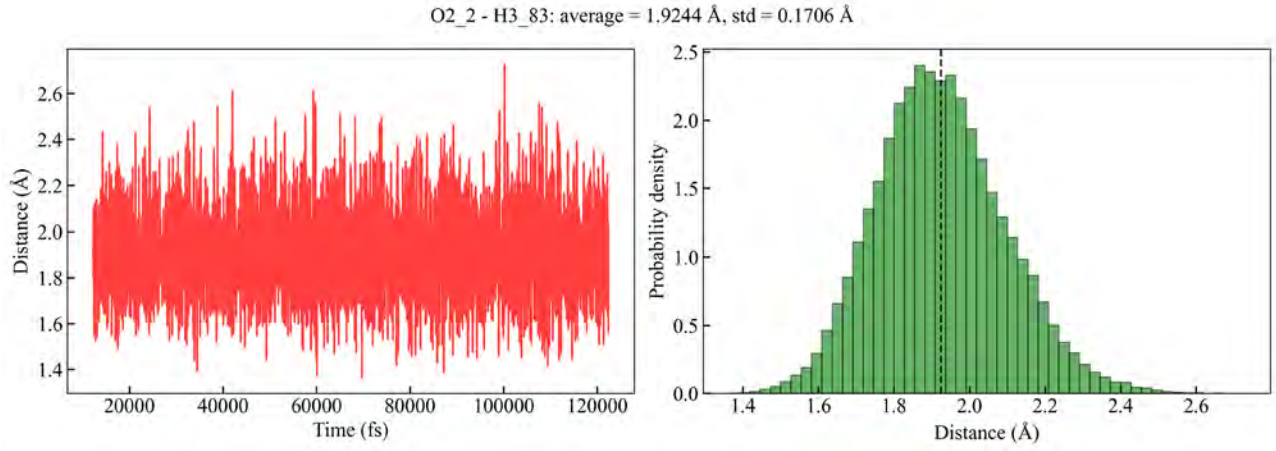
O2_152 - H3_229

Average distance = 1.9202 Å; standard deviation = 0.1687 Å; number of points = 110177



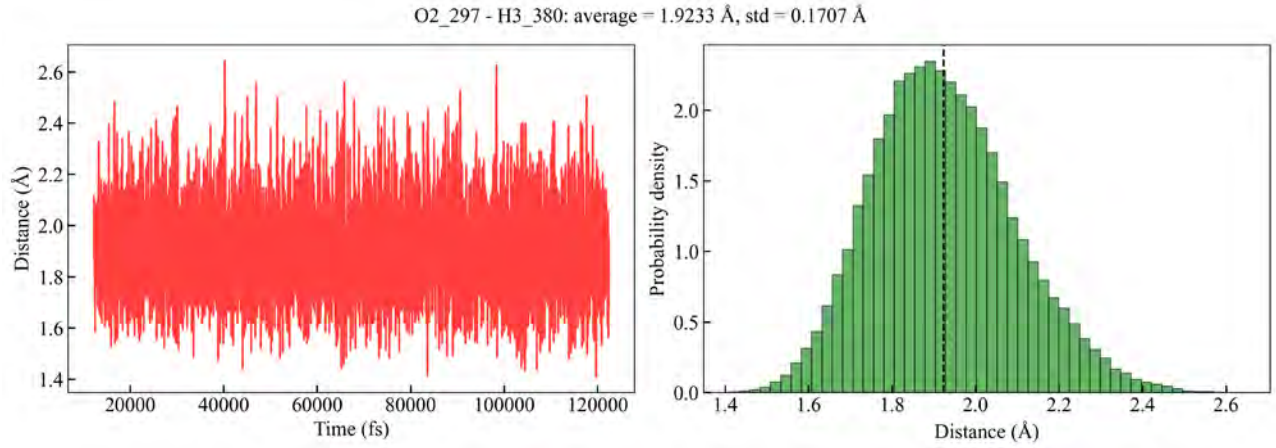
O2_2 - H3_83

Average distance = 1.9244 Å; standard deviation = 0.1706 Å; number of points = 110177



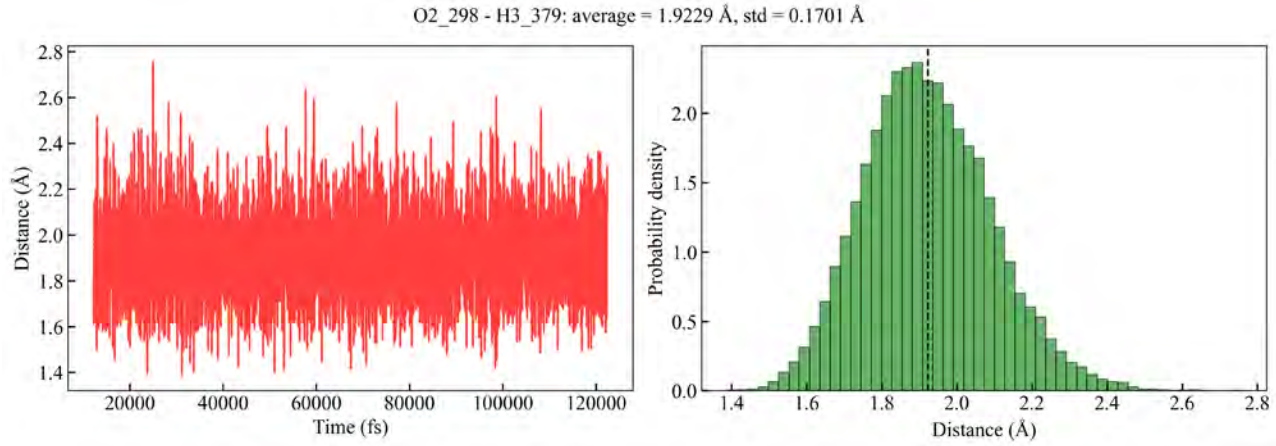
O2_297 - H3_380

Average distance = 1.9233 Å; standard deviation = 0.1707 Å; number of points = 110177



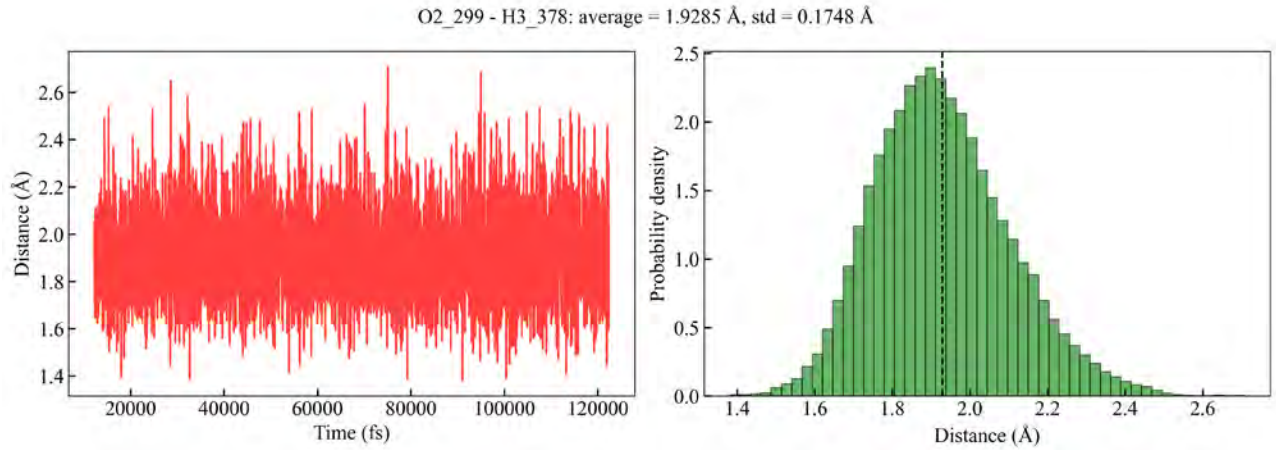
O2_298 - H3_379

Average distance = 1.9229 Å; standard deviation = 0.1701 Å; number of points = 110177



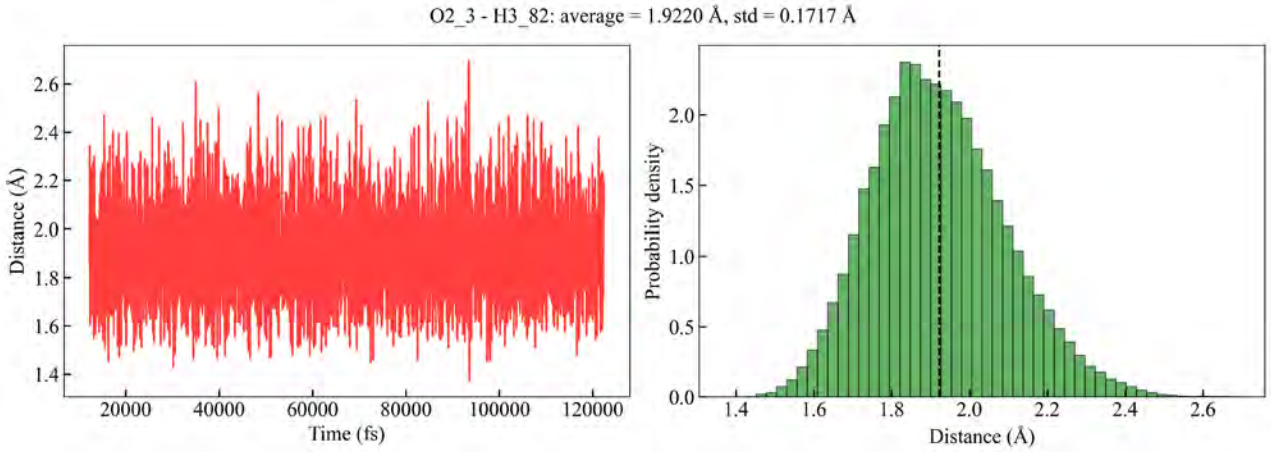
O2_299 - H3_378

Average distance = 1.9285 Å; standard deviation = 0.1748 Å; number of points = 110177



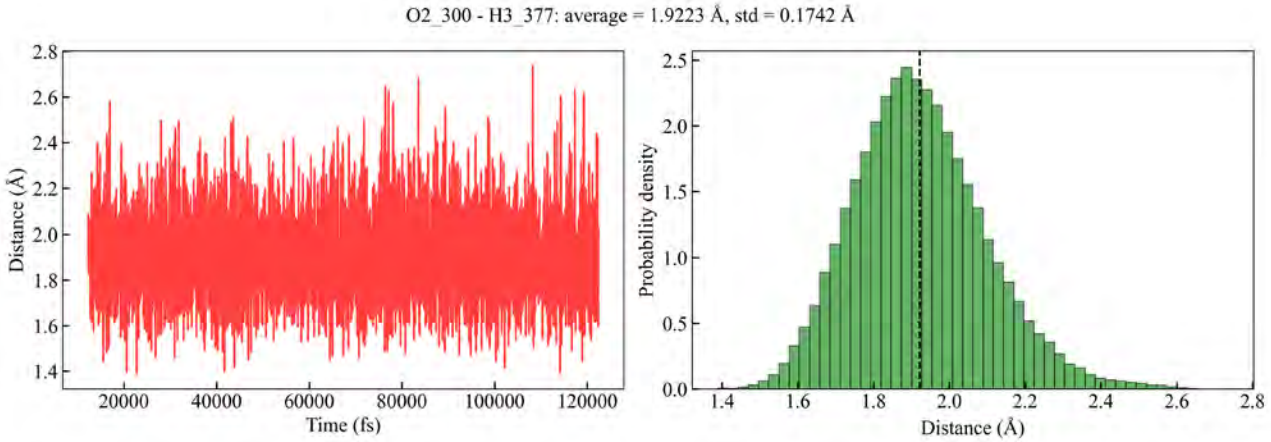
O2_3 - H3_82

Average distance = 1.9220 Å; standard deviation = 0.1717 Å; number of points = 110177



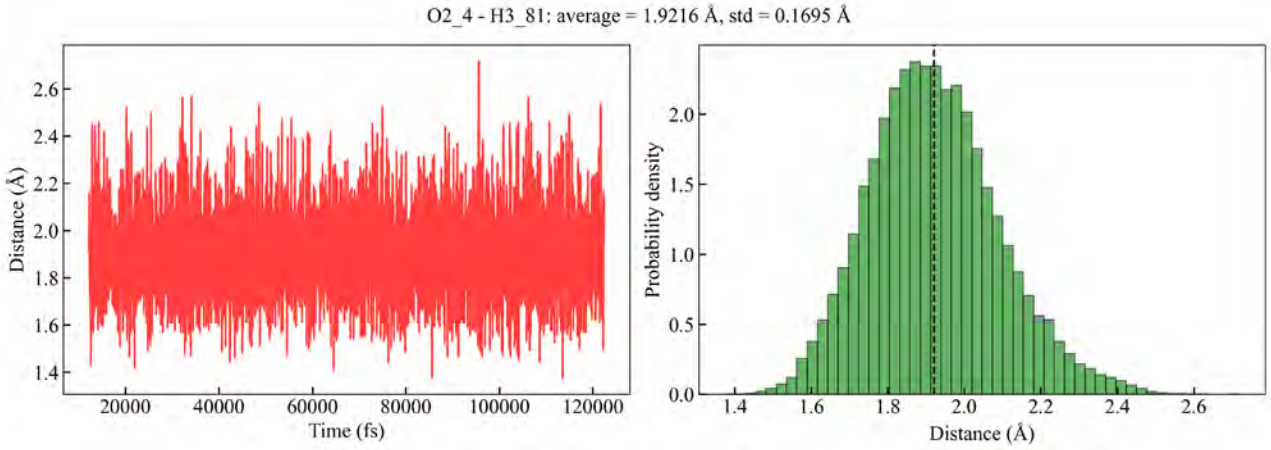
O2_300 - H3_377

Average distance = 1.9223 Å; standard deviation = 0.1742 Å; number of points = 110177



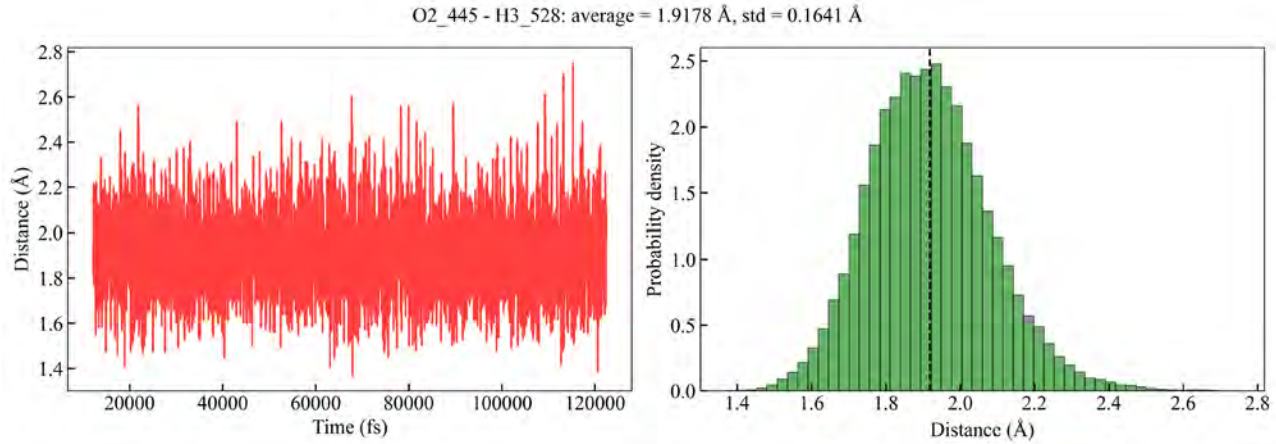
O2_4 - H3_81

Average distance = 1.9216 Å; standard deviation = 0.1695 Å; number of points = 110177



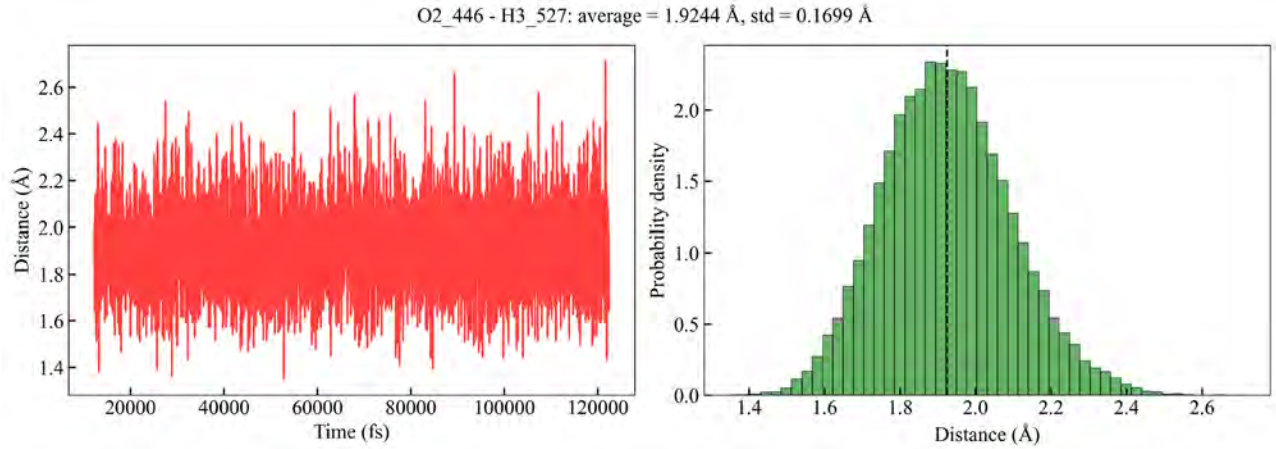
O2_445 - H3_528

Average distance = 1.9178 Å; standard deviation = 0.1641 Å; number of points = 110177



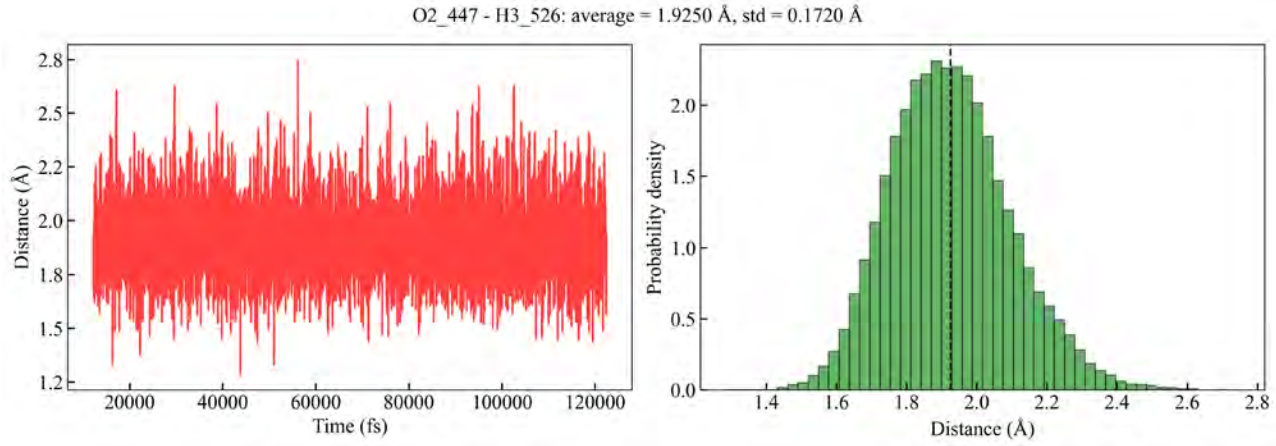
O2_446 - H3_527

Average distance = 1.9244 Å; standard deviation = 0.1699 Å; number of points = 110177



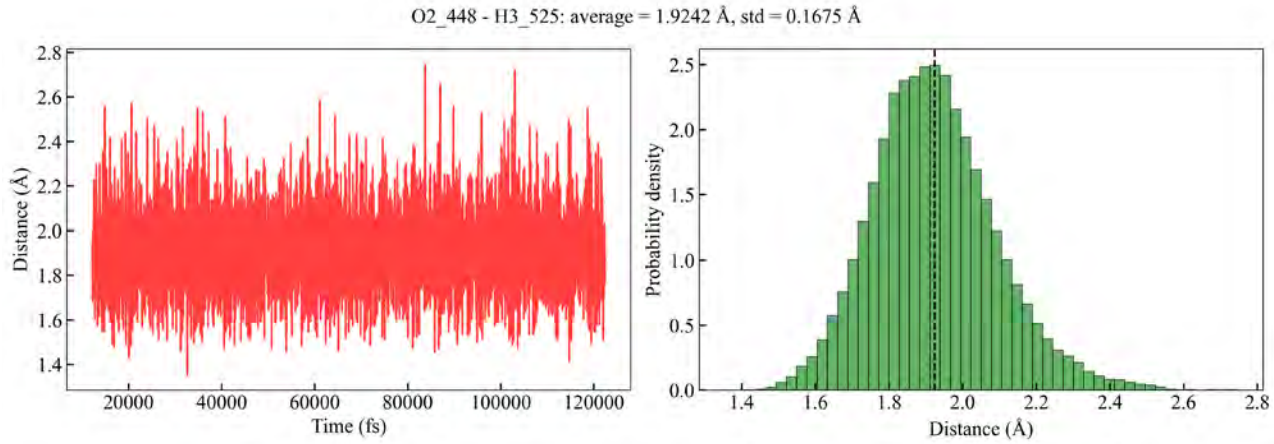
O2_447 - H3_526

Average distance = 1.9250 Å; standard deviation = 0.1720 Å; number of points = 110177



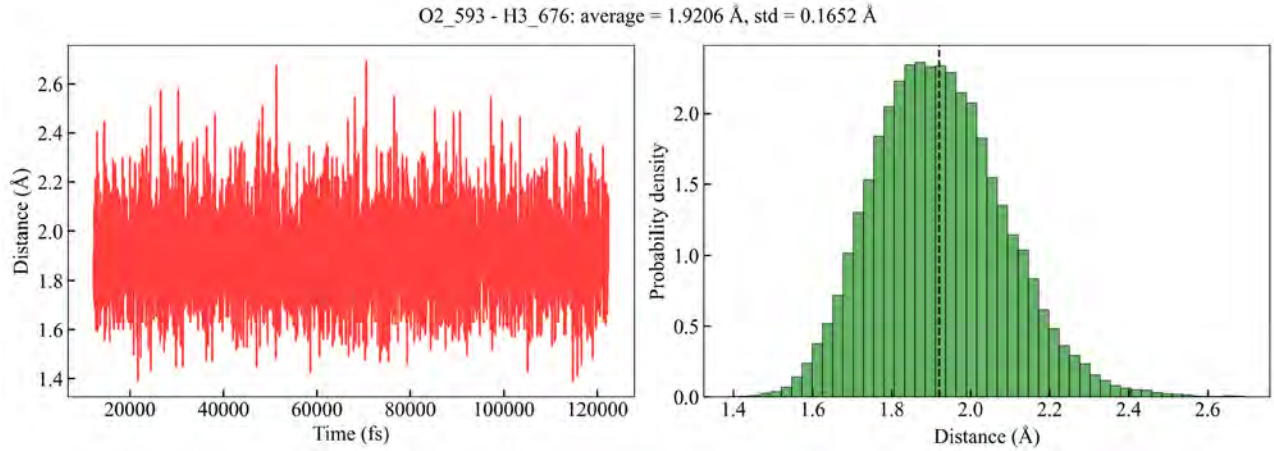
O2_448 - H3_525

Average distance = 1.9242 Å; standard deviation = 0.1675 Å; number of points = 110177



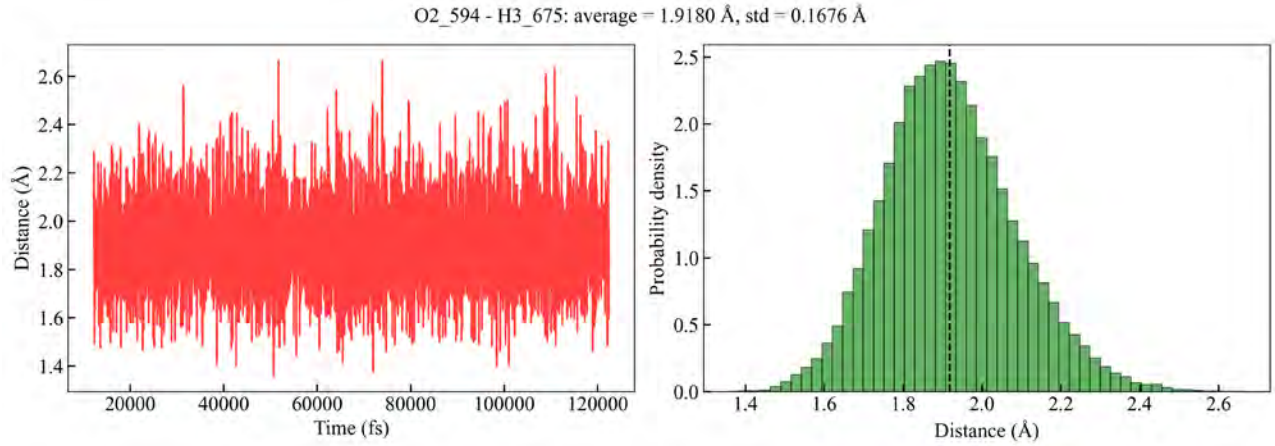
O2_593 - H3_676

Average distance = 1.9206 Å; standard deviation = 0.1652 Å; number of points = 110177



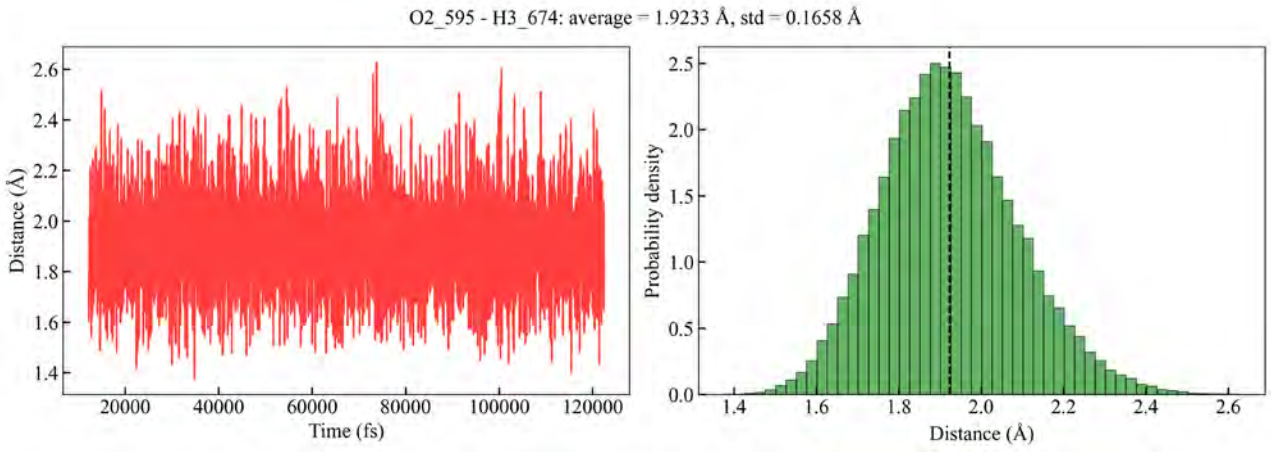
O2_594 - H3_675

Average distance = 1.9180 Å; standard deviation = 0.1676 Å; number of points = 110177



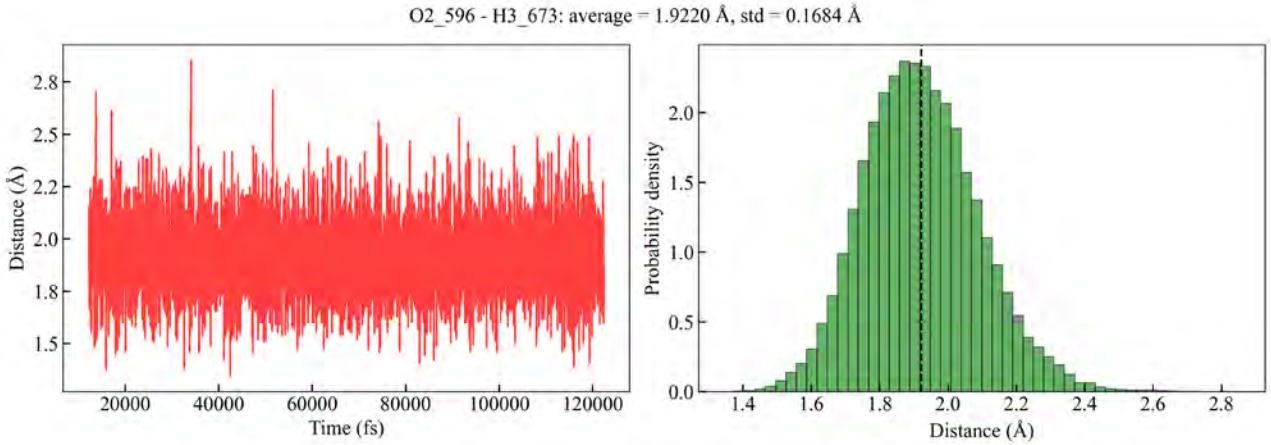
O2_595 - H3_674

Average distance = 1.9233 Å; standard deviation = 0.1658 Å; number of points = 110177



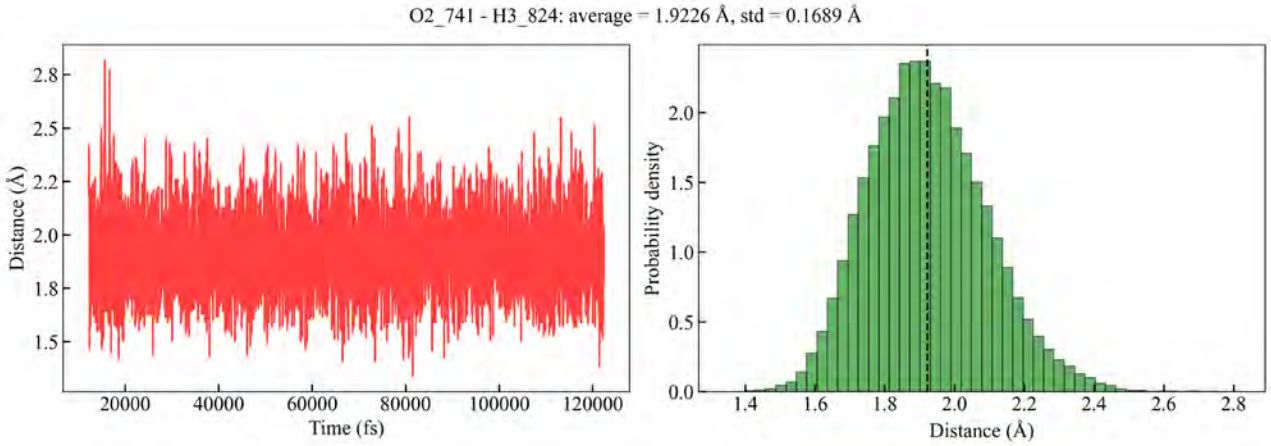
O2_596 - H3_673

Average distance = 1.9220 Å; standard deviation = 0.1684 Å; number of points = 110177



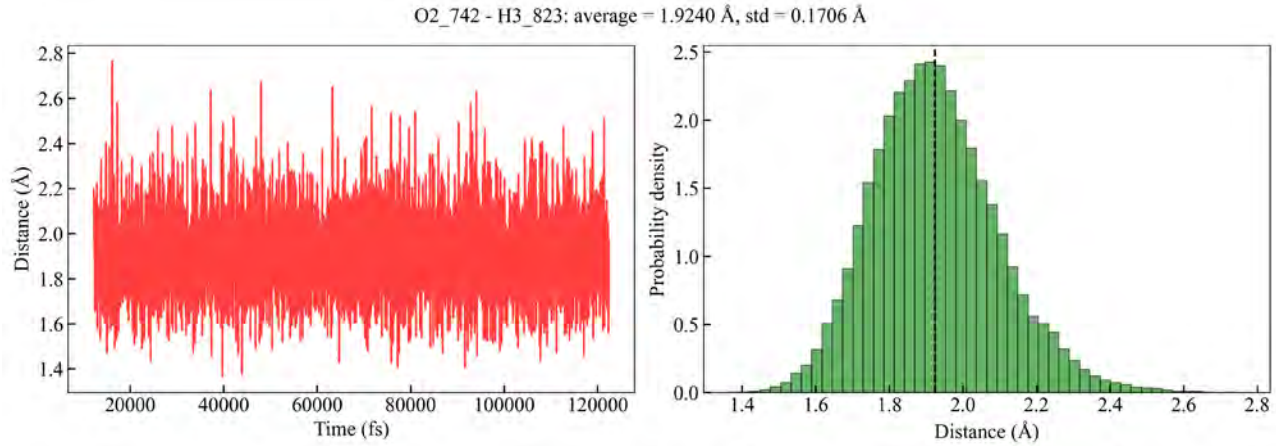
O2_741 - H3_824

Average distance = 1.9226 Å; standard deviation = 0.1689 Å; number of points = 110177



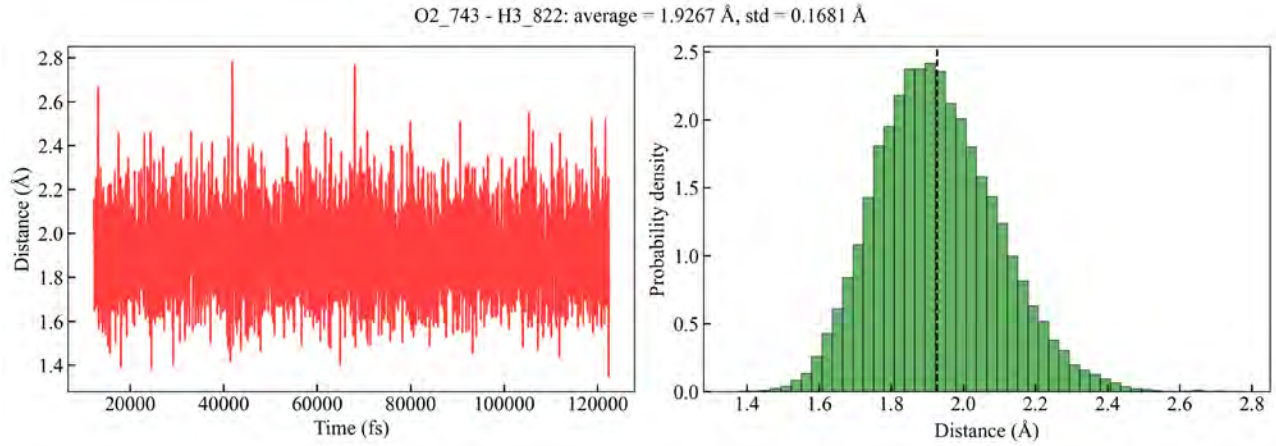
O2_742 - H3_823

Average distance = 1.9240 Å; standard deviation = 0.1706 Å; number of points = 110177



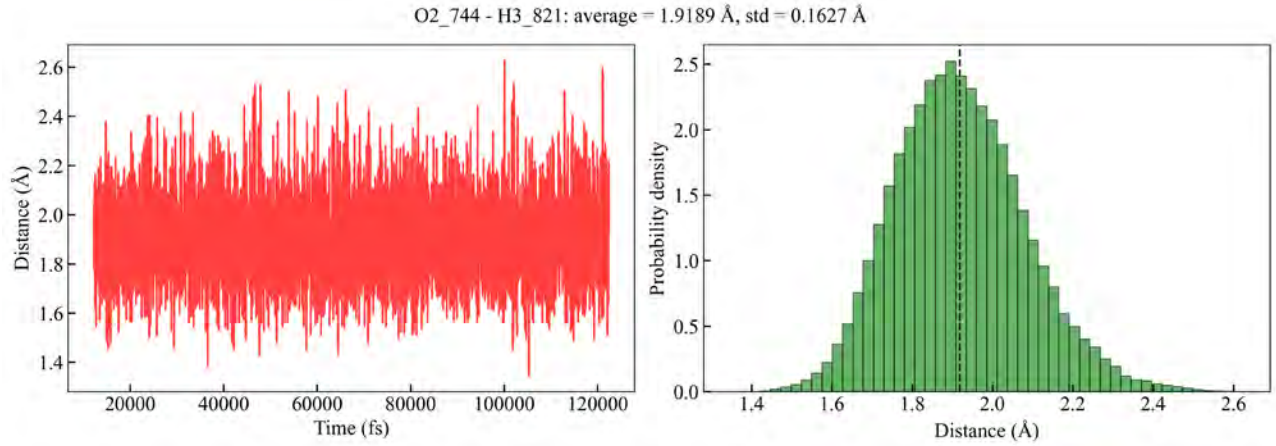
O2_743 - H3_822

Average distance = 1.9267 Å; standard deviation = 0.1681 Å; number of points = 110177



O2_744 - H3_821

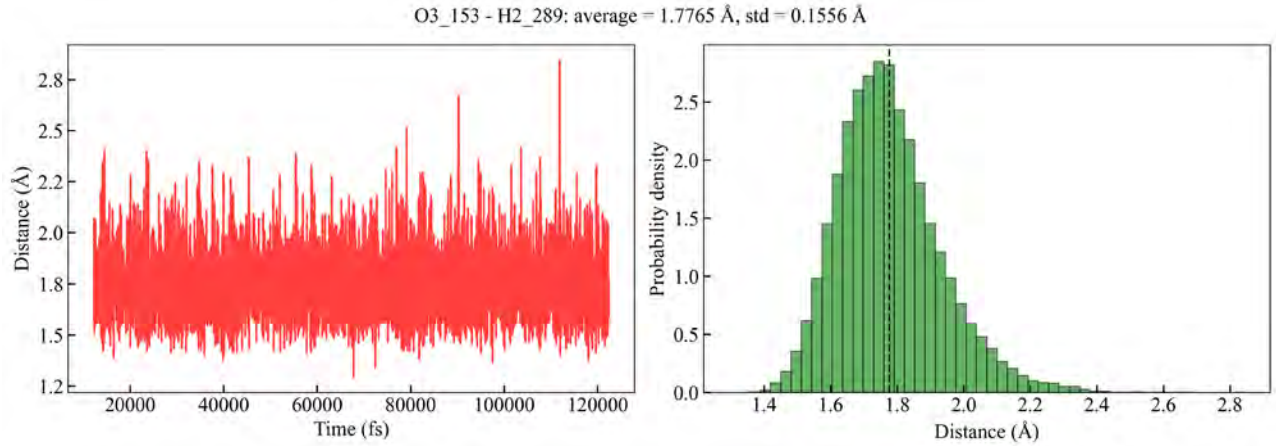
Average distance = 1.9189 Å; standard deviation = 0.1627 Å; number of points = 110177



O3 - H2

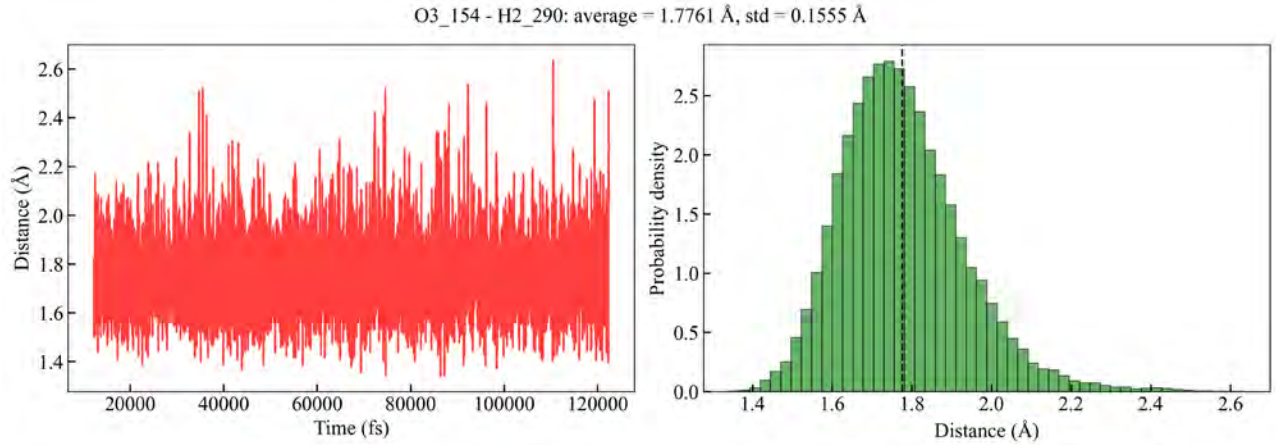
O3_153 - H2_289

Average distance = 1.7765 Å; standard deviation = 0.1556 Å; number of points = 110177



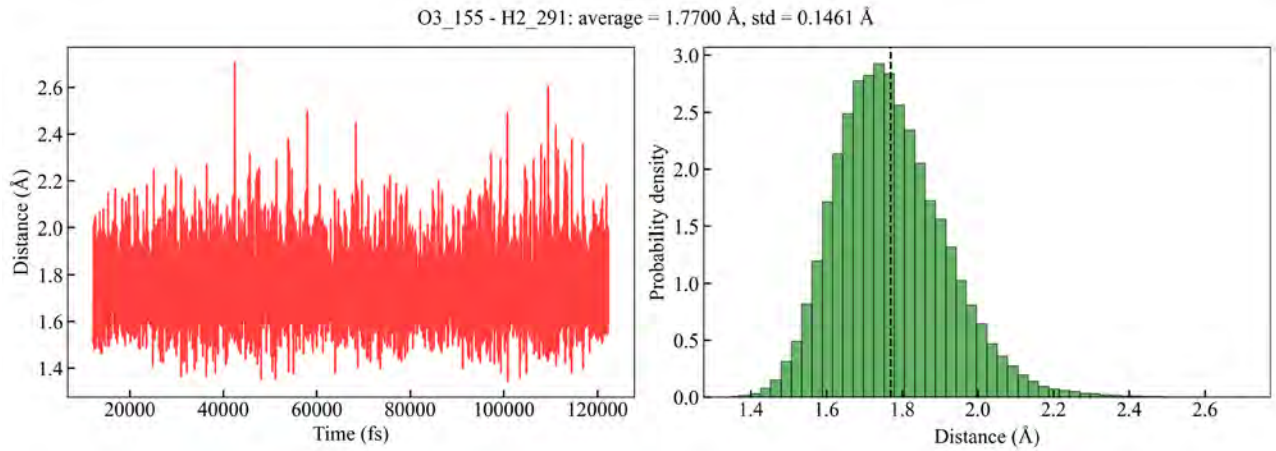
O3_154 - H2_290

Average distance = 1.7761 Å; standard deviation = 0.1555 Å; number of points = 110177



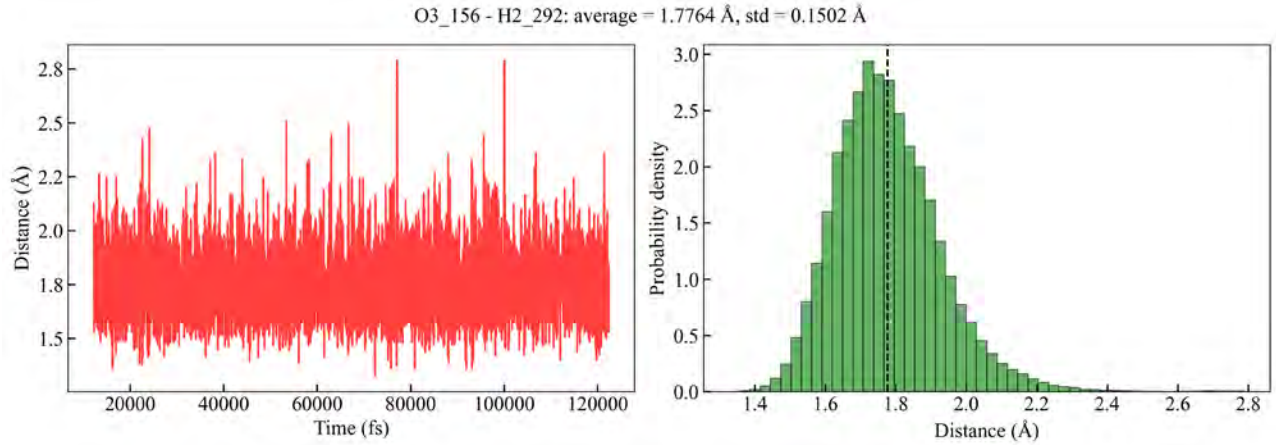
O3_155 - H2_291

Average distance = 1.7700 Å; standard deviation = 0.1461 Å; number of points = 110177



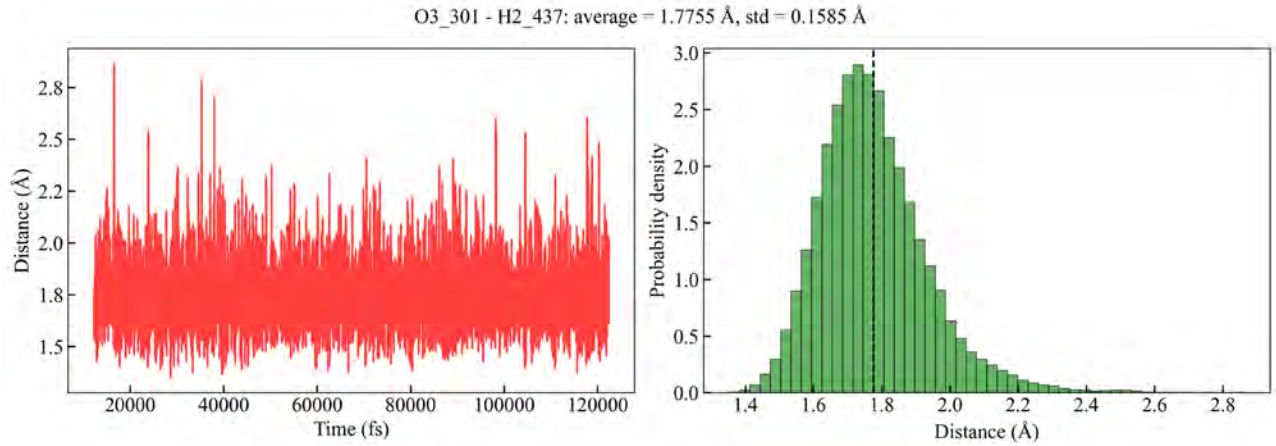
O3_156 - H2_292

Average distance = 1.7764 Å; standard deviation = 0.1502 Å; number of points = 110177



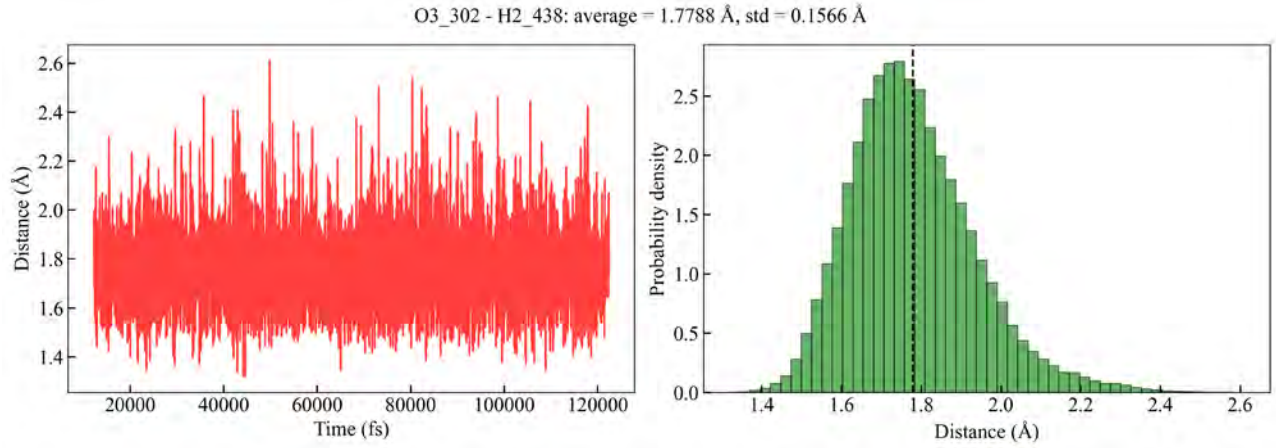
O3_301 - H2_437

Average distance = 1.7755 Å; standard deviation = 0.1585 Å; number of points = 110177



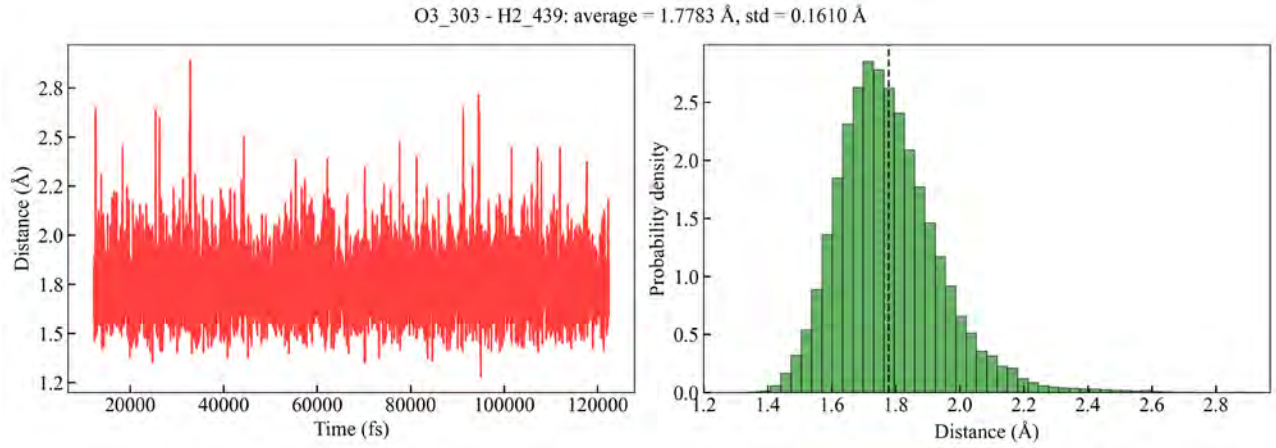
O3_302 - H2_438

Average distance = 1.7788 Å; standard deviation = 0.1566 Å; number of points = 110177



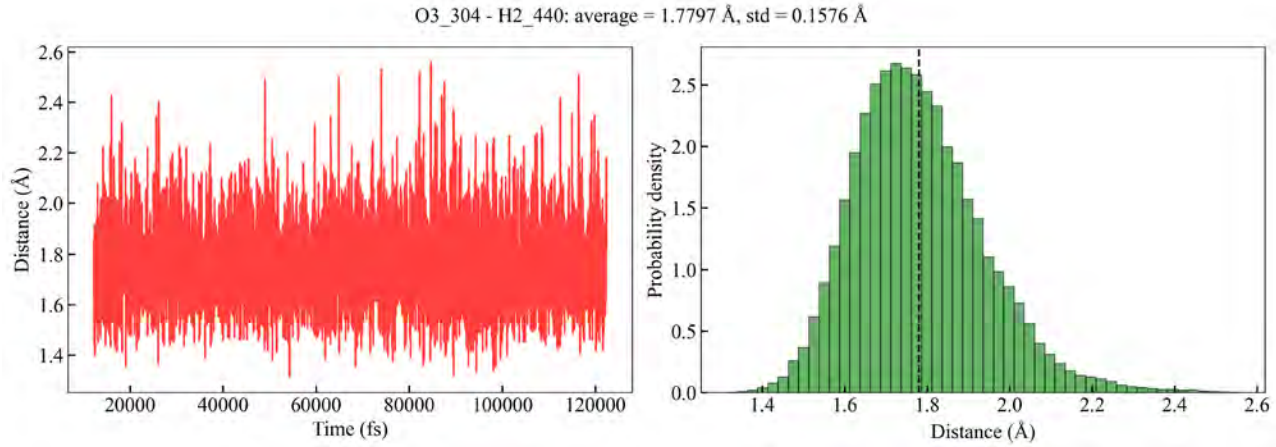
O3_303 - H2_439

Average distance = 1.7783 Å; standard deviation = 0.1610 Å; number of points = 110177



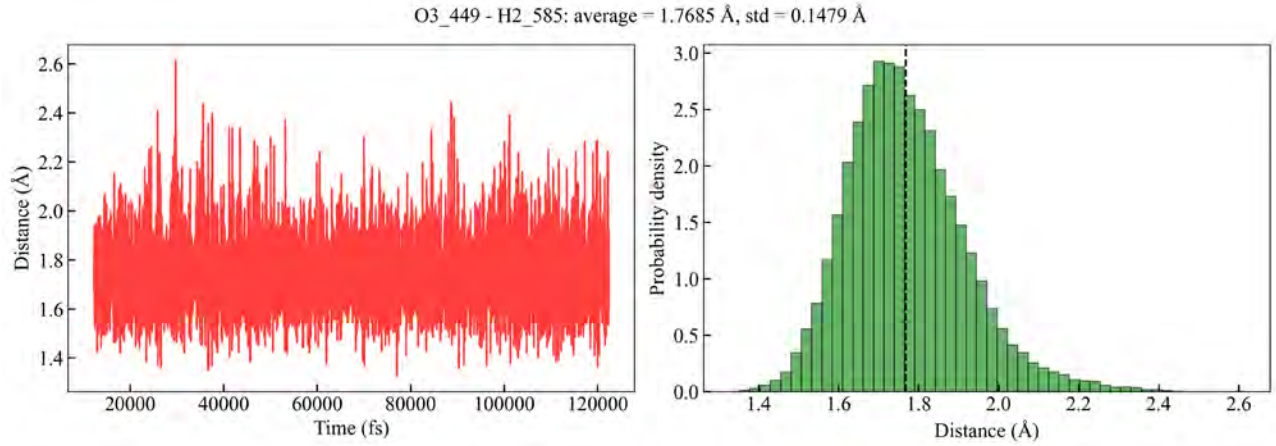
O3_304 - H2_440

Average distance = 1.7797 Å; standard deviation = 0.1576 Å; number of points = 110177



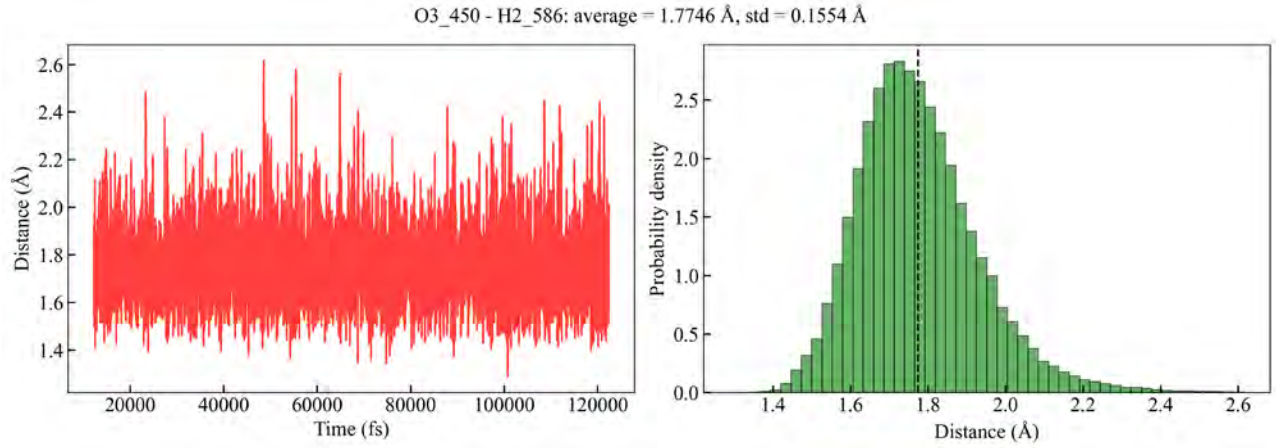
O3_449 - H2_585

Average distance = 1.7685 Å; standard deviation = 0.1479 Å; number of points = 110177



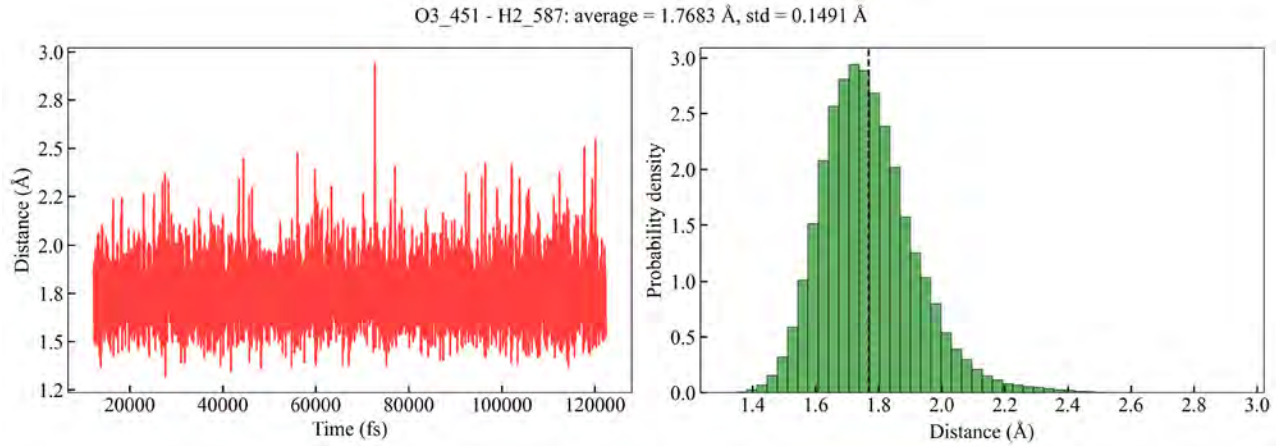
O3_450 - H2_586

Average distance = 1.7746 Å; standard deviation = 0.1554 Å; number of points = 110177



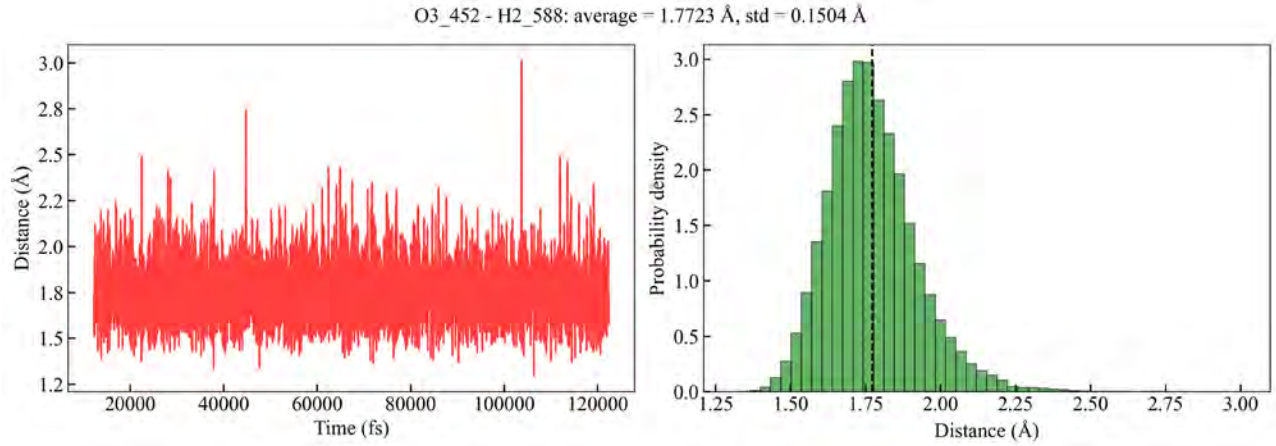
O3_451 - H2_587

Average distance = 1.7683 Å; standard deviation = 0.1491 Å; number of points = 110177



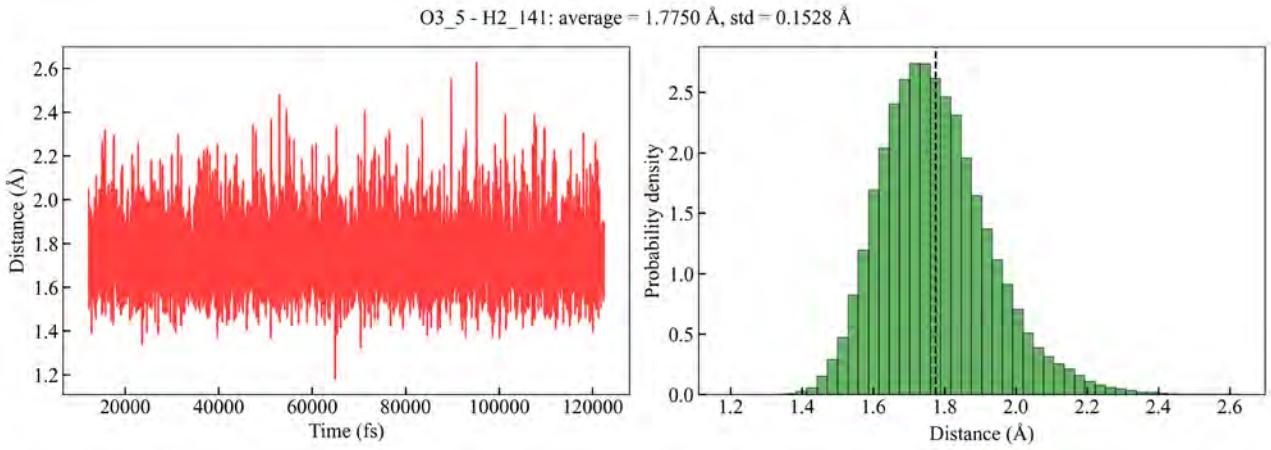
O3_452 - H2_588

Average distance = 1.7723 Å; standard deviation = 0.1504 Å; number of points = 110177



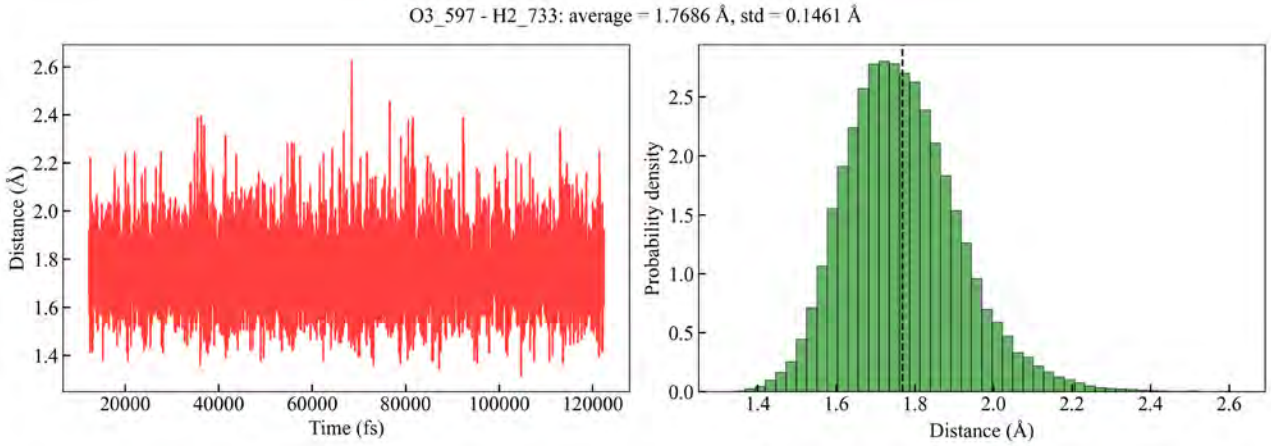
O3_5 - H2_141

Average distance = 1.7750 Å; standard deviation = 0.1528 Å; number of points = 110177



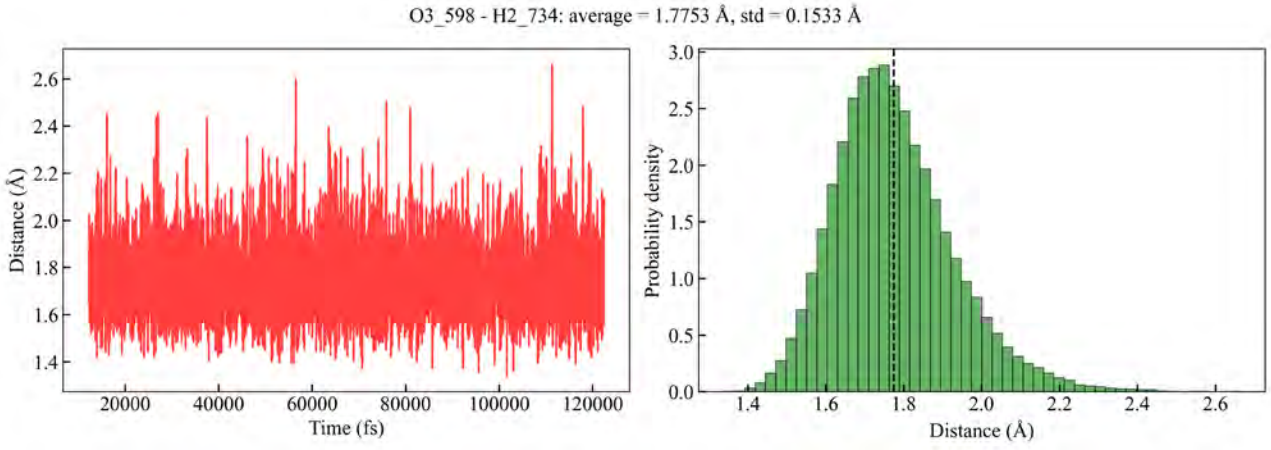
O3_597 - H2_733

Average distance = 1.7686 Å; standard deviation = 0.1461 Å; number of points = 110177



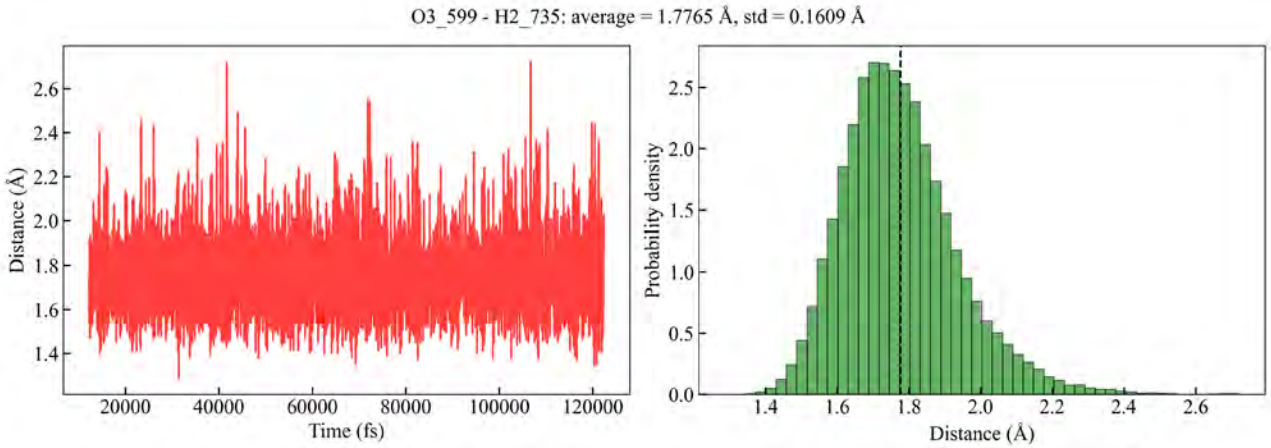
O3_598 - H2_734

Average distance = 1.7753 Å; standard deviation = 0.1533 Å; number of points = 110177



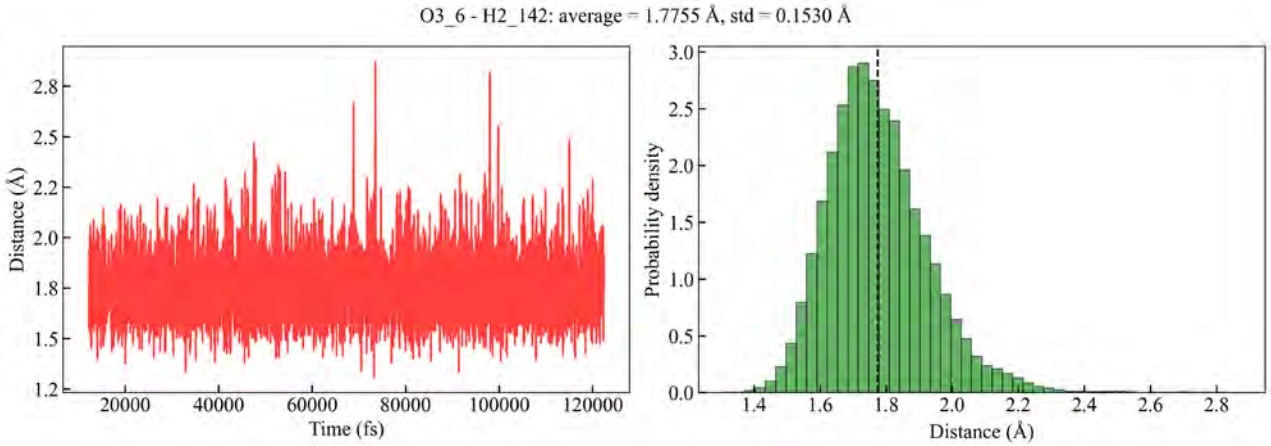
O3_599 - H2_735

Average distance = 1.7765 Å; standard deviation = 0.1609 Å; number of points = 110177



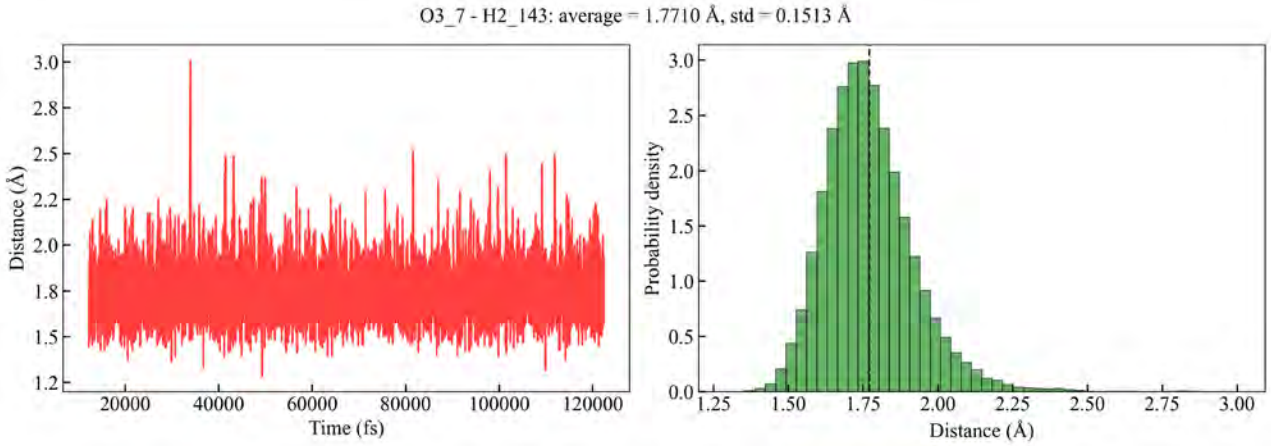
O3_6 - H2_142

Average distance = 1.7755 Å; standard deviation = 0.1530 Å; number of points = 110177



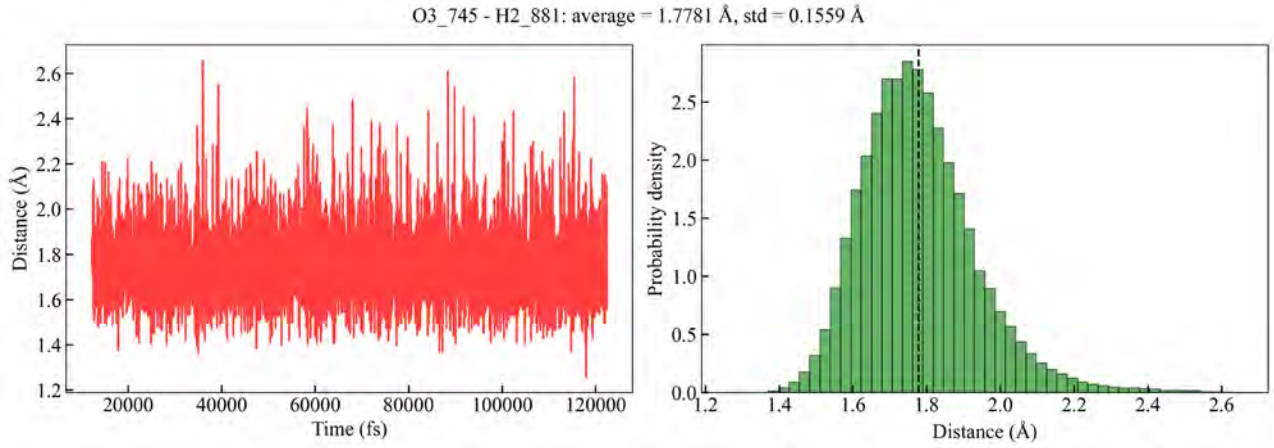
O3_7 - H2_143

Average distance = 1.7710 Å; standard deviation = 0.1513 Å; number of points = 110177



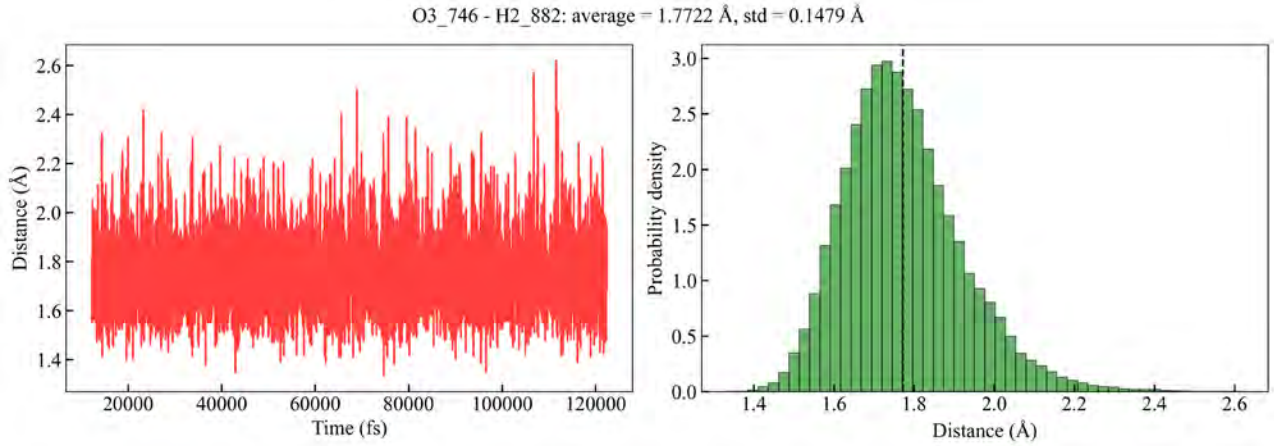
O3_745 - H2_881

Average distance = 1.7781 Å; standard deviation = 0.1559 Å; number of points = 110177



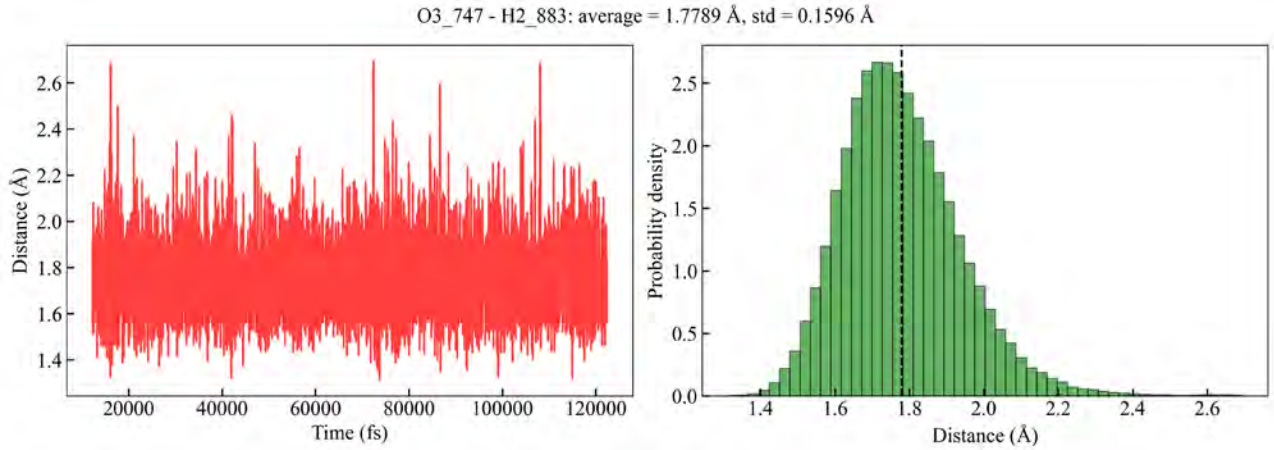
O3_746 - H2_882

Average distance = 1.7722 Å; standard deviation = 0.1479 Å; number of points = 110177



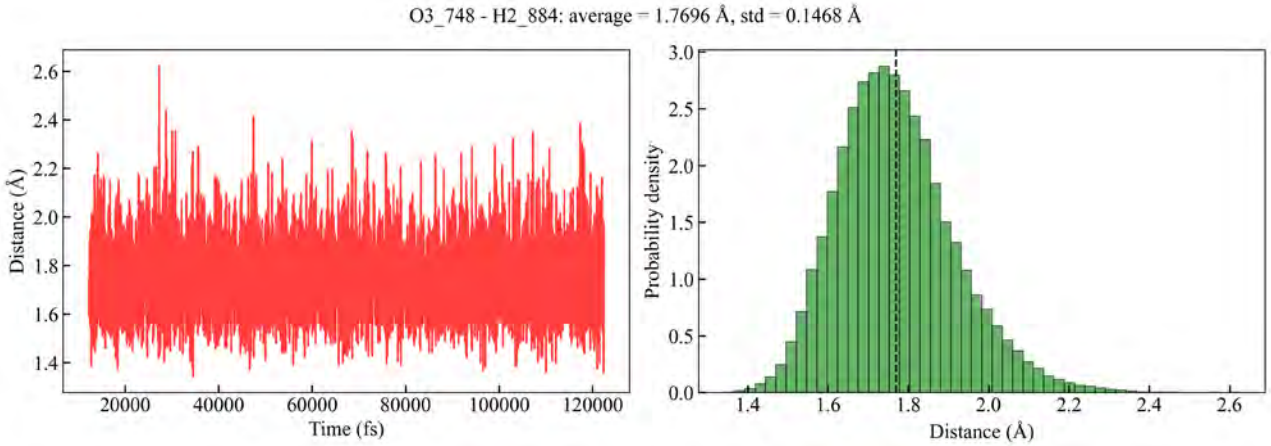
O3_747 - H2_883

Average distance = 1.7789 Å; standard deviation = 0.1596 Å; number of points = 110177



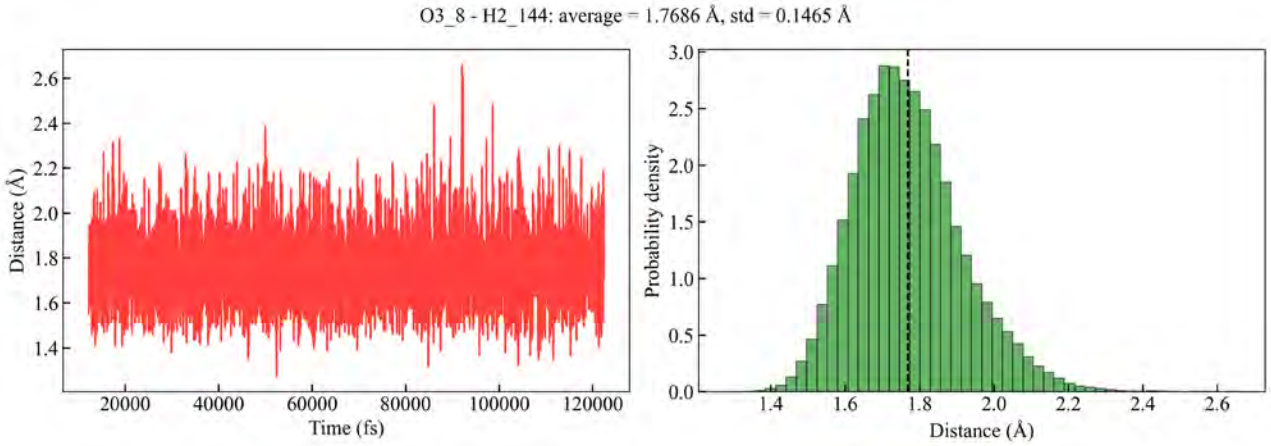
O3_748 - H2_884

Average distance = 1.7696 Å; standard deviation = 0.1468 Å; number of points = 110177



O3_8 - H2_144

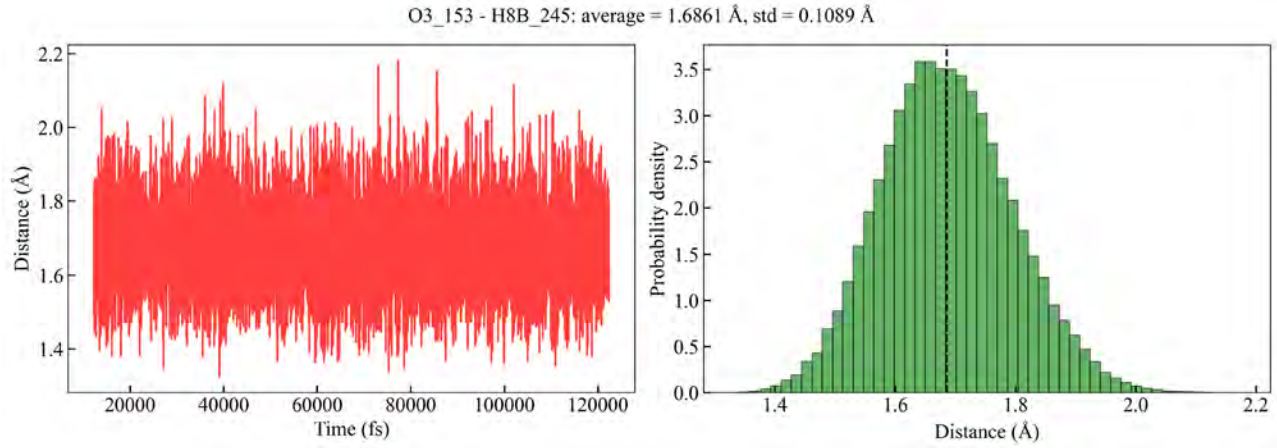
Average distance = 1.7686 Å; standard deviation = 0.1465 Å; number of points = 110177



O3 - H8B

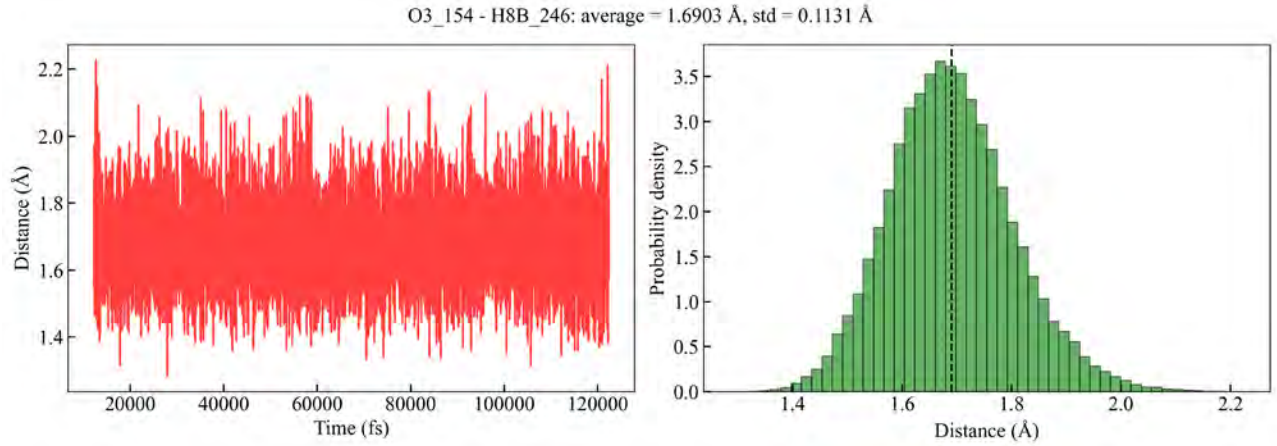
O3_153 - H8B_245

Average distance = 1.6861 Å; standard deviation = 0.1089 Å; number of points = 110177



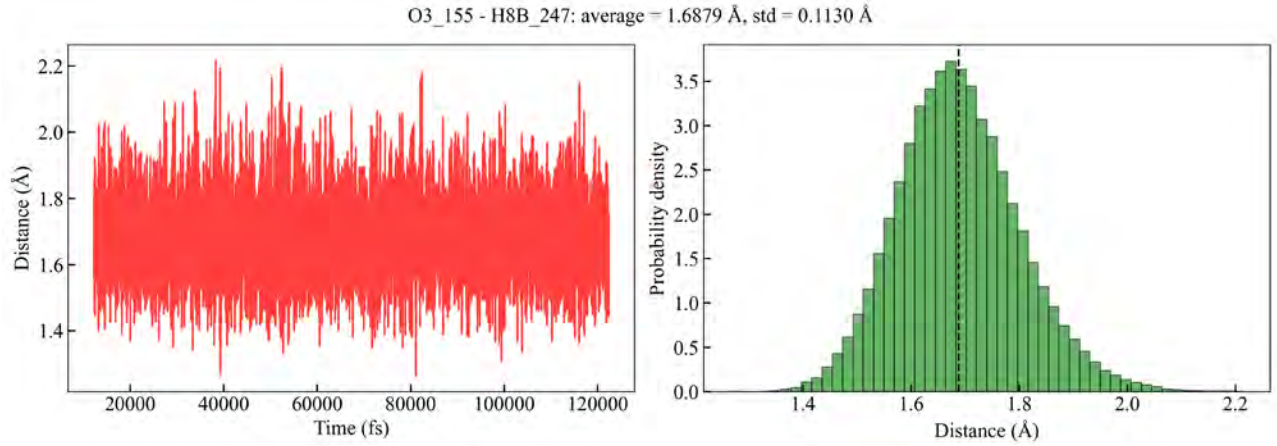
O3_154 - H8B_246

Average distance = 1.6903 Å; standard deviation = 0.1131 Å; number of points = 110177



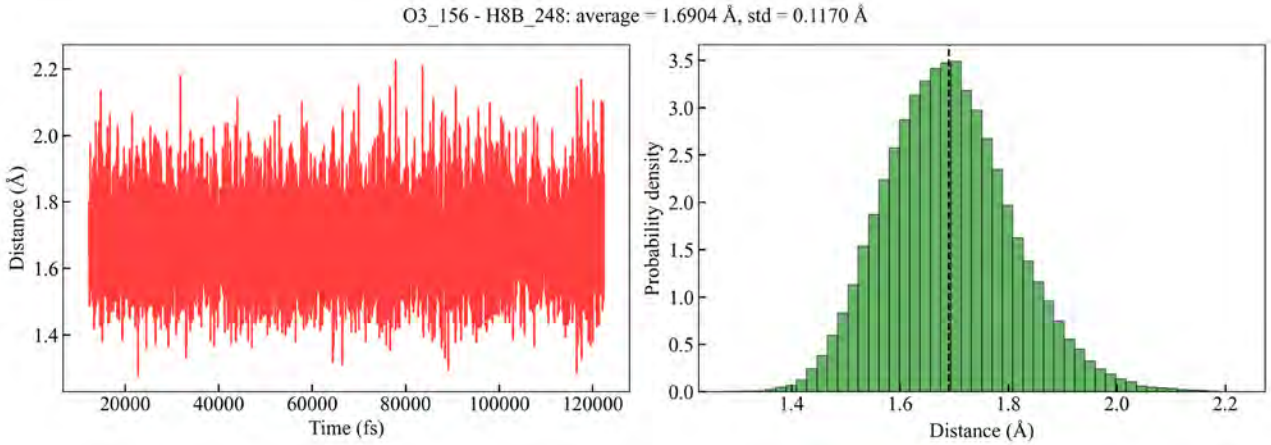
O3_155 - H8B_247

Average distance = 1.6879 Å; standard deviation = 0.1130 Å; number of points = 110177



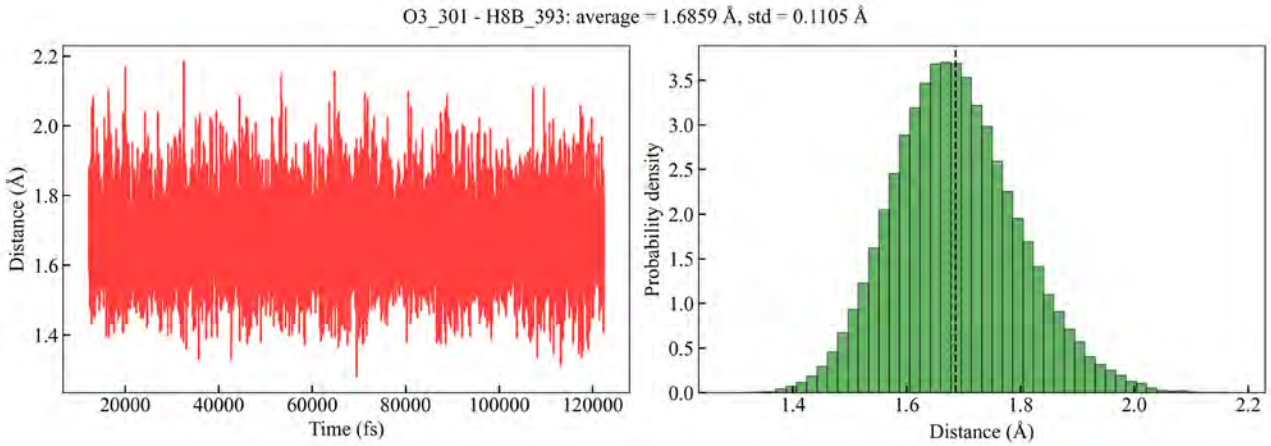
O3_156 - H8B_248

Average distance = 1.6904 Å; standard deviation = 0.1170 Å; number of points = 110177



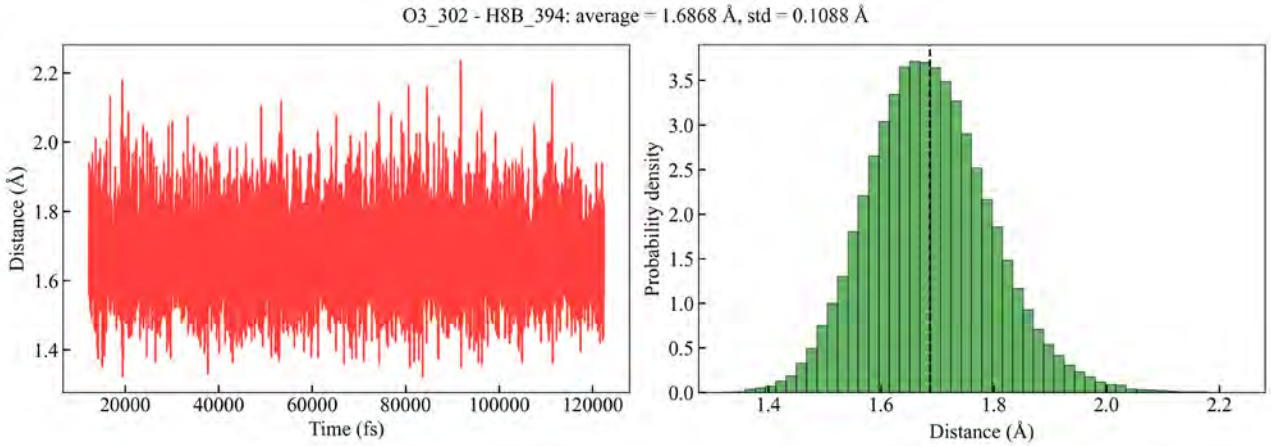
O3_301 - H8B_393

Average distance = 1.6859 Å; standard deviation = 0.1105 Å; number of points = 110177



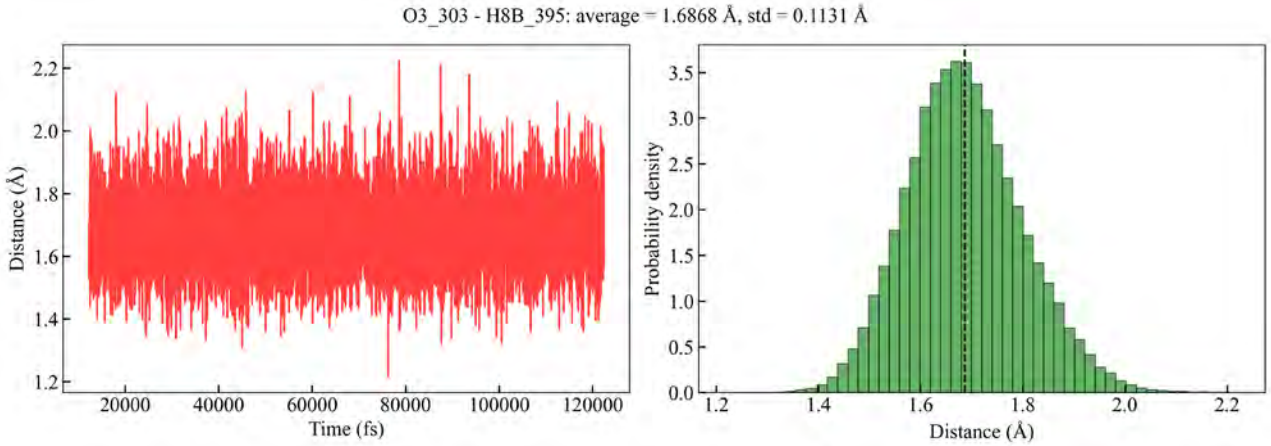
O3_302 - H8B_394

Average distance = 1.6868 Å; standard deviation = 0.1088 Å; number of points = 110177



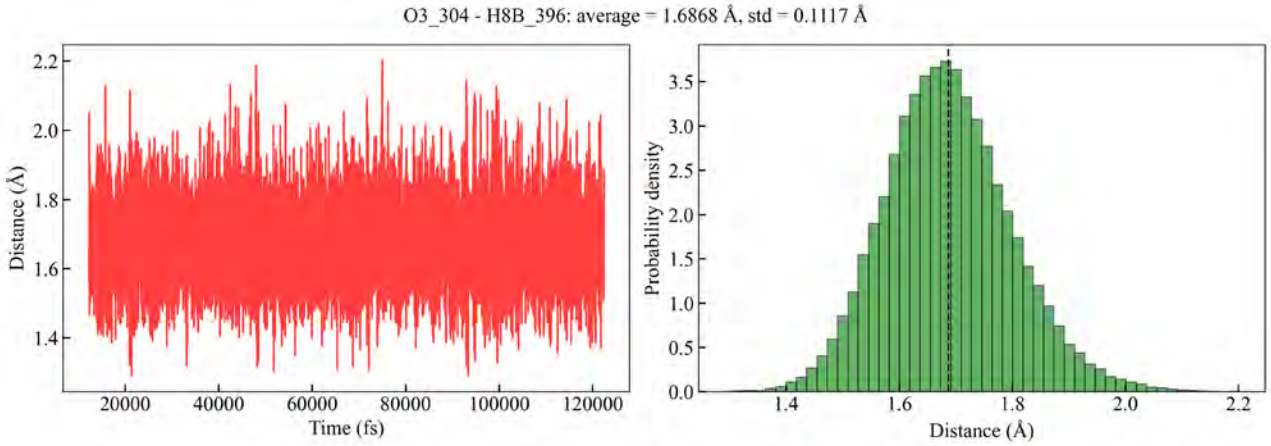
O3_303 - H8B_395

Average distance = 1.6868 Å; standard deviation = 0.1131 Å; number of points = 110177



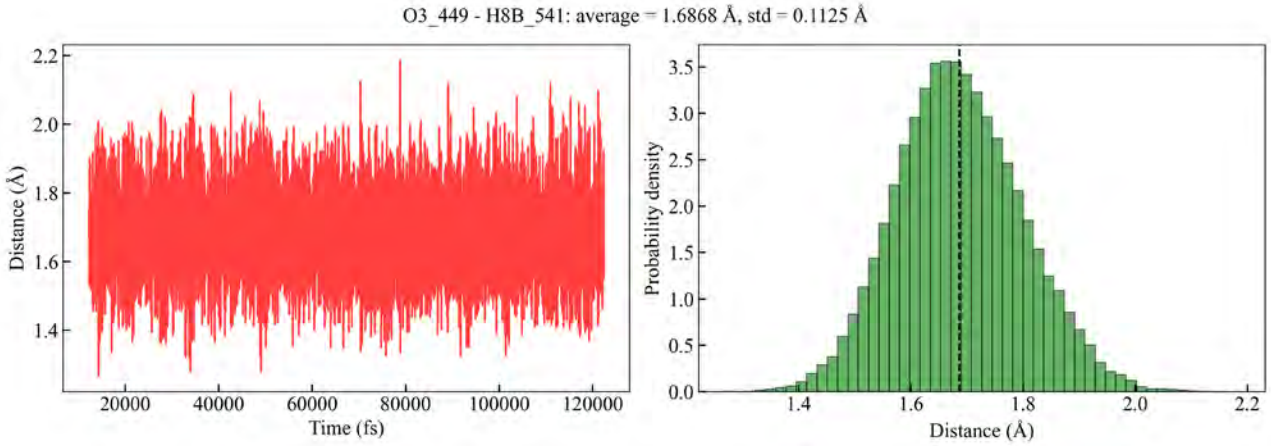
O3_304 - H8B_396

Average distance = 1.6868 Å; standard deviation = 0.1117 Å; number of points = 110177



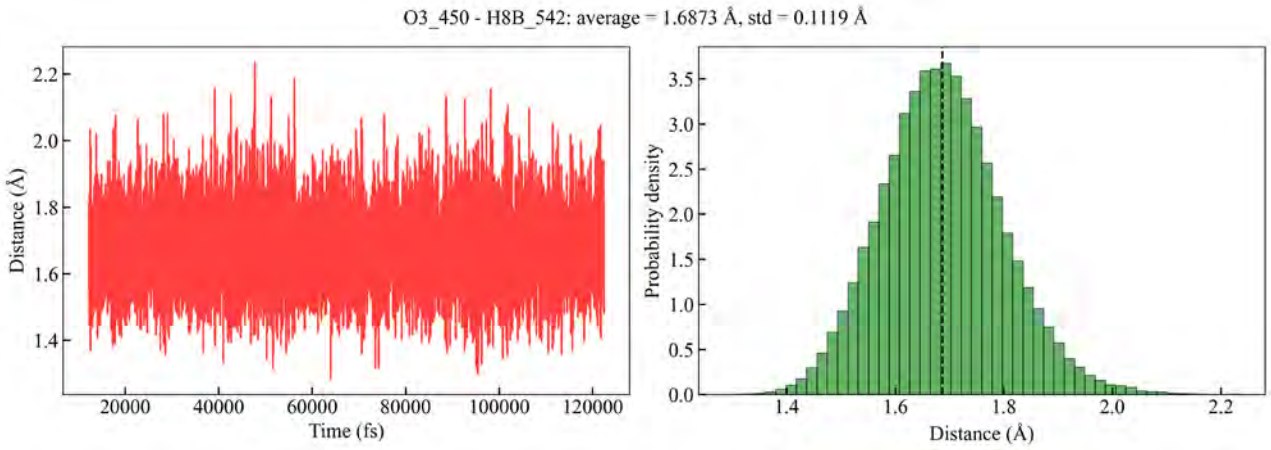
O3_449 - H8B_541

Average distance = 1.6868 Å; standard deviation = 0.1125 Å; number of points = 110177



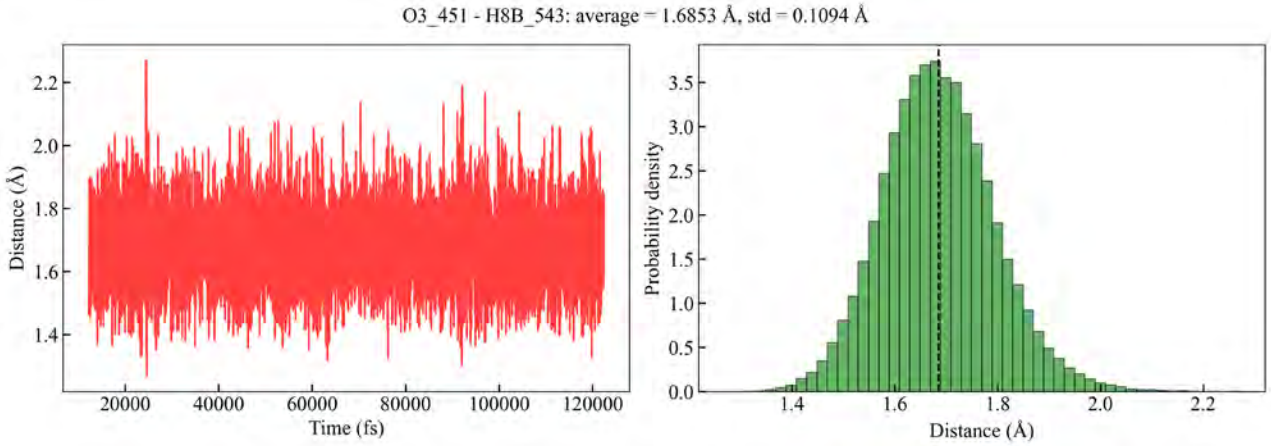
O3_450 - H8B_542

Average distance = 1.6873 Å; standard deviation = 0.1119 Å; number of points = 110177



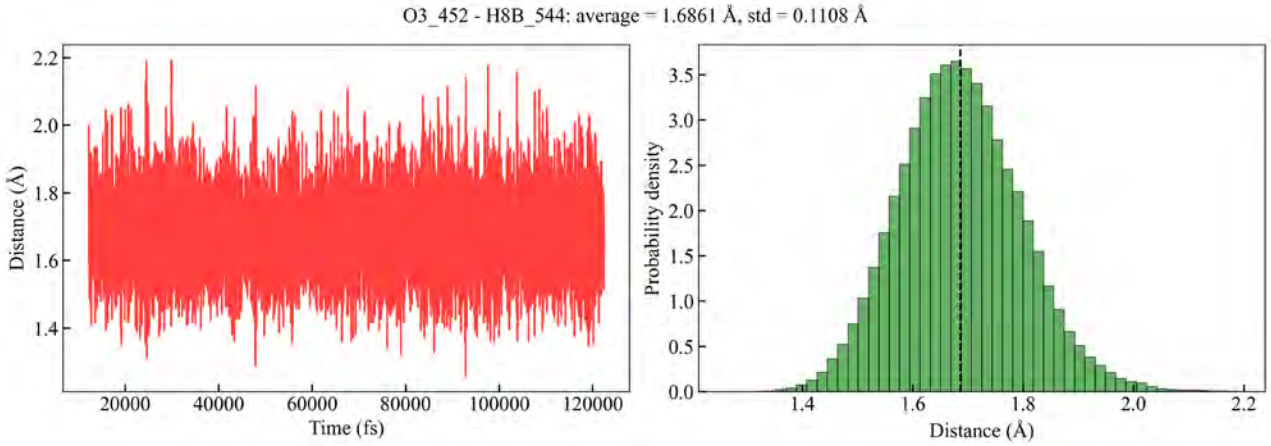
O3_451 - H8B_543

Average distance = 1.6853 Å; standard deviation = 0.1094 Å; number of points = 110177



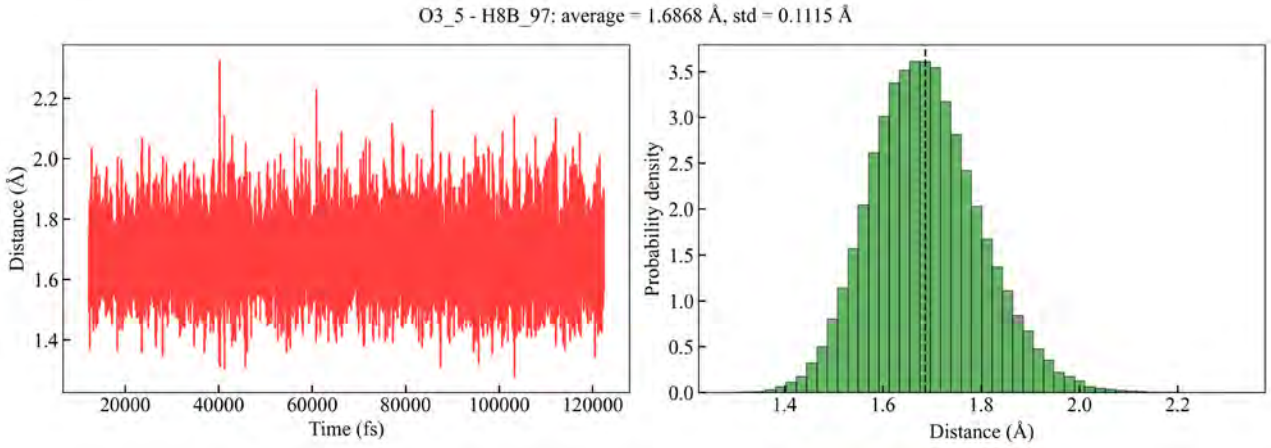
O3_452 - H8B_544

Average distance = 1.6861 Å; standard deviation = 0.1108 Å; number of points = 110177



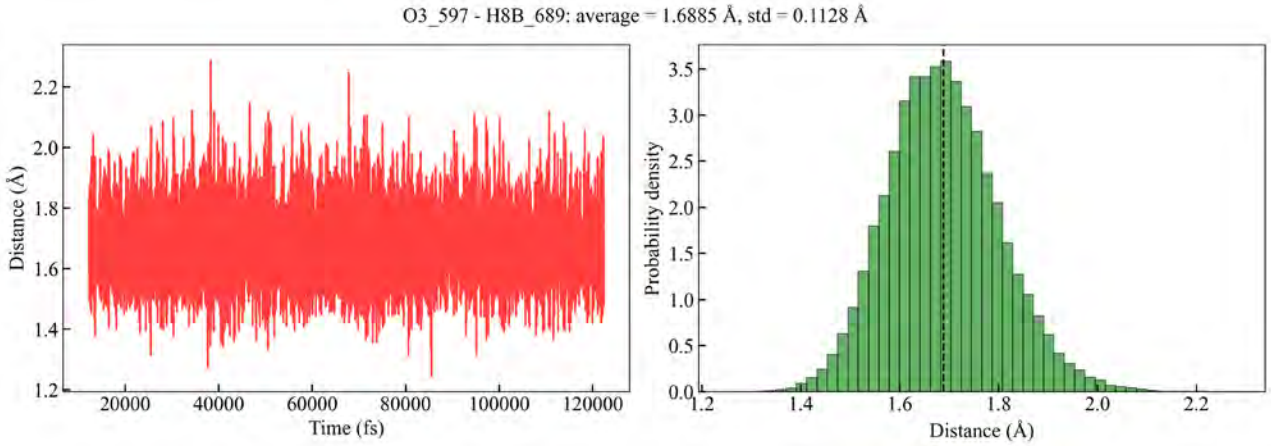
O3_5 - H8B_97

Average distance = 1.6868 Å; standard deviation = 0.1115 Å; number of points = 110177



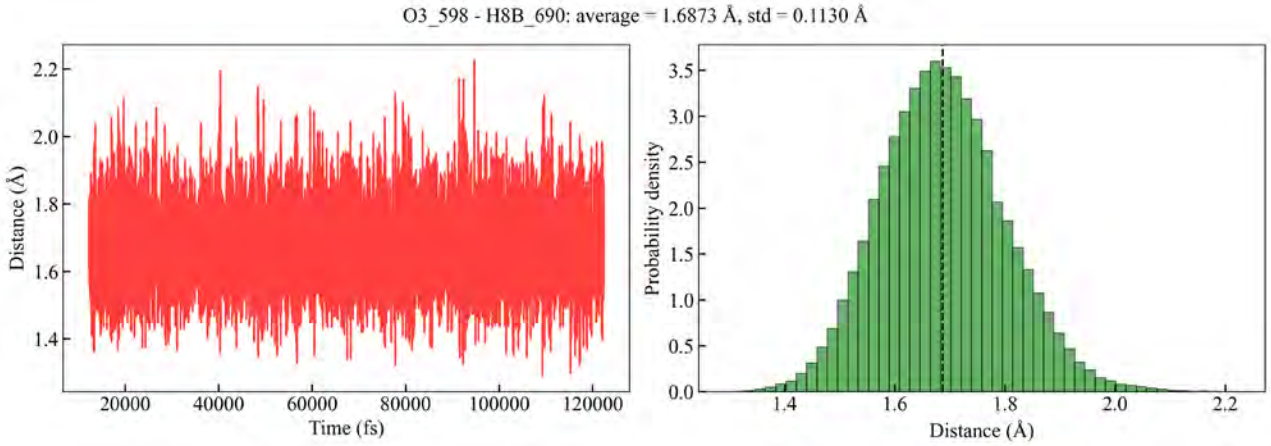
O3_597 - H8B_689

Average distance = 1.6885 Å; standard deviation = 0.1128 Å; number of points = 110177



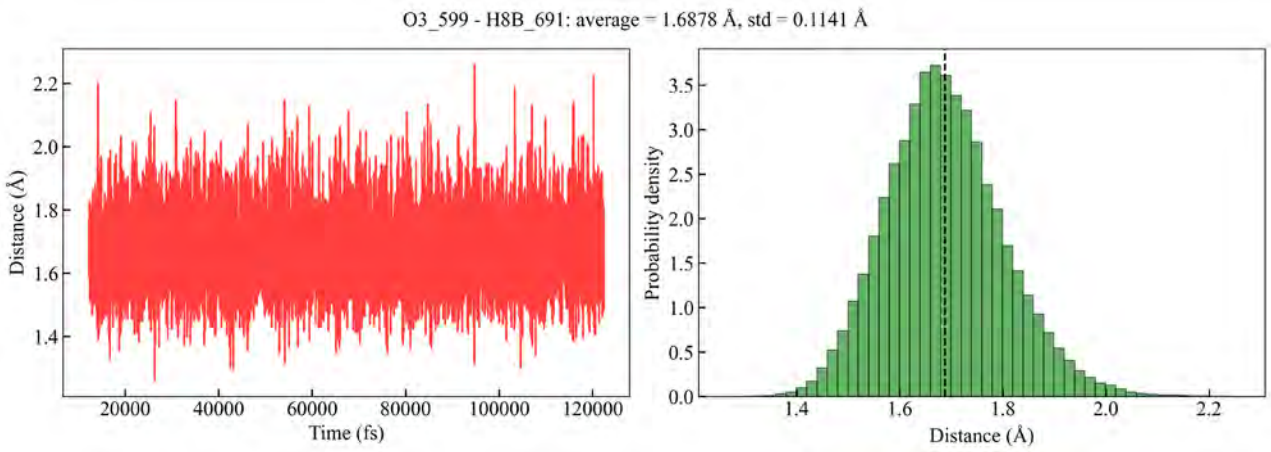
O3_598 - H8B_690

Average distance = 1.6873 Å; standard deviation = 0.1130 Å; number of points = 110177



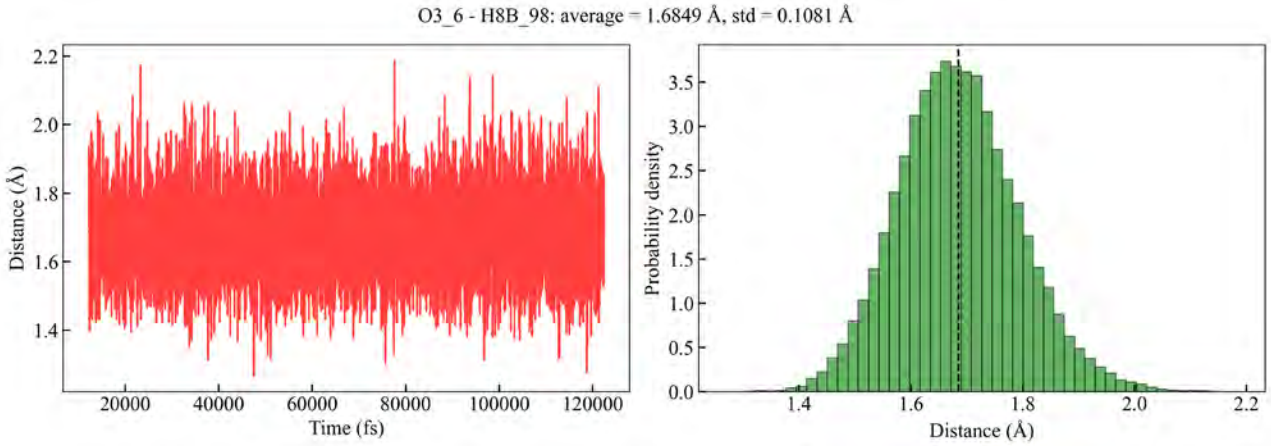
O3_599 - H8B_691

Average distance = 1.6878 Å; standard deviation = 0.1141 Å; number of points = 110177



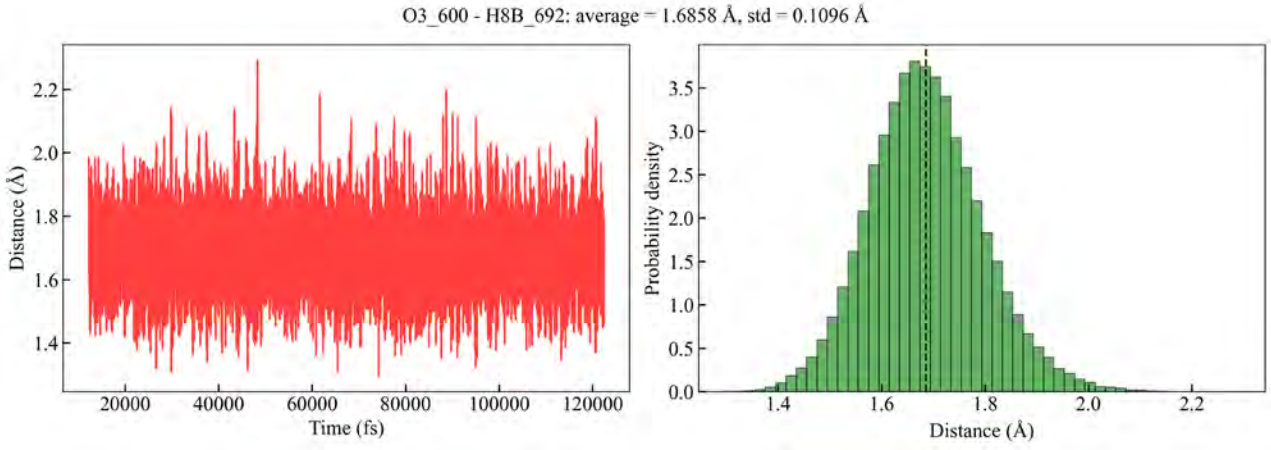
O3_6 - H8B_98

Average distance = 1.6849 Å; standard deviation = 0.1081 Å; number of points = 110177



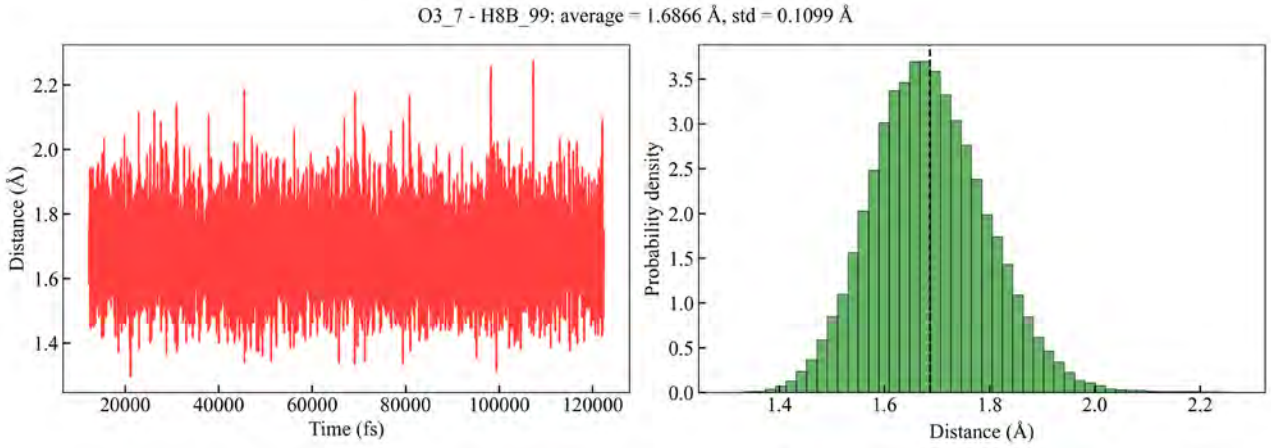
O3_600 - H8B_692

Average distance = 1.6858 Å; standard deviation = 0.1096 Å; number of points = 110177



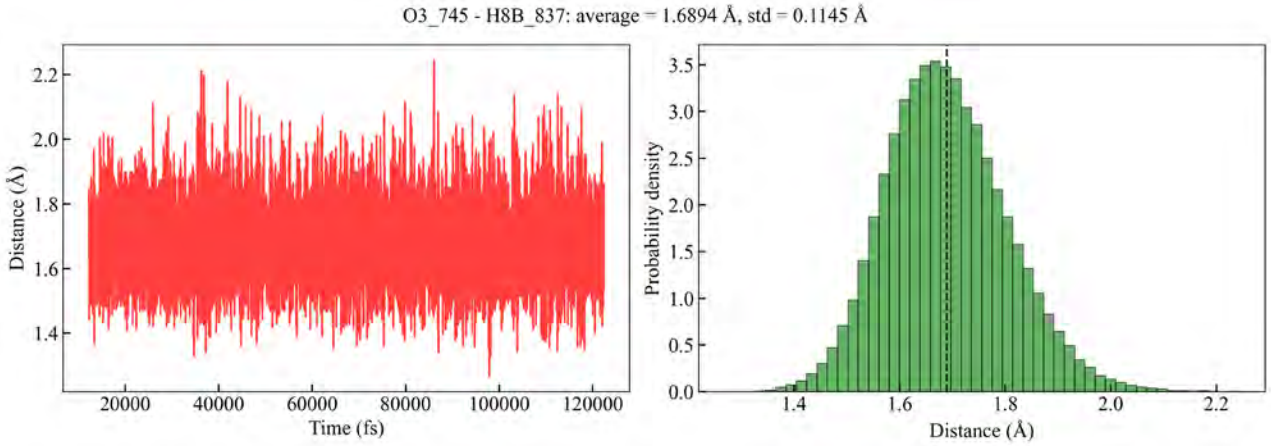
O3_7 - H8B_99

Average distance = 1.6866 Å; standard deviation = 0.1099 Å; number of points = 110177



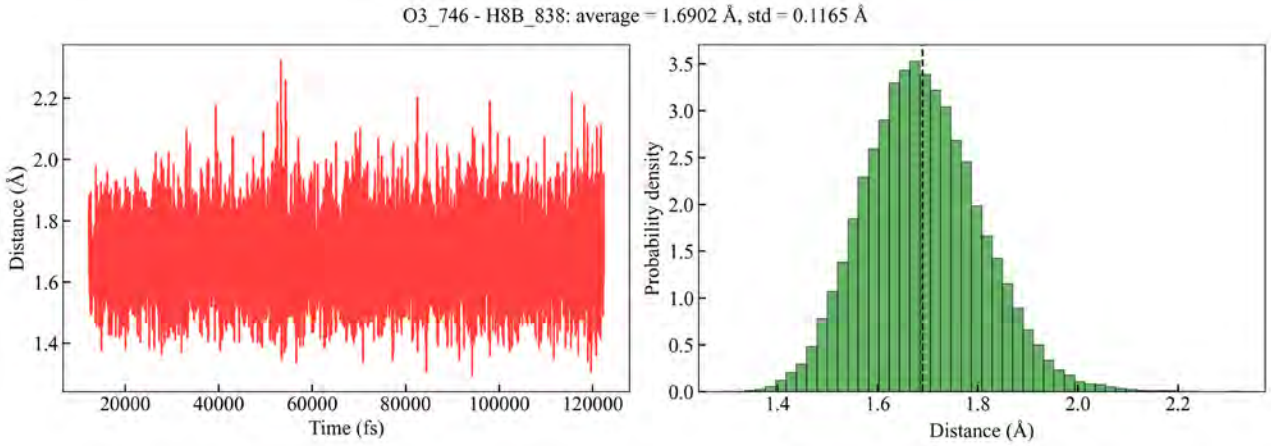
O3_745 - H8B_837

Average distance = 1.6894 Å; standard deviation = 0.1145 Å; number of points = 110177



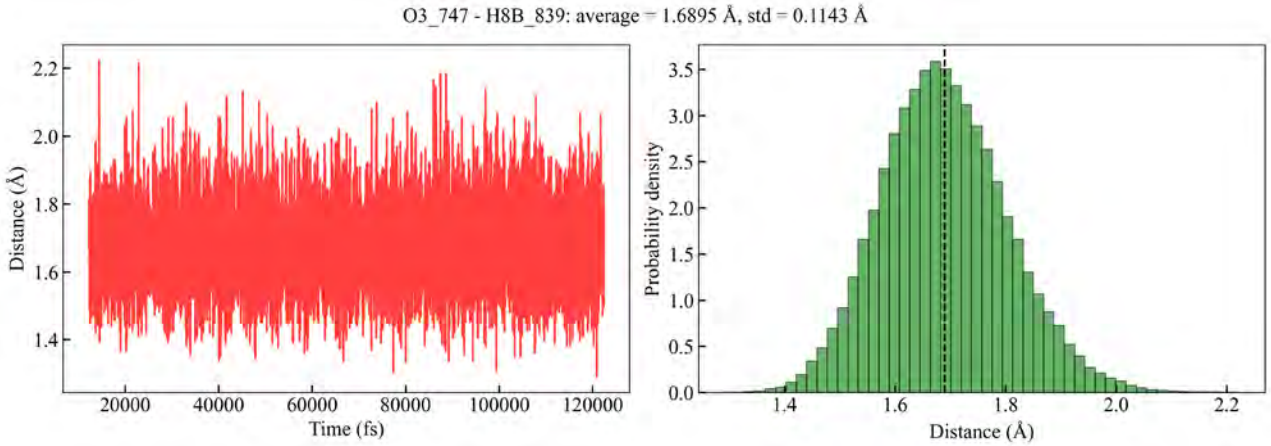
O3_746 - H8B_838

Average distance = 1.6902 Å; standard deviation = 0.1165 Å; number of points = 110177



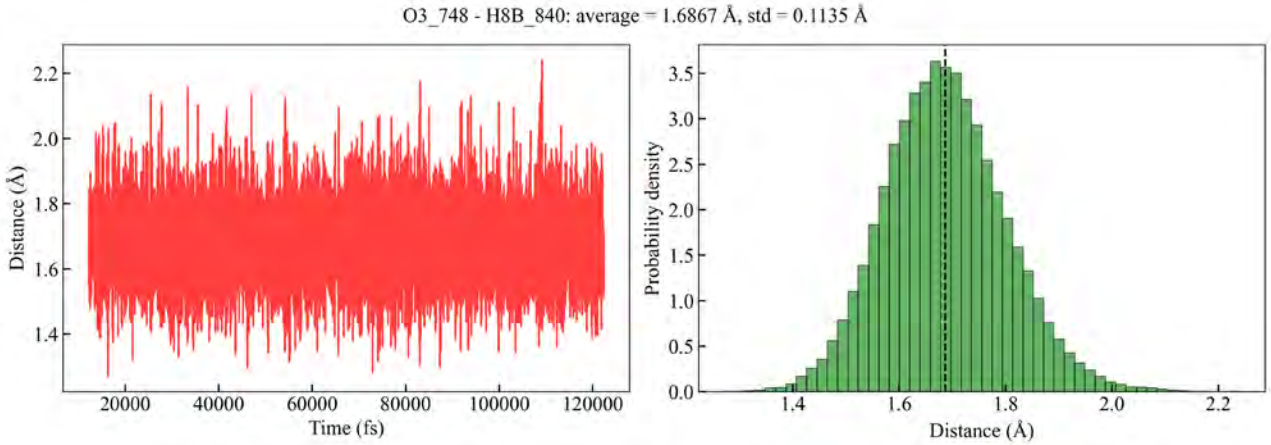
O3_747 - H8B_839

Average distance = 1.6895 Å; standard deviation = 0.1143 Å; number of points = 110177



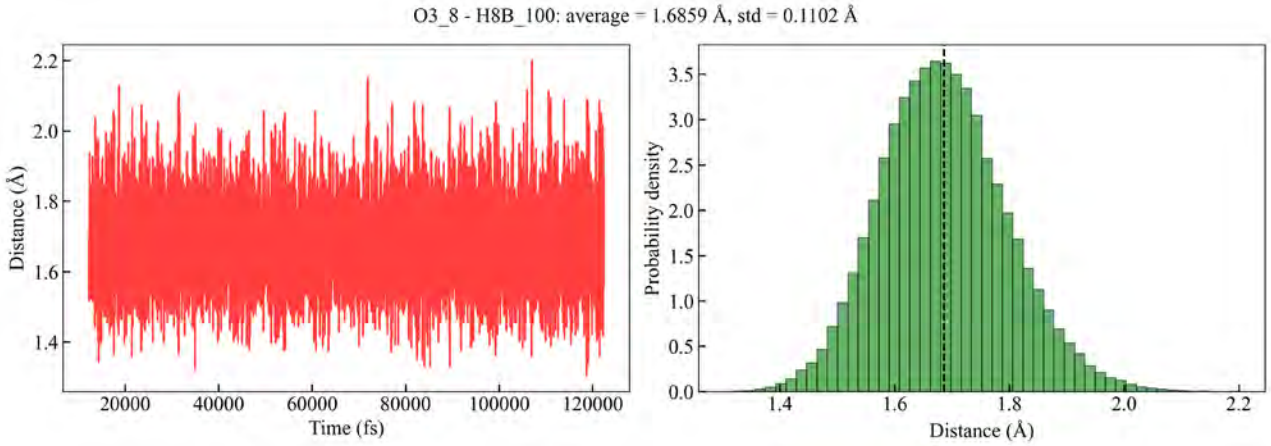
O3_748 - H8B_840

Average distance = 1.6867 Å; standard deviation = 0.1135 Å; number of points = 110177



O3_8 - H8B_100

Average distance = 1.6859 Å; standard deviation = 0.1102 Å; number of points = 110177



3.2.5. P3 at 400 K - Bond Distance Analysis

Table S22. Individual time-averaged hydrogen-involving atomic distances for all equivalent proton environments in the P3 bulk AIMD trajectory at 400 K.

Bond type	Average distance (Å)	Standard dev. σ (Å)	Number of points
O1_10 - H2D1_93	1.9679	0.2267	100046
O1_11 - H2D1_96	1.9652	0.2228	100046
O1_12 - H2D1_95	1.9569	0.2110	100046
O1_157 - H2D1_242	1.9504	0.2049	100046
O1_158 - H2D1_241	1.9642	0.2100	100046
O1_159 - H2D1_244	1.9665	0.2251	100046
O1_160 - H2D1_243	1.9644	0.2205	100046
O1_305 - H2D1_390	1.9581	0.2112	100046
O1_306 - H2D1_389	1.9639	0.2203	100046
O1_307 - H2D1_392	1.9565	0.2121	100046
O1_308 - H2D1_391	1.9591	0.2159	100046
O1_453 - H2D1_538	1.9691	0.2210	100046
O1_454 - H2D1_537	1.9604	0.2113	100046
O1_455 - H2D1_540	1.9593	0.2075	100046
O1_456 - H2D1_539	1.9586	0.2105	100046
O1_601 - H2D1_686	1.9607	0.2165	100046
O1_602 - H2D1_685	1.9603	0.2065	100046
O1_603 - H2D1_688	1.9506	0.2130	100046
O1_604 - H2D1_687	1.9558	0.2100	100046
O1_749 - H2D1_834	1.9651	0.2216	100046
O1_750 - H2D1_833	1.9650	0.2152	100046
O1_751 - H2D1_836	1.9635	0.2167	100046
O1_752 - H2D1_835	1.9610	0.2142	100046
O1_9 - H2D1_94	1.9582	0.2158	100046
O1_10 - H6_110	1.7492	0.1680	100046
O1_11 - H6_259	1.7530	0.1687	100046
O1_12 - H6_260	1.7483	0.1674	100046
O1_157 - H6_257	1.7580	0.1716	100046
O1_158 - H6_258	1.7576	0.1688	100046
O1_159 - H6_111	1.7542	0.1719	100046
O1_160 - H6_112	1.7502	0.1701	100046
O1_305 - H6_405	1.7552	0.1658	100046
O1_306 - H6_406	1.7551	0.1742	100046
O1_307 - H6_555	1.7579	0.1708	100046
O1_308 - H6_556	1.7582	0.1754	100046
O1_453 - H6_553	1.7527	0.1677	100046
O1_454 - H6_554	1.7562	0.1712	100046
O1_455 - H6_407	1.7567	0.1757	100046
O1_456 - H6_408	1.7583	0.1750	100046
O1_601 - H6_701	1.7567	0.1760	100046
O1_602 - H6_702	1.7535	0.1659	100046
O1_603 - H6_851	1.7570	0.1679	100046
O1_604 - H6_852	1.7511	0.1693	100046
O1_749 - H6_849	1.7543	0.1691	100046
O1_750 - H6_850	1.7524	0.1718	100046
O1_751 - H6_703	1.7538	0.1626	100046
O1_752 - H6_704	1.7555	0.1681	100046
O1_9 - H6_109	1.7545	0.1673	100046
O1_10 - H7_138	2.0566	0.3514	100046

O1_11 - H7_139	2.0761	0.3780	100046
O1_12 - H7_140	2.5490	0.5983	100046
O1_157 - H7_285	2.9381	0.4327	100046
O1_159 - H7_287	3.0606	0.2561	100046
O1_160 - H7_288	2.0437	0.3220	100046
O1_305 - H7_433	2.3210	0.5546	100046
O1_306 - H7_434	2.0200	0.2949	100046
O1_307 - H7_435	2.1788	0.4795	100046
O1_308 - H7_436	2.0253	0.3064	100046
O1_453 - H7_581	2.1207	0.4172	100046
O1_454 - H7_582	2.0307	0.3207	100046
O1_456 - H7_584	2.3794	0.5755	100046
O1_601 - H7_729	2.3367	0.5743	100046
O1_603 - H7_731	2.5876	0.5860	100046
O1_604 - H7_732	2.0486	0.3426	100046
O1_750 - H7_878	2.9574	0.4030	100046
O1_751 - H7_879	2.0317	0.3096	100046
O1_752 - H7_880	2.6473	0.5734	100046
O1_9 - H7_137	2.3574	0.5624	100046
O2_1 - H1_135	1.8420	0.2004	100046
O2_149 - H1_283	1.8264	0.1809	100046
O2_150 - H1_284	1.8344	0.1871	100046
O2_151 - H1_281	1.8421	0.2012	100046
O2_152 - H1_282	1.8372	0.1894	100046
O2_2 - H1_136	1.8415	0.2007	100046
O2_297 - H1_431	1.8386	0.1884	100046
O2_298 - H1_432	1.8291	0.1857	100046
O2_299 - H1_429	1.8345	0.1834	100046
O2_3 - H1_133	1.8441	0.1963	100046
O2_300 - H1_430	1.8342	0.1858	100046
O2_4 - H1_134	1.8278	0.1812	100046
O2_445 - H1_579	1.8339	0.1891	100046
O2_446 - H1_580	1.8369	0.1890	100046
O2_447 - H1_577	1.8387	0.1877	100046
O2_448 - H1_578	1.8325	0.1860	100046
O2_593 - H1_727	1.8352	0.1917	100046
O2_594 - H1_728	1.8255	0.1723	100046
O2_595 - H1_725	1.8297	0.1820	100046
O2_596 - H1_726	1.8291	0.1830	100046
O2_741 - H1_875	1.8376	0.1888	100046
O2_742 - H1_876	1.8341	0.1932	100046
O2_743 - H1_873	1.8329	0.1861	100046
O2_744 - H1_874	1.8330	0.1861	100046
O2_1 - H1A_114	1.7633	0.1740	100046
O2_149 - H1A_262	1.7711	0.1809	100046
O2_150 - H1A_261	1.7686	0.1696	100046
O2_151 - H1A_264	1.7692	0.1746	100046
O2_152 - H1A_263	1.7709	0.1701	100046
O2_2 - H1A_113	1.7649	0.1704	100046
O2_297 - H1A_410	1.7641	0.1681	100046
O2_298 - H1A_409	1.7641	0.1689	100046
O2_299 - H1A_412	1.7622	0.1675	100046
O2_3 - H1A_116	1.7661	0.1701	100046

O2_300 - H1A_411	1.7666	0.1711	100046
O2_4 - H1A_115	1.7663	0.1642	100046
O2_445 - H1A_558	1.7653	0.1675	100046
O2_446 - H1A_557	1.7668	0.1737	100046
O2_447 - H1A_560	1.7644	0.1690	100046
O2_448 - H1A_559	1.7642	0.1661	100046
O2_593 - H1A_706	1.7647	0.1723	100046
O2_594 - H1A_705	1.7653	0.1725	100046
O2_595 - H1A_708	1.7651	0.1763	100046
O2_596 - H1A_707	1.7649	0.1672	100046
O2_741 - H1A_854	1.7590	0.1634	100046
O2_742 - H1A_853	1.7626	0.1711	100046
O2_743 - H1A_856	1.7659	0.1713	100046
O2_744 - H1A_855	1.7620	0.1667	100046
O2_1 - H3_84	1.9369	0.1988	100046
O2_149 - H3_232	1.9369	0.1960	100046
O2_150 - H3_231	1.9380	0.1960	100046
O2_151 - H3_230	1.9344	0.2008	100046
O2_152 - H3_229	1.9375	0.1976	100046
O2_2 - H3_83	1.9299	0.1901	100046
O2_297 - H3_380	1.9291	0.1877	100046
O2_298 - H3_379	1.9451	0.2165	100046
O2_299 - H3_378	1.9367	0.1912	100046
O2_3 - H3_82	1.9465	0.1997	100046
O2_300 - H3_377	1.9412	0.1915	100046
O2_4 - H3_81	1.9430	0.2029	100046
O2_445 - H3_528	1.9318	0.1897	100046
O2_446 - H3_527	1.9401	0.1972	100046
O2_447 - H3_526	1.9346	0.1962	100046
O2_448 - H3_525	1.9347	0.1908	100046
O2_593 - H3_676	1.9452	0.1998	100046
O2_594 - H3_675	1.9414	0.1915	100046
O2_595 - H3_674	1.9420	0.1982	100046
O2_596 - H3_673	1.9357	0.2031	100046
O2_741 - H3_824	1.9434	0.2020	100046
O2_742 - H3_823	1.9418	0.1984	100046
O2_743 - H3_822	1.9367	0.1931	100046
O2_744 - H3_821	1.9344	0.1936	100046
O3_153 - H2_289	1.8045	0.1878	100046
O3_154 - H2_290	1.8083	0.1917	100046
O3_155 - H2_291	1.8050	0.1866	100046
O3_156 - H2_292	1.8041	0.1872	100046
O3_301 - H2_437	1.8062	0.1887	100046
O3_302 - H2_438	1.8133	0.1910	100046
O3_303 - H2_439	1.8117	0.2007	100046
O3_304 - H2_440	1.7999	0.1749	100046
O3_449 - H2_585	1.8048	0.1806	100046
O3_450 - H2_586	1.8142	0.2003	100046
O3_451 - H2_587	1.8121	0.1874	100046
O3_452 - H2_588	1.8026	0.1808	100046
O3_5 - H2_141	1.8105	0.1933	100046
O3_597 - H2_733	1.8061	0.1857	100046
O3_598 - H2_734	1.8043	0.1848	100046

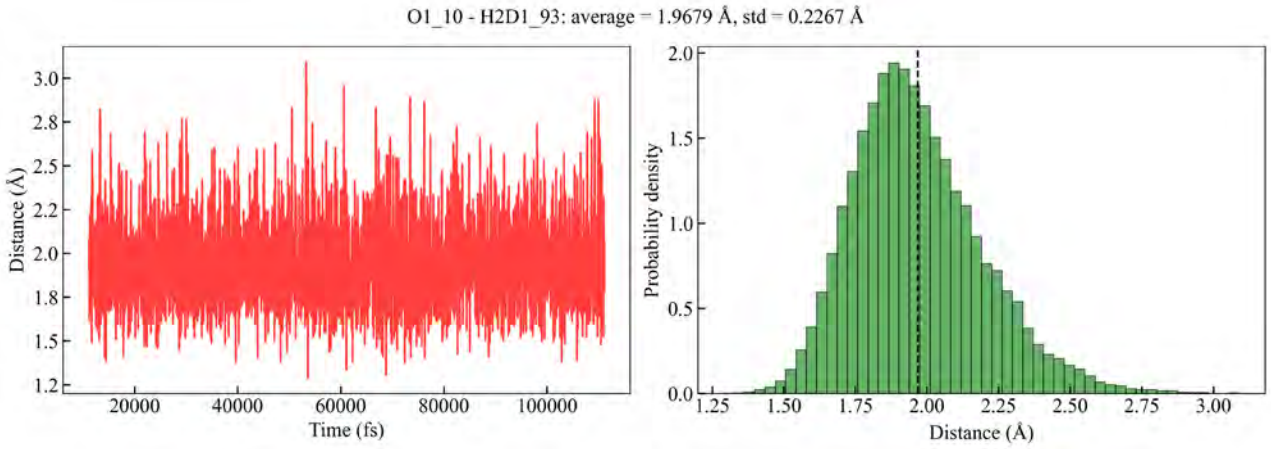
O3_599 - H2_735	1.8121	0.2053	100046
O3_6 - H2_142	1.8034	0.1868	100046
O3_600 - H2_736	1.8106	0.1916	100046
O3_7 - H2_143	1.8146	0.1922	100046
O3_745 - H2_881	1.8080	0.1882	100046
O3_746 - H2_882	1.8113	0.1982	100046
O3_747 - H2_883	1.8024	0.1790	100046
O3_748 - H2_884	1.8058	0.1804	100046
O3_8 - H2_144	1.8058	0.1891	100046
O3_153 - H8B_245	1.6930	0.1279	100046
O3_154 - H8B_246	1.6940	0.1309	100046
O3_155 - H8B_247	1.6906	0.1286	100046
O3_156 - H8B_248	1.6916	0.1264	100046
O3_301 - H8B_393	1.6926	0.1313	100046
O3_302 - H8B_394	1.6958	0.1311	100046
O3_303 - H8B_395	1.6938	0.1310	100046
O3_304 - H8B_396	1.6943	0.1282	100046
O3_449 - H8B_541	1.6957	0.1281	100046
O3_450 - H8B_542	1.6929	0.1269	100046
O3_451 - H8B_543	1.6946	0.1301	100046
O3_452 - H8B_544	1.6966	0.1317	100046
O3_5 - H8B_97	1.6930	0.1265	100046
O3_597 - H8B_689	1.6932	0.1317	100046
O3_598 - H8B_690	1.6938	0.1289	100046
O3_599 - H8B_691	1.6916	0.1258	100046
O3_6 - H8B_98	1.6946	0.1325	100046
O3_600 - H8B_692	1.6915	0.1273	100046
O3_7 - H8B_99	1.6928	0.1281	100046
O3_745 - H8B_837	1.6945	0.1267	100046
O3_746 - H8B_838	1.6926	0.1256	100046
O3_747 - H8B_839	1.6938	0.1312	100046
O3_748 - H8B_840	1.6949	0.1295	100046
O3_8 - H8B_100	1.6963	0.1327	100046

Bond Distance Plots

O1 - H2D1

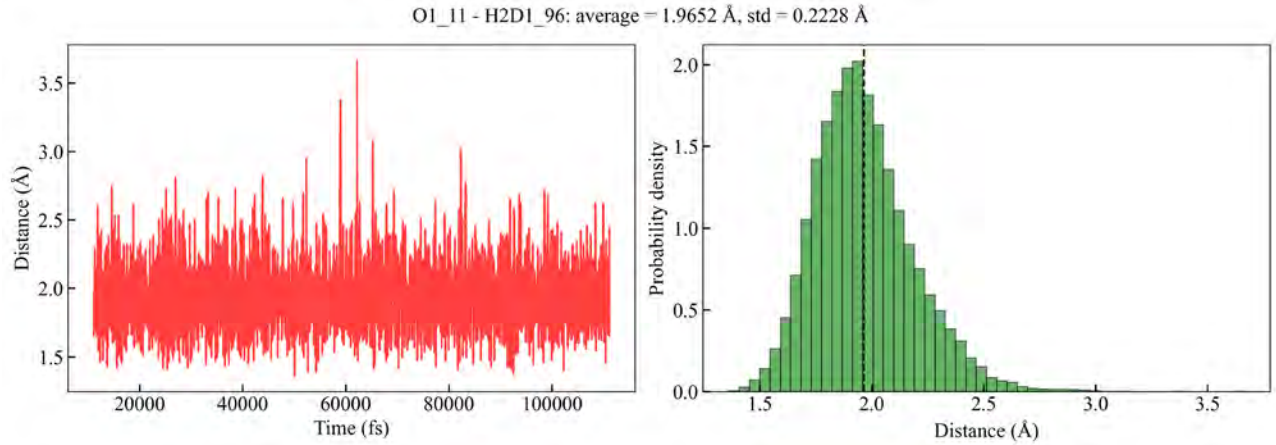
O1_10 - H2D1_93

Average distance = 1.9679 Å; standard deviation = 0.2267 Å; number of points = 100046



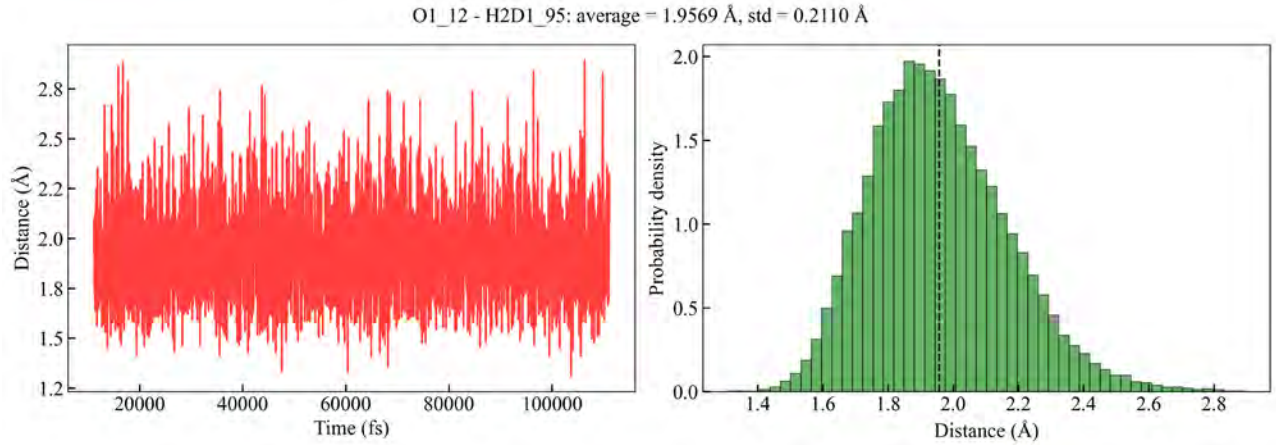
O1_11 - H2D1_96

Average distance = 1.9652 Å; standard deviation = 0.2228 Å; number of points = 100046



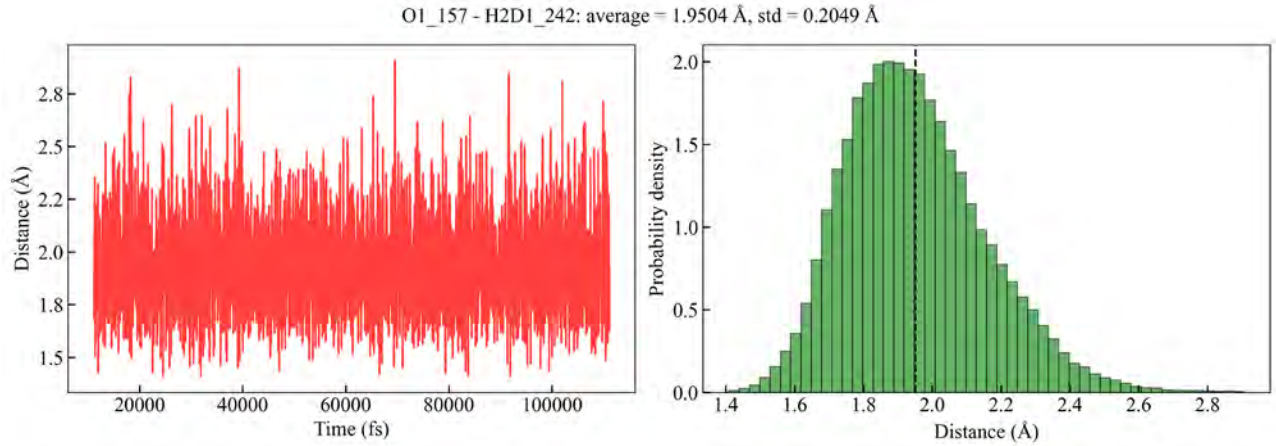
O1_12 - H2D1_95

Average distance = 1.9569 Å; standard deviation = 0.2110 Å; number of points = 100046



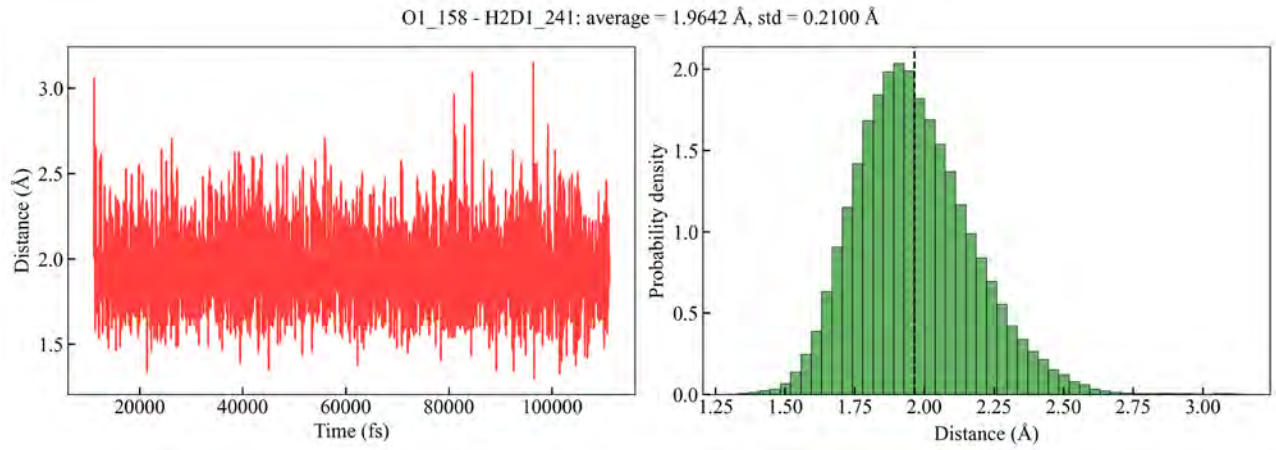
O1_157 - H2D1_242

Average distance = 1.9504 Å; standard deviation = 0.2049 Å; number of points = 100046



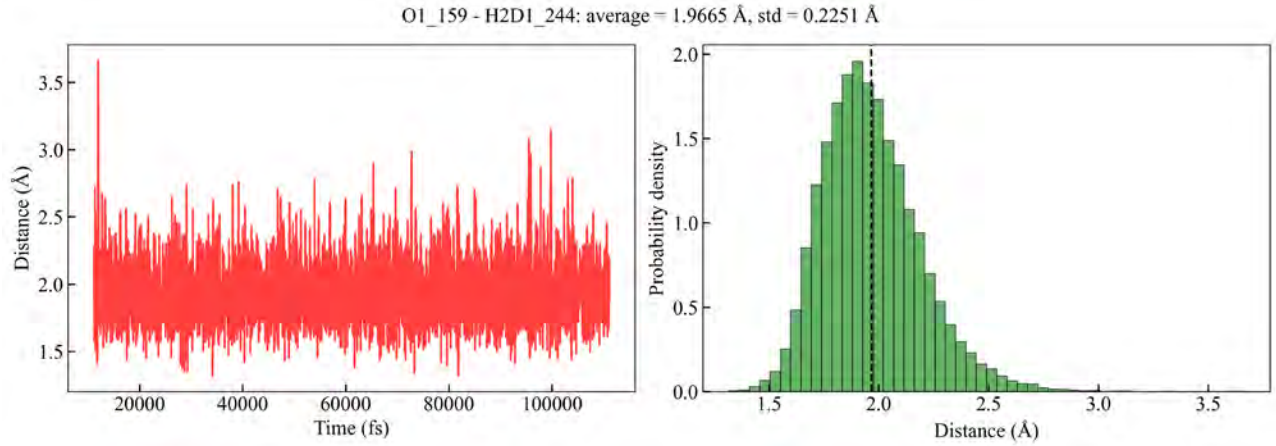
O1_158 - H2D1_241

Average distance = 1.9642 Å; standard deviation = 0.2100 Å; number of points = 100046



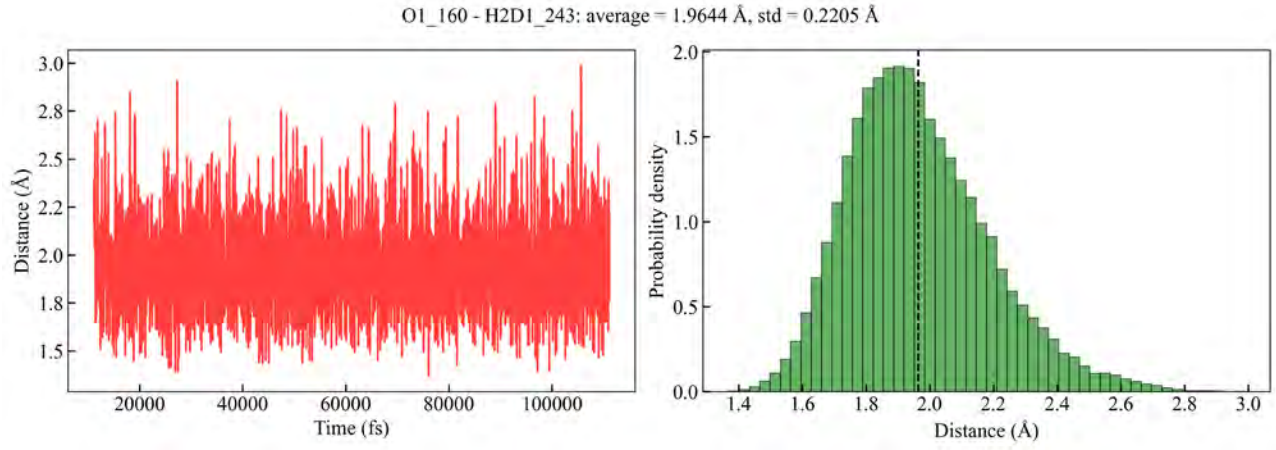
O1_159 - H2D1_244

Average distance = 1.9665 Å; standard deviation = 0.2251 Å; number of points = 100046



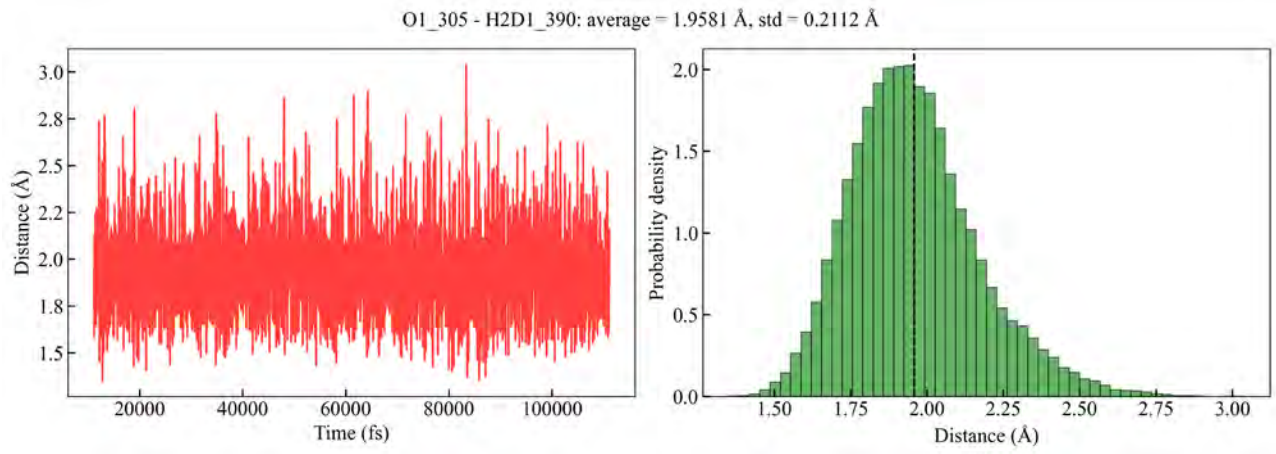
O1_160 - H2D1_243

Average distance = 1.9644 Å; standard deviation = 0.2205 Å; number of points = 100046



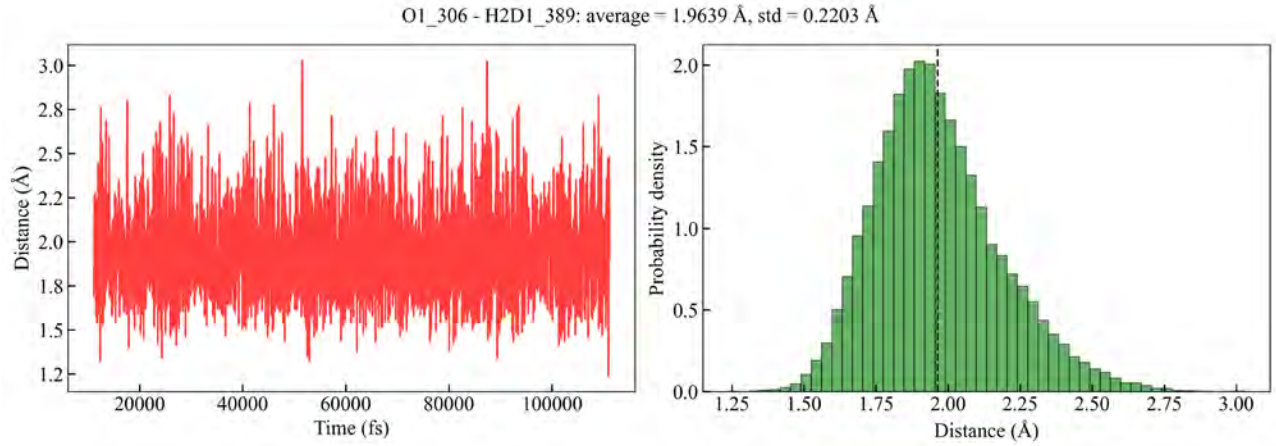
O1_305 - H2D1_390

Average distance = 1.9581 Å; standard deviation = 0.2112 Å; number of points = 100046



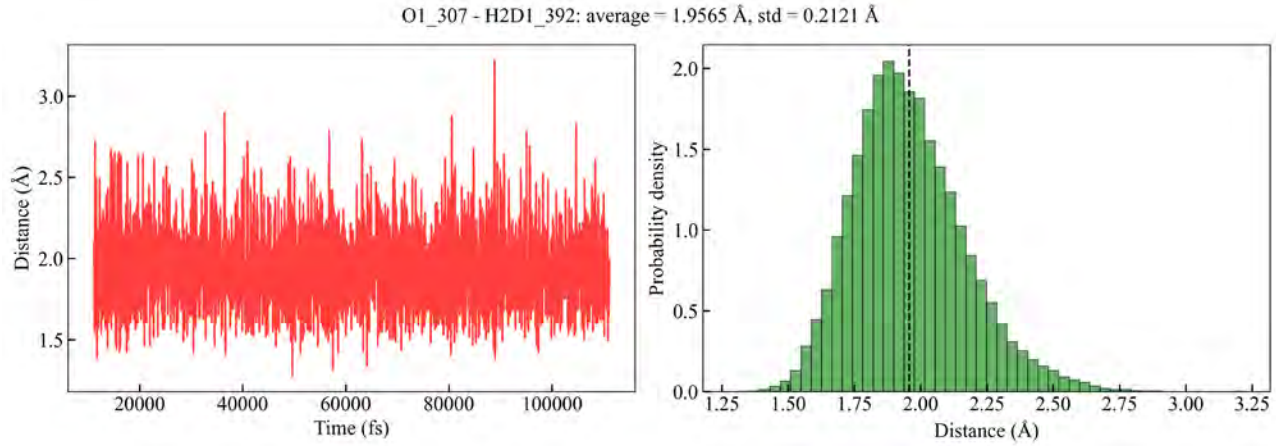
O1_306 - H2D1_389

Average distance = 1.9639 Å; standard deviation = 0.2203 Å; number of points = 100046



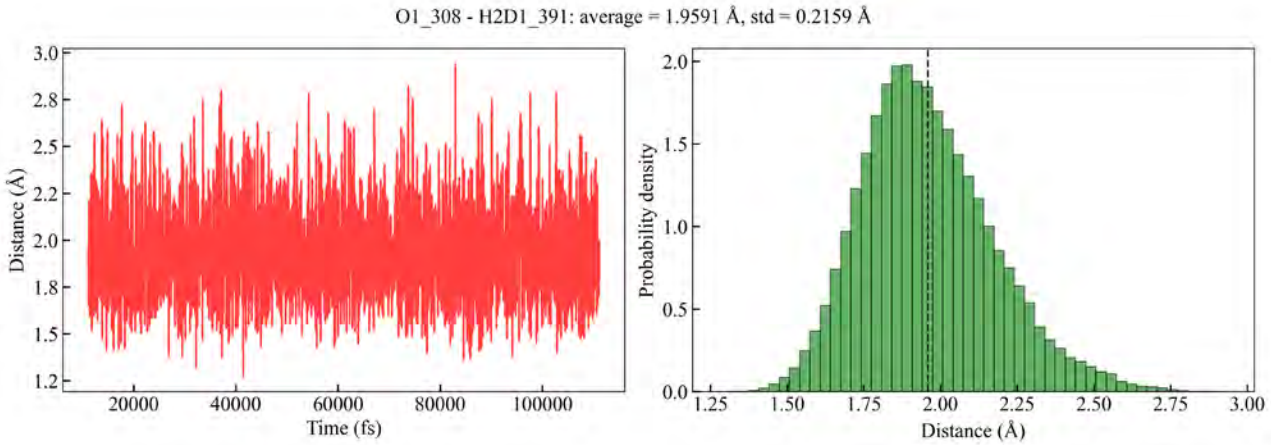
O1_307 - H2D1_392

Average distance = 1.9565 Å; standard deviation = 0.2121 Å; number of points = 100046



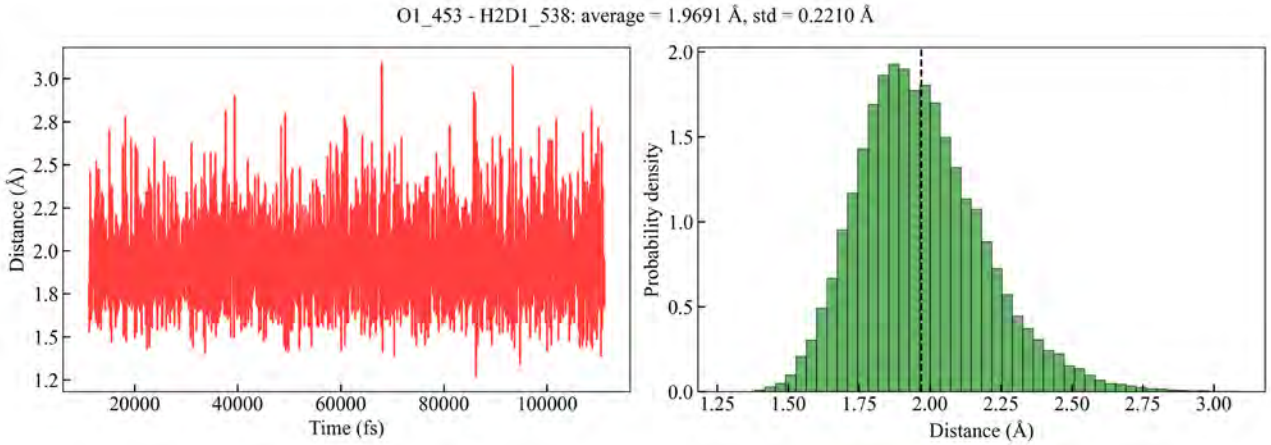
O1_308 - H2D1_391

Average distance = 1.9591 Å; standard deviation = 0.2159 Å; number of points = 100046



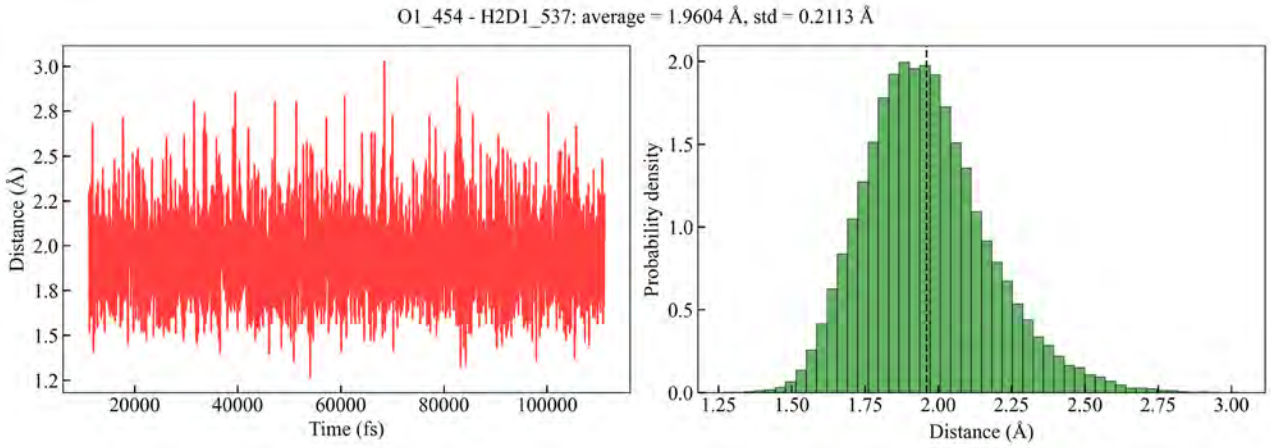
O1_453 - H2D1_538

Average distance = 1.9691 Å; standard deviation = 0.2210 Å; number of points = 100046



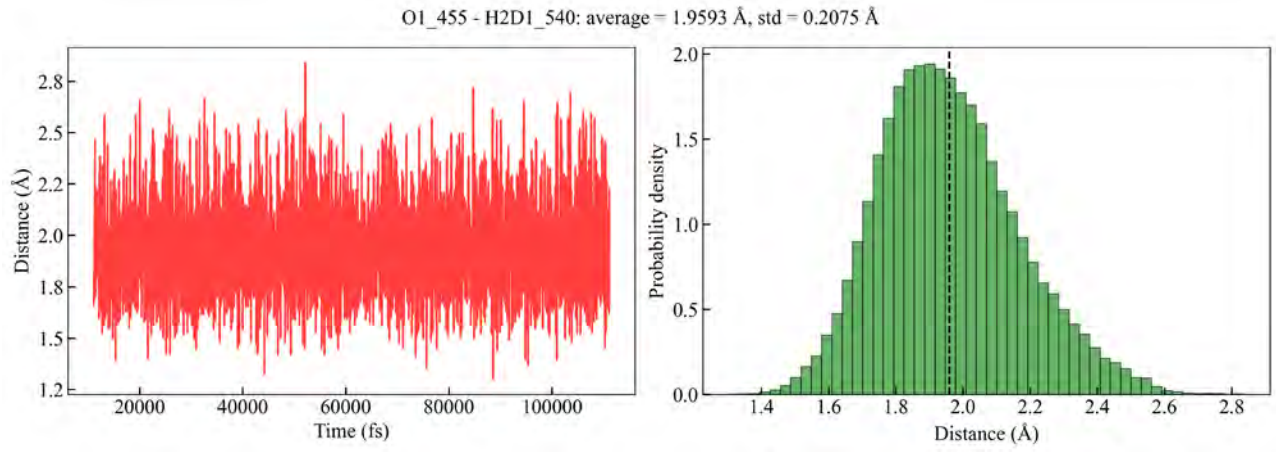
O1_454 - H2D1_537

Average distance = 1.9604 Å; standard deviation = 0.2113 Å; number of points = 100046



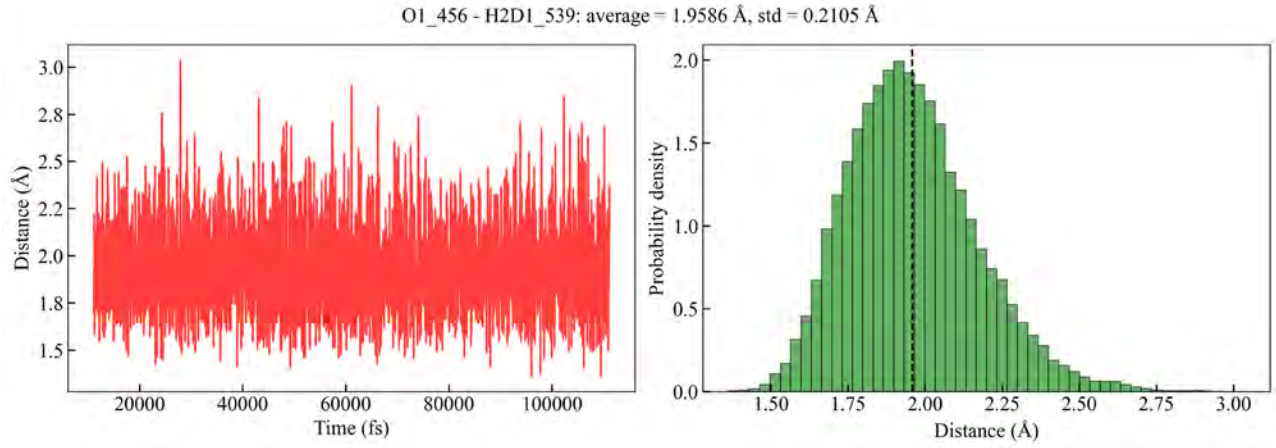
O1_455 - H2D1_540

Average distance = 1.9593 Å; standard deviation = 0.2075 Å; number of points = 100046



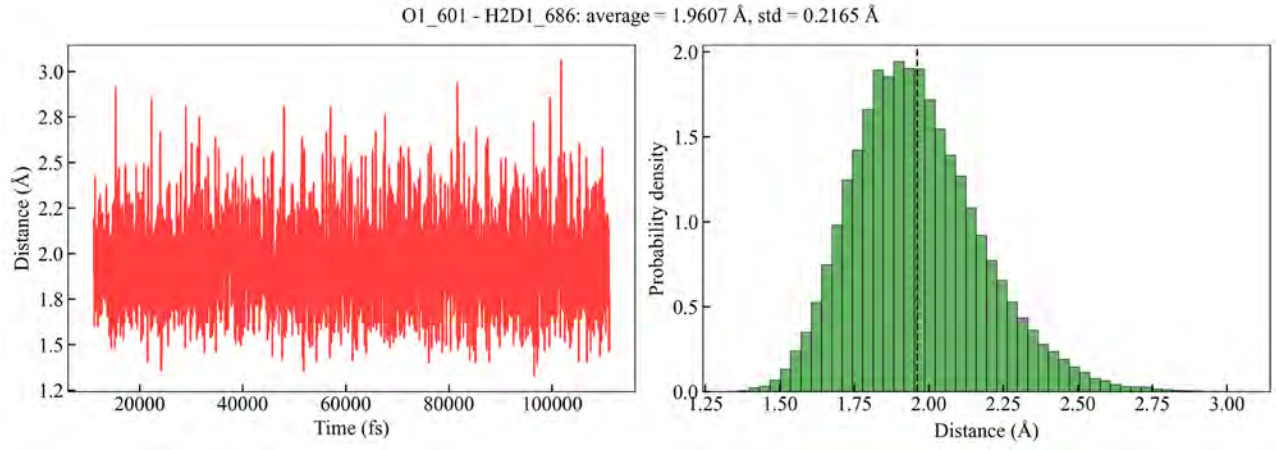
O1_456 - H2D1_539

Average distance = 1.9586 Å; standard deviation = 0.2105 Å; number of points = 100046



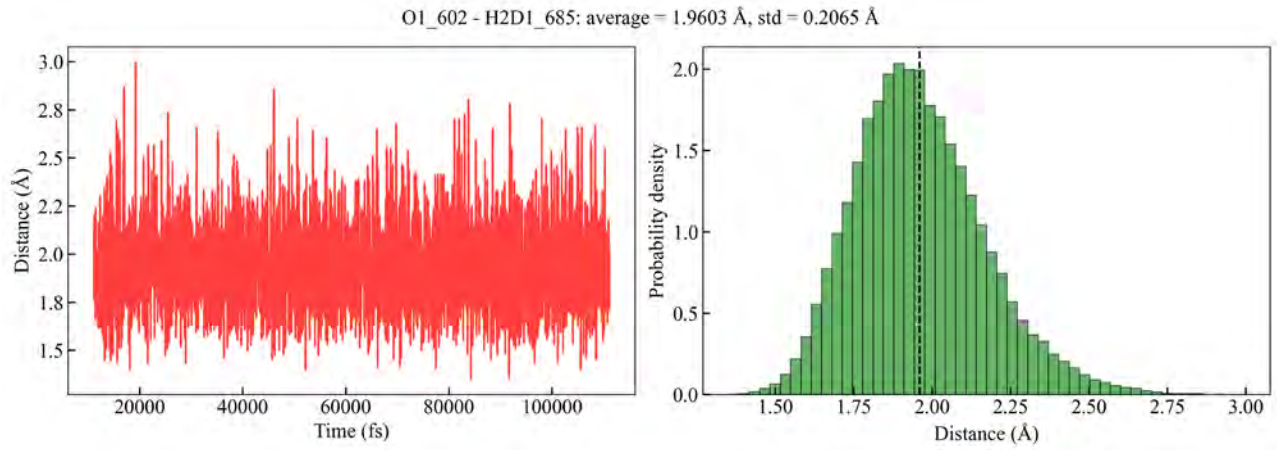
O1_601 - H2D1_686

Average distance = 1.9607 Å; standard deviation = 0.2165 Å; number of points = 100046



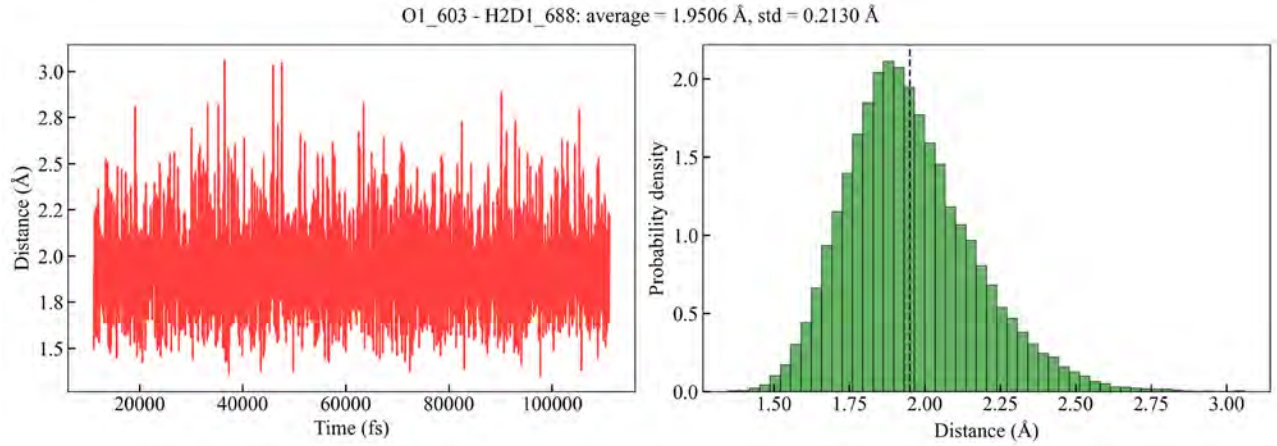
O1_602 - H2D1_685

Average distance = 1.9603 Å; standard deviation = 0.2065 Å; number of points = 100046



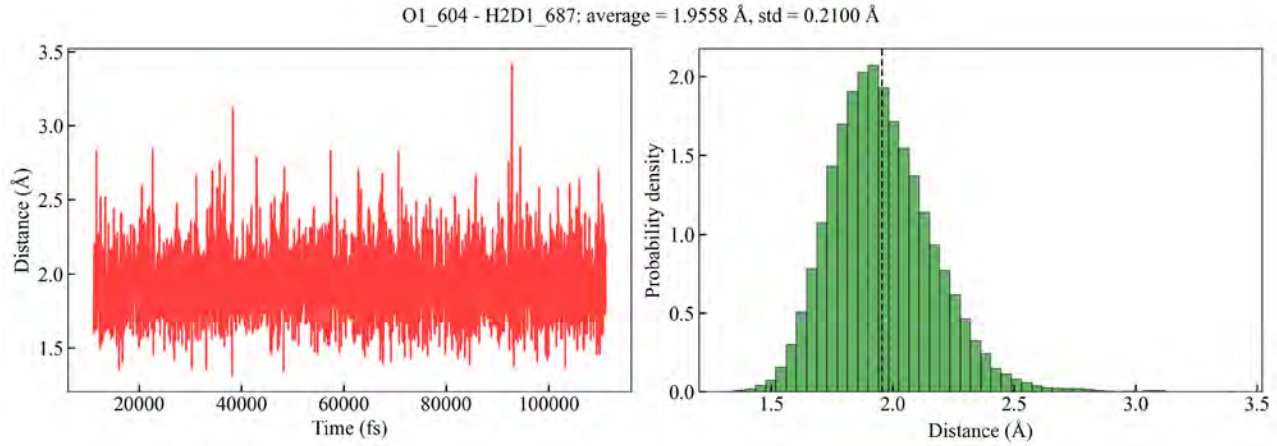
O1_603 - H2D1_688

Average distance = 1.9506 Å; standard deviation = 0.2130 Å; number of points = 100046



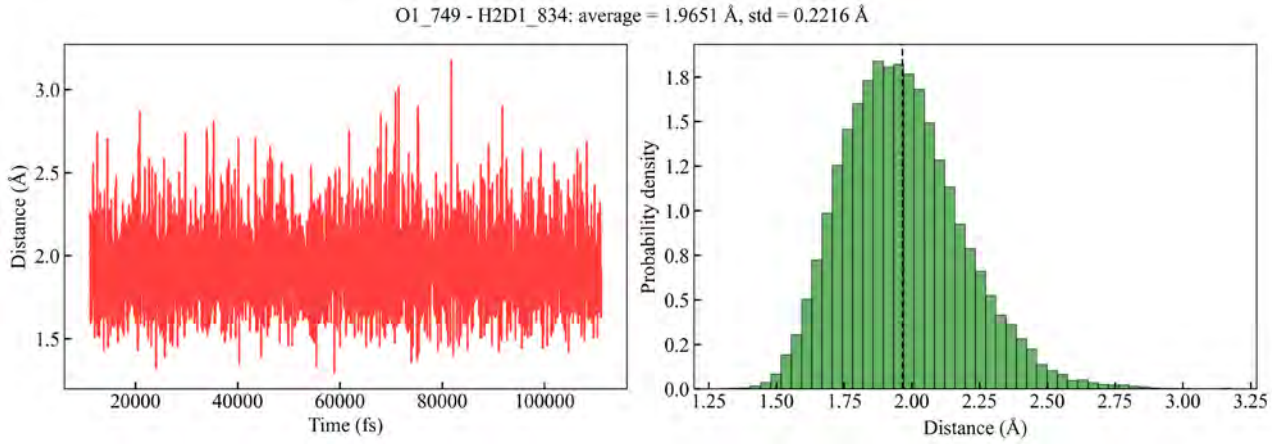
O1_604 - H2D1_687

Average distance = 1.9558 Å; standard deviation = 0.2100 Å; number of points = 100046



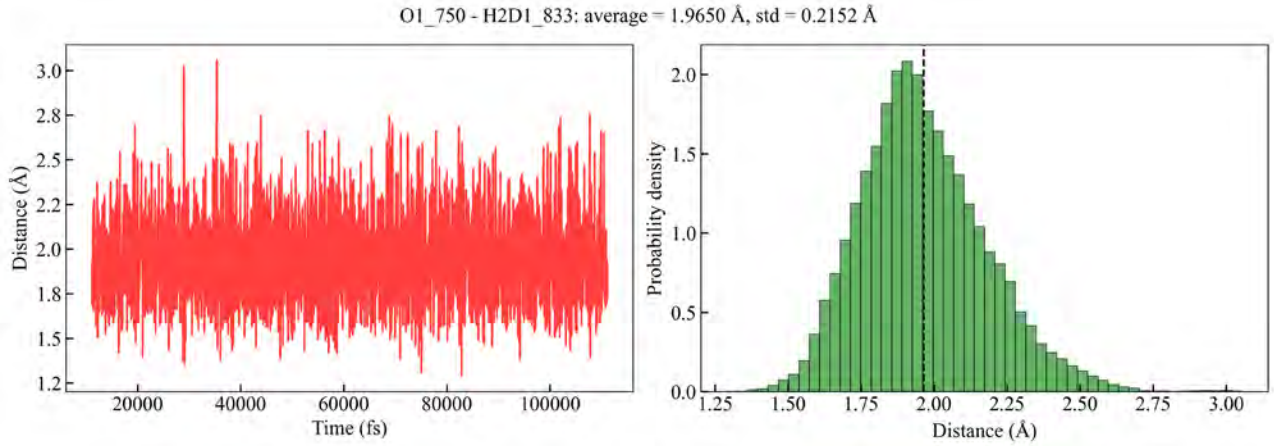
O1_749 - H2D1_834

Average distance = 1.9651 Å; standard deviation = 0.2216 Å; number of points = 100046



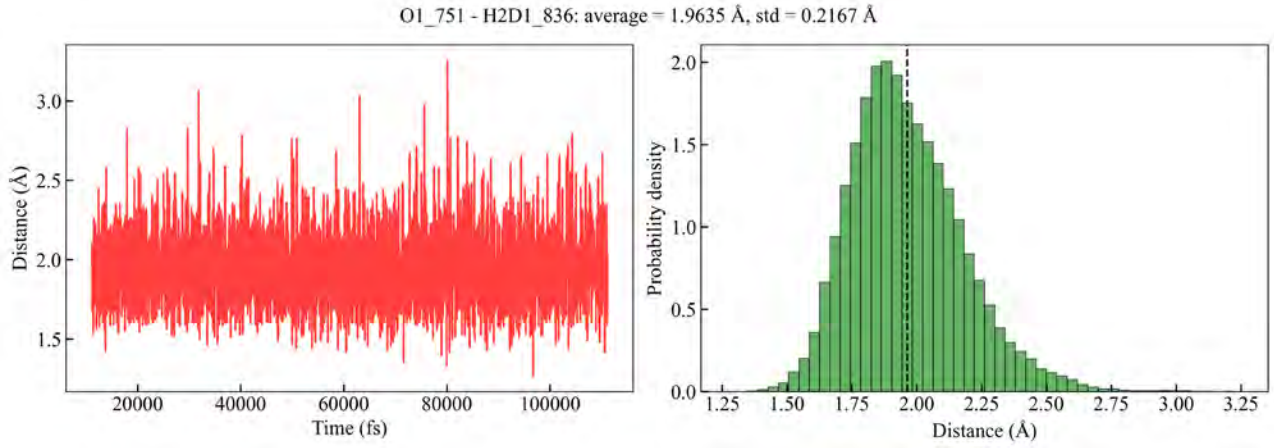
O1_750 - H2D1_833

Average distance = 1.9650 Å; standard deviation = 0.2152 Å; number of points = 100046



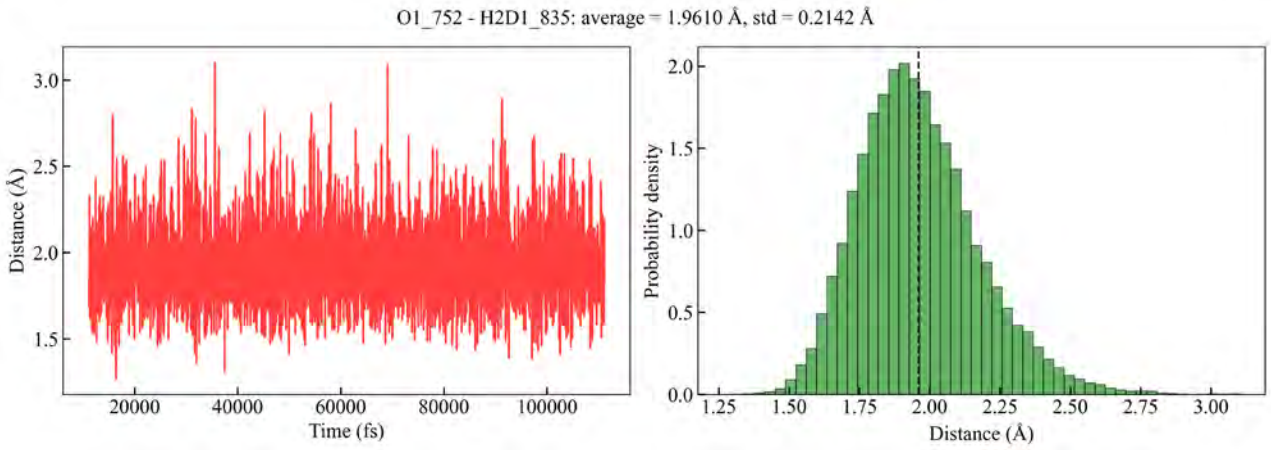
O1_751 - H2D1_836

Average distance = 1.9635 Å; standard deviation = 0.2167 Å; number of points = 100046



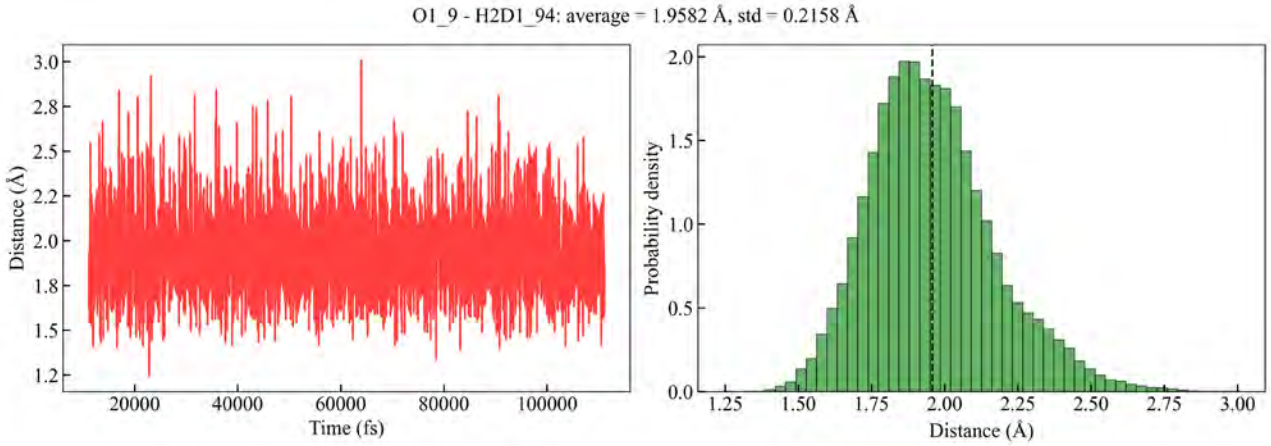
O1_752 - H2D1_835

Average distance = 1.9610 Å; standard deviation = 0.2142 Å; number of points = 100046



O1_9 - H2D1_94

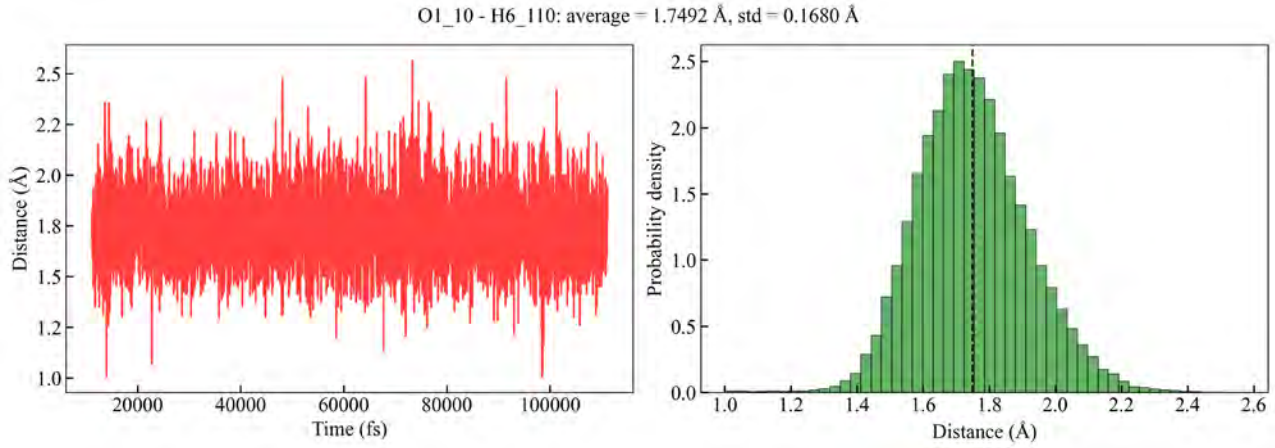
Average distance = 1.9582 Å; standard deviation = 0.2158 Å; number of points = 100046



O1 - H6

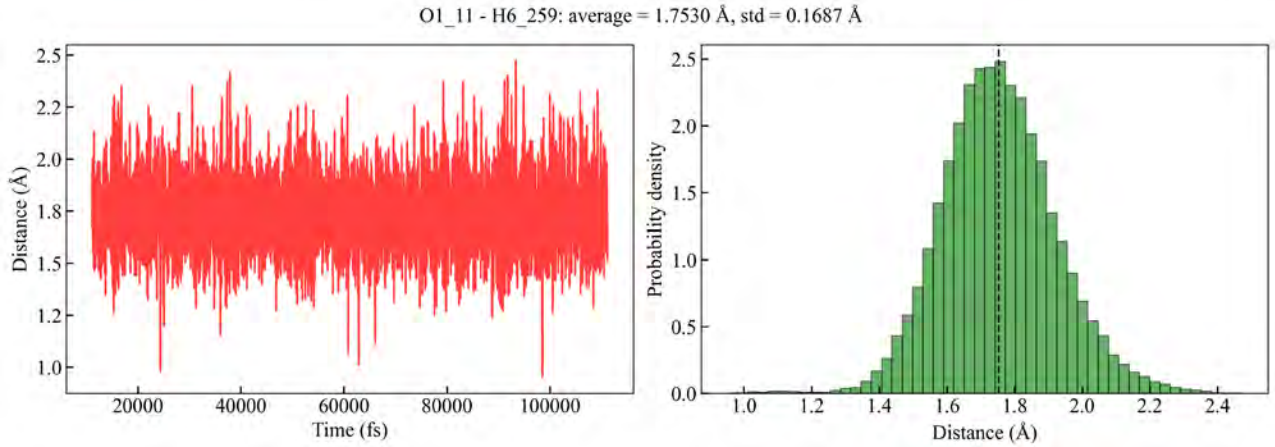
O1_10 - H6_110

Average distance = 1.7492 Å; standard deviation = 0.1680 Å; number of points = 100046



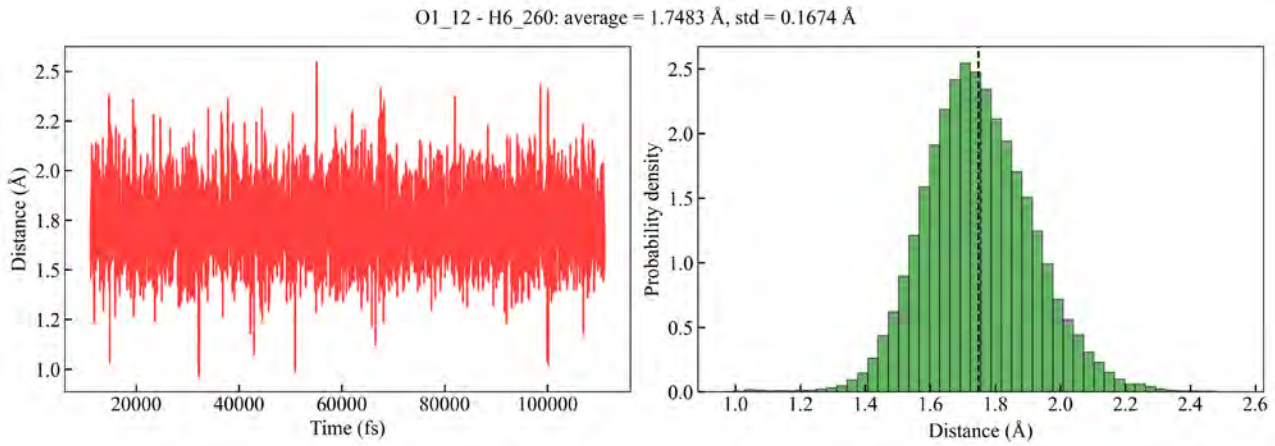
O1_11 - H6_259

Average distance = 1.7530 Å; standard deviation = 0.1687 Å; number of points = 100046



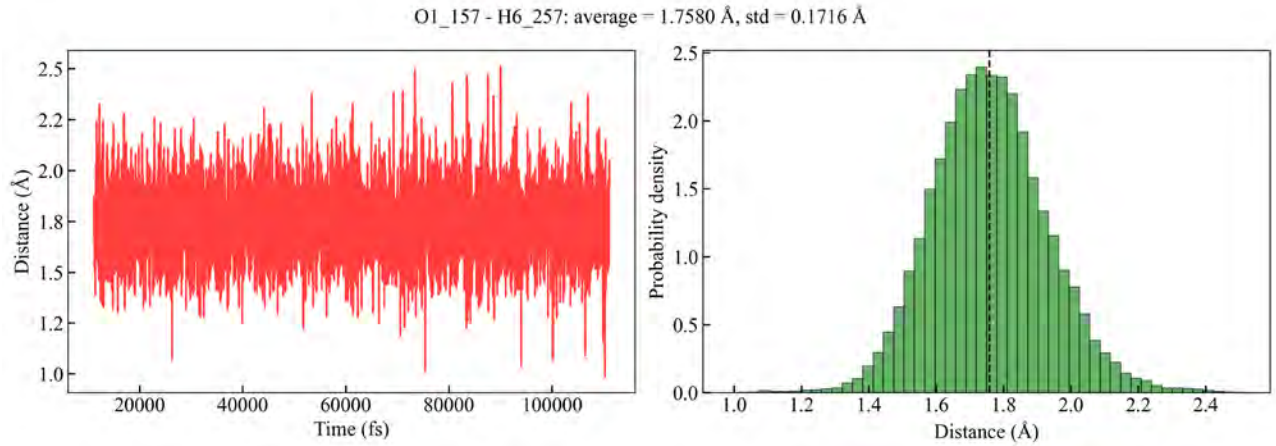
O1_12 - H6_260

Average distance = 1.7483 Å; standard deviation = 0.1674 Å; number of points = 100046



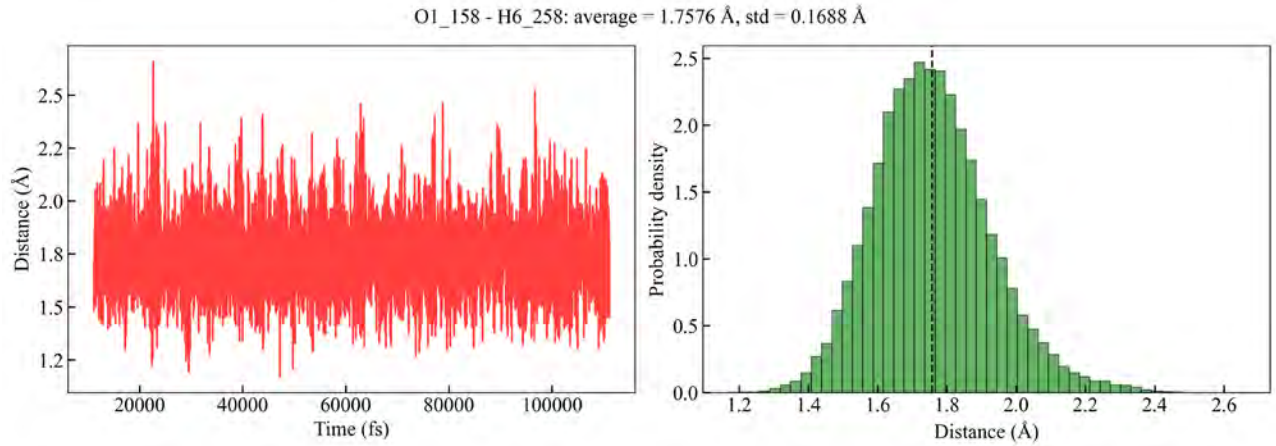
O1_157 - H6_257

Average distance = 1.7580 Å; standard deviation = 0.1716 Å; number of points = 100046



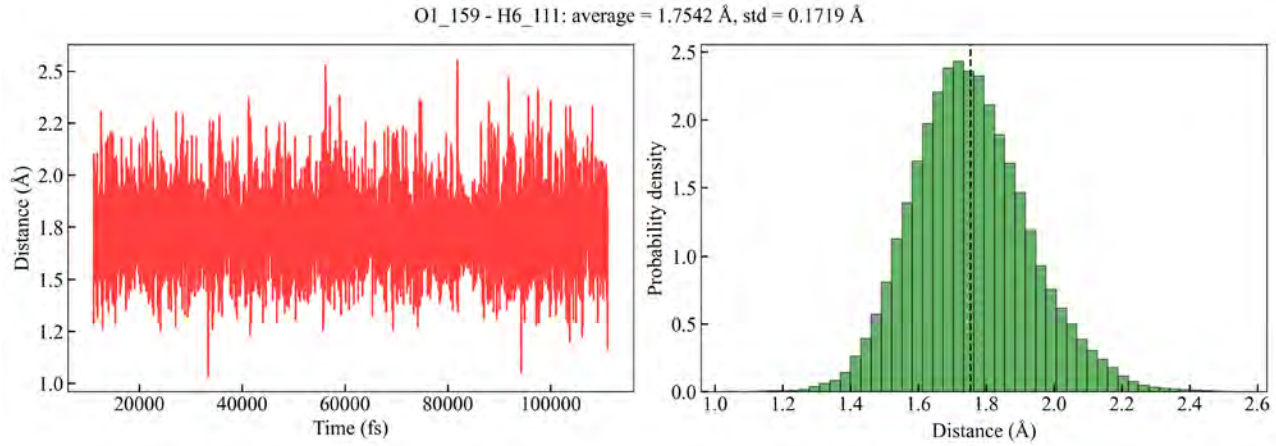
O1_158 - H6_258

Average distance = 1.7576 Å; standard deviation = 0.1688 Å; number of points = 100046



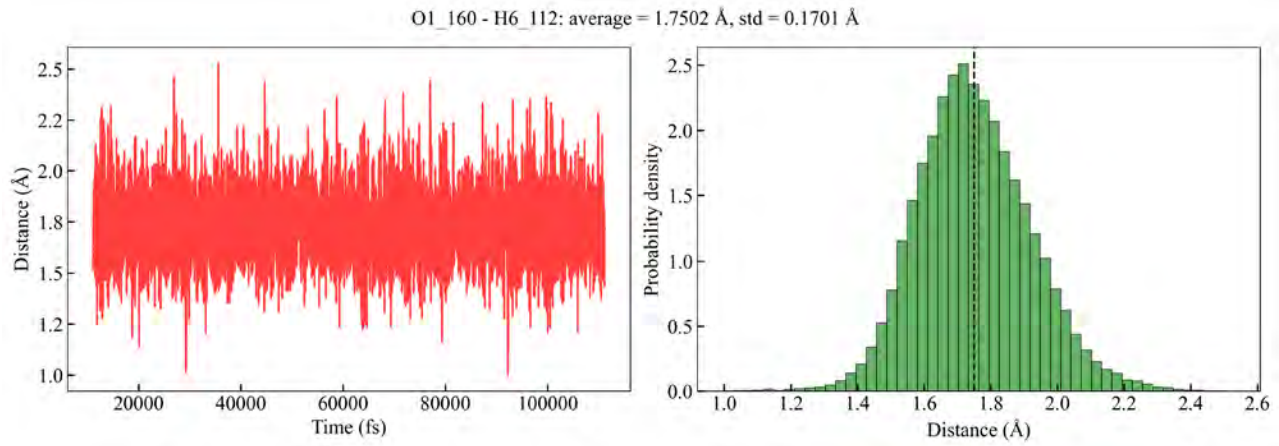
O1_159 - H6_111

Average distance = 1.7542 Å; standard deviation = 0.1719 Å; number of points = 100046



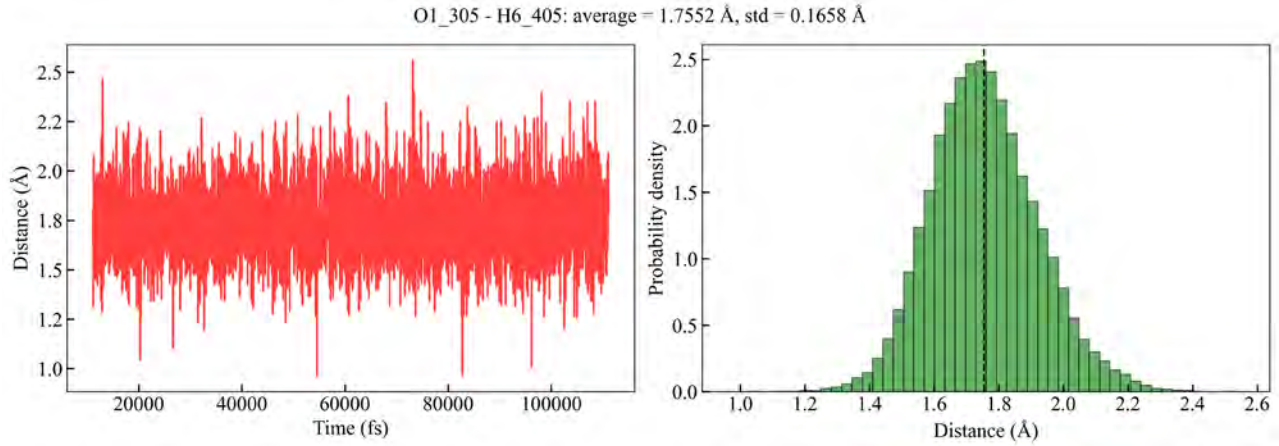
O1_160 - H6_112

Average distance = 1.7502 Å; standard deviation = 0.1701 Å; number of points = 100046



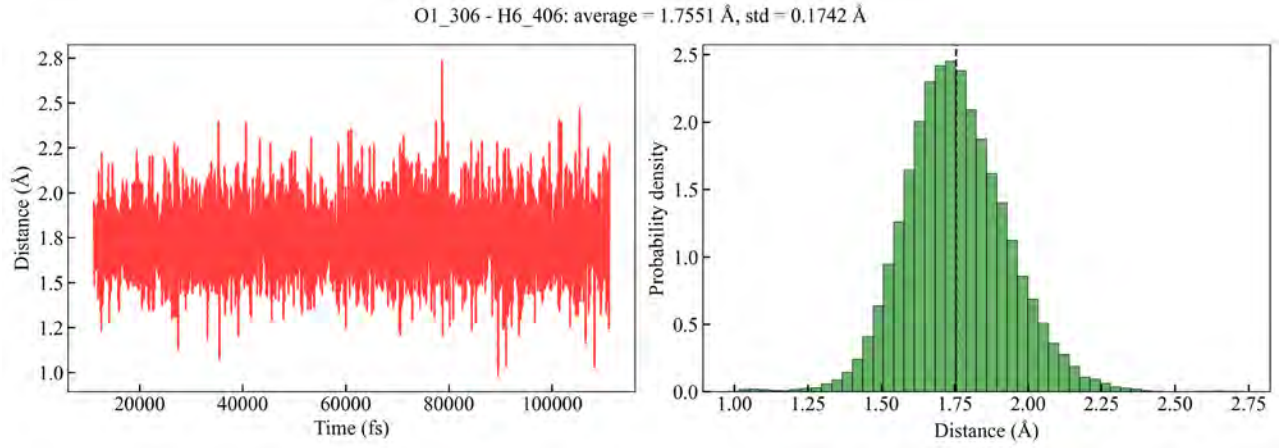
O1_305 - H6_405

Average distance = 1.7552 Å; standard deviation = 0.1658 Å; number of points = 100046



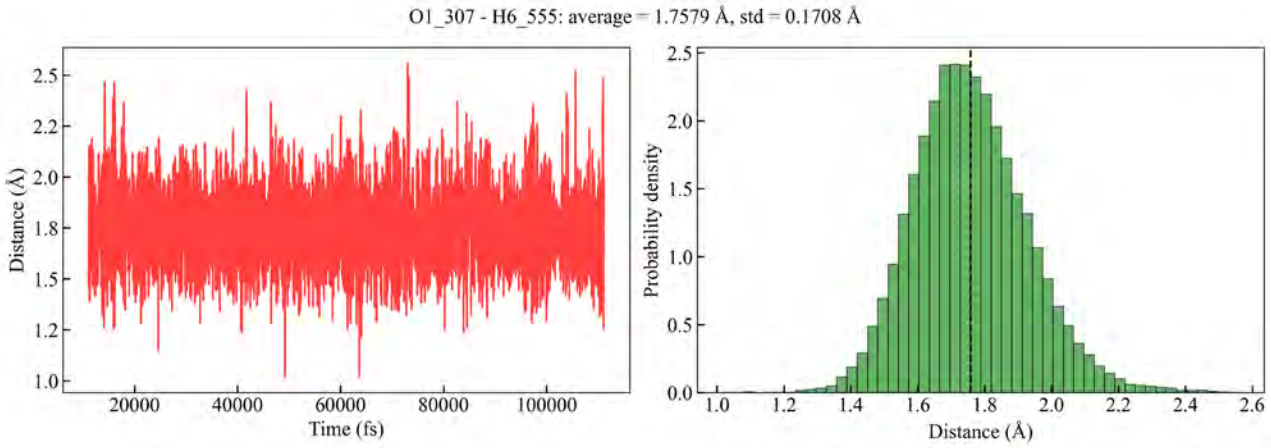
O1_306 - H6_406

Average distance = 1.7551 Å; standard deviation = 0.1742 Å; number of points = 100046



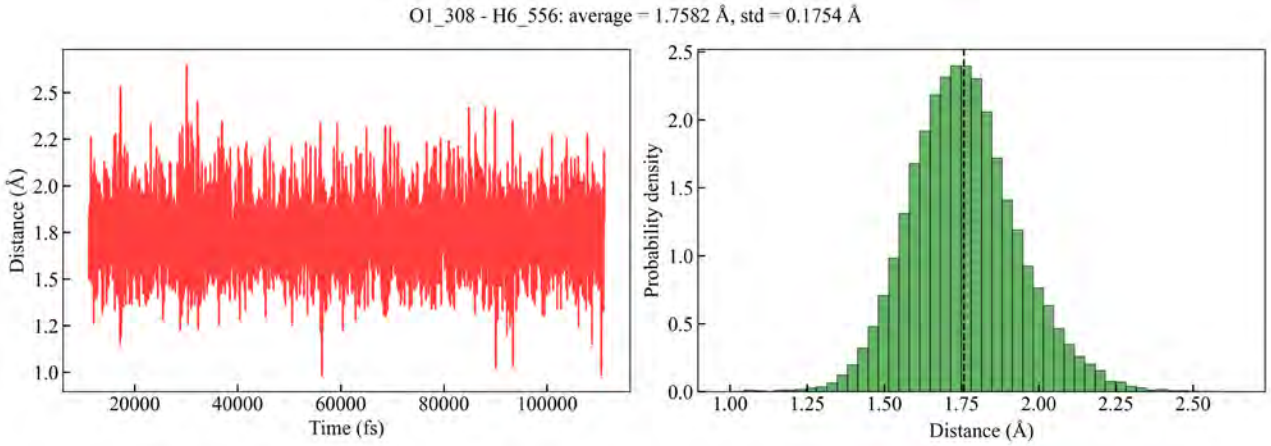
O1_307 - H6_555

Average distance = 1.7579 Å; standard deviation = 0.1708 Å; number of points = 100046



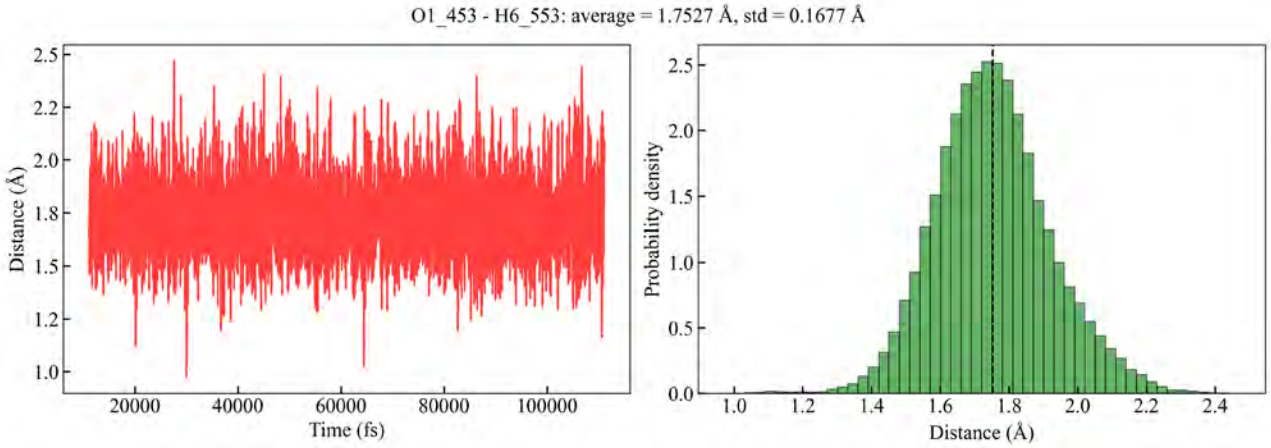
O1_308 - H6_556

Average distance = 1.7582 Å; standard deviation = 0.1754 Å; number of points = 100046



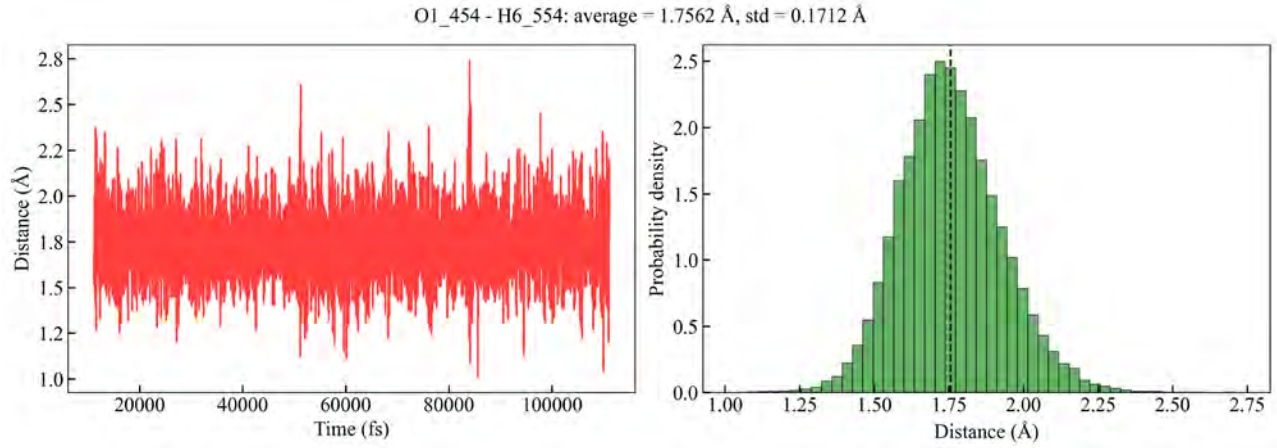
O1_453 - H6_553

Average distance = 1.7527 Å; standard deviation = 0.1677 Å; number of points = 100046



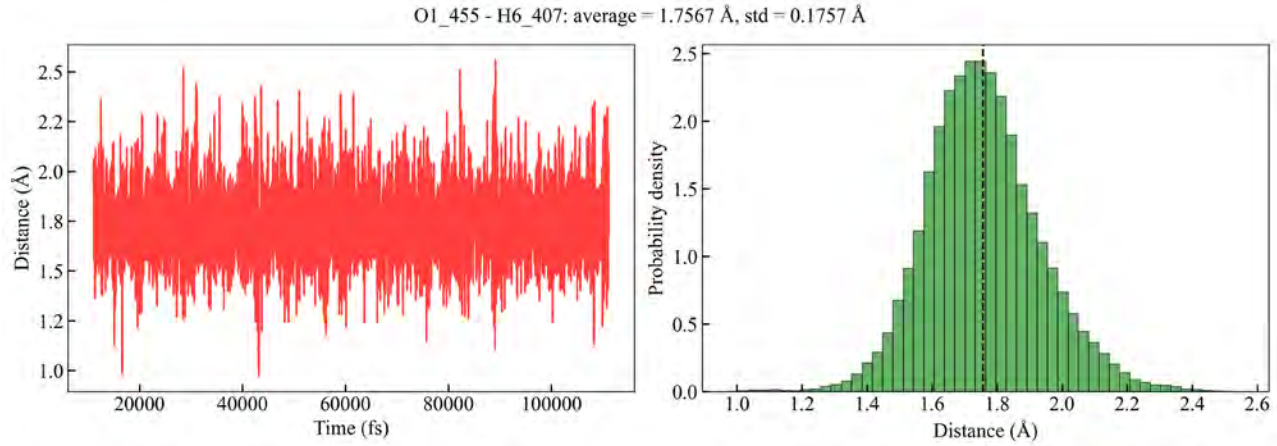
O1_454 - H6_554

Average distance = 1.7562 Å; standard deviation = 0.1712 Å; number of points = 100046



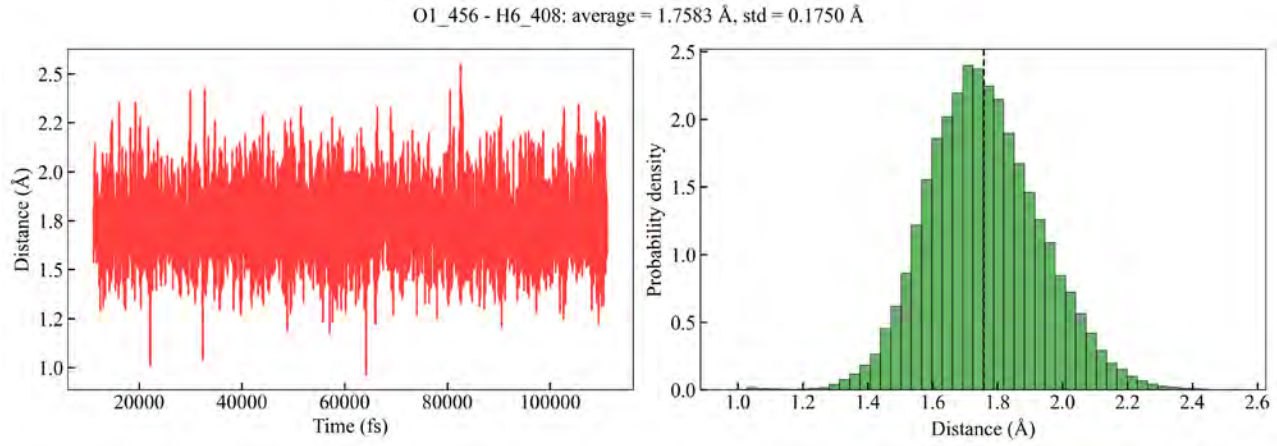
O1_455 - H6_407

Average distance = 1.7567 Å; standard deviation = 0.1757 Å; number of points = 100046



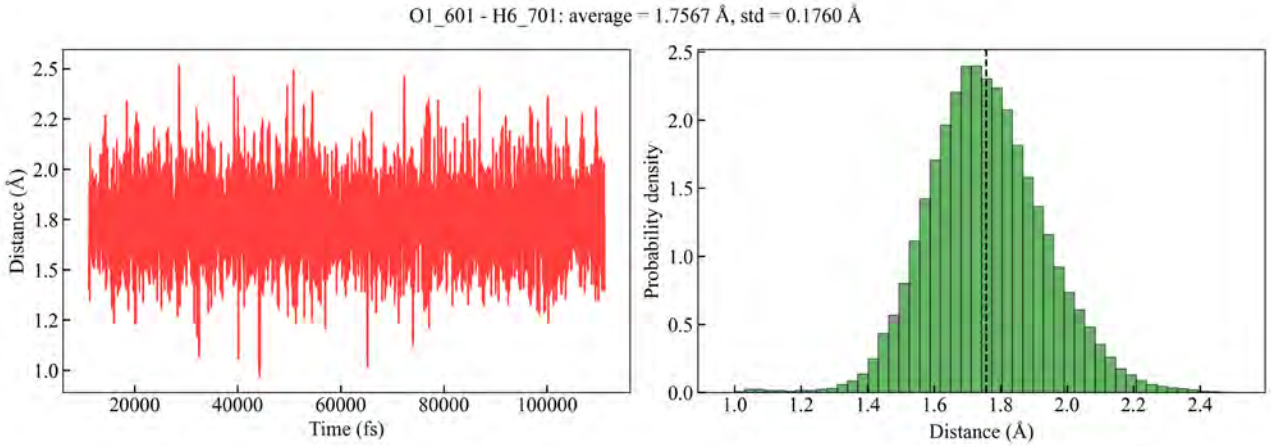
O1_456 - H6_408

Average distance = 1.7583 Å; standard deviation = 0.1750 Å; number of points = 100046



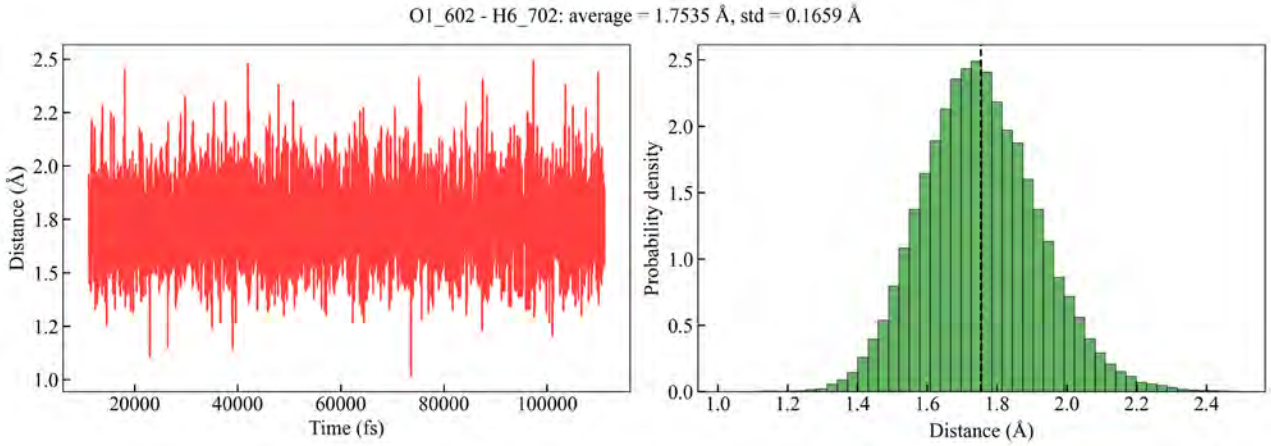
O1_601 - H6_701

Average distance = 1.7567 Å; standard deviation = 0.1760 Å; number of points = 100046



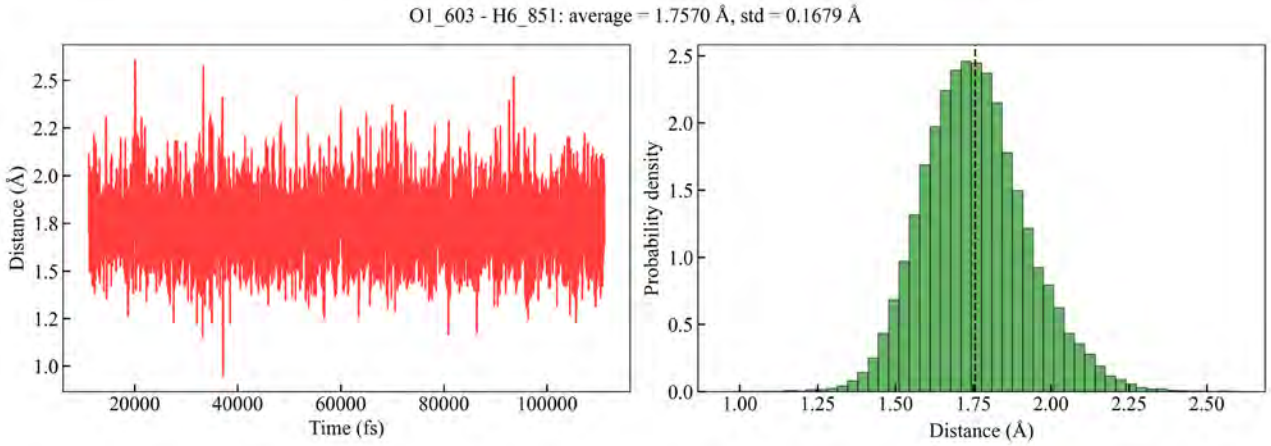
O1_602 - H6_702

Average distance = 1.7535 Å; standard deviation = 0.1659 Å; number of points = 100046



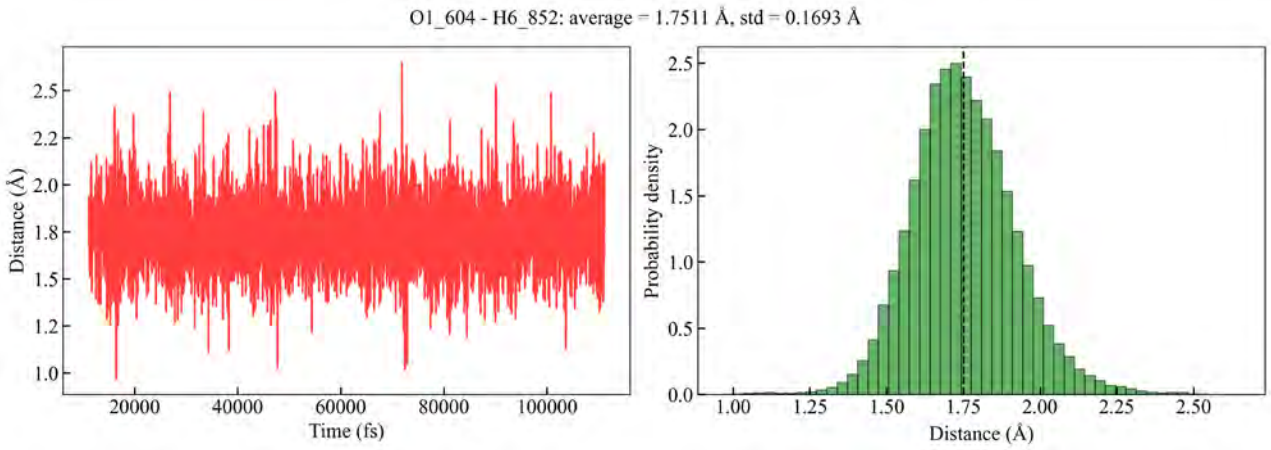
O1_603 - H6_851

Average distance = 1.7570 Å; standard deviation = 0.1679 Å; number of points = 100046



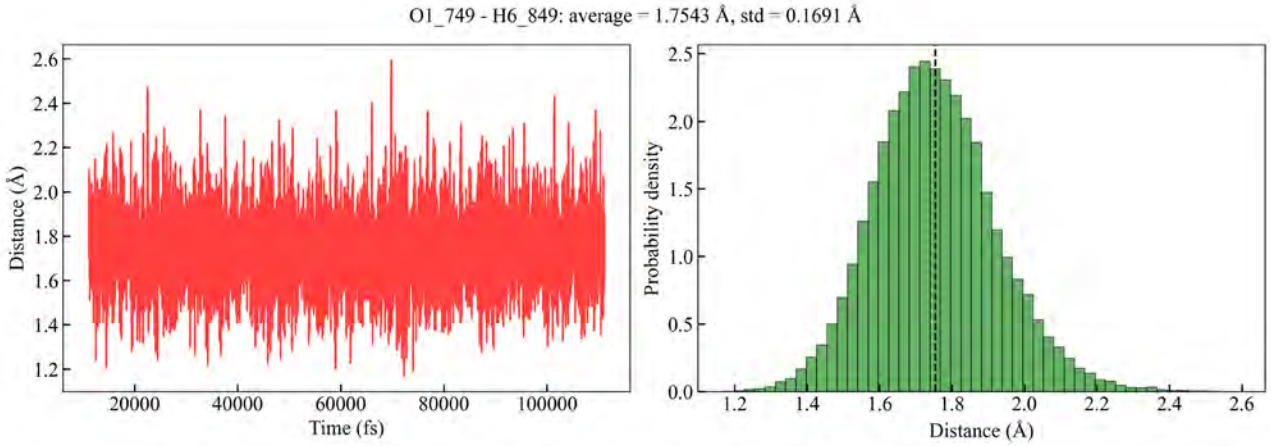
O1_604 - H6_852

Average distance = 1.7511 Å; standard deviation = 0.1693 Å; number of points = 100046



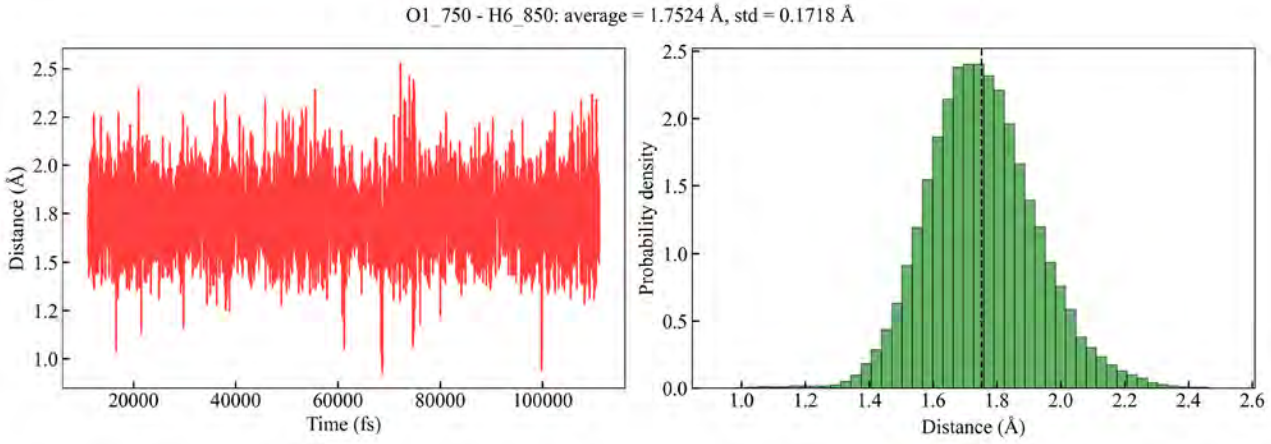
O1_749 - H6_849

Average distance = 1.7543 Å; standard deviation = 0.1691 Å; number of points = 100046



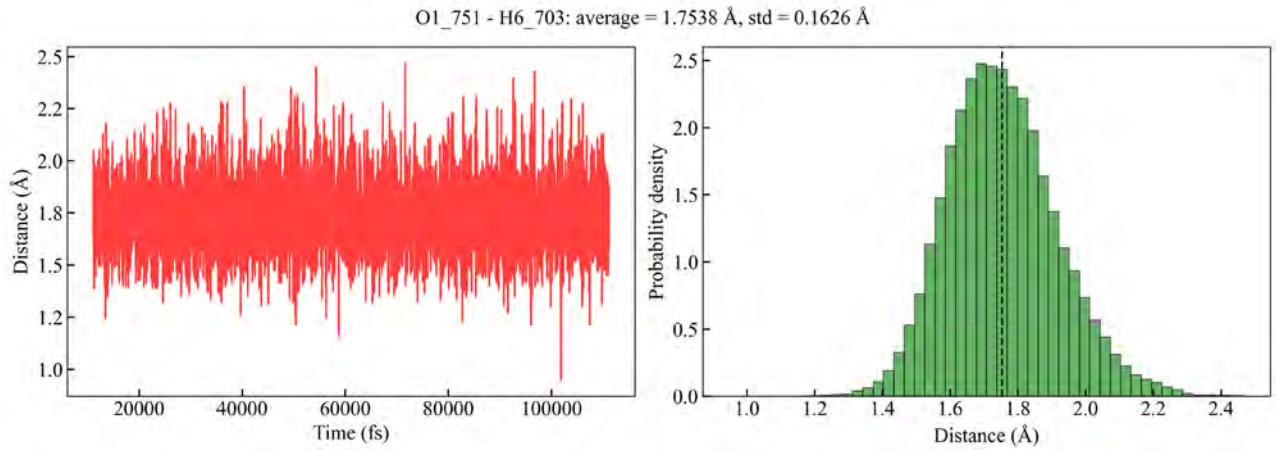
O1_750 - H6_850

Average distance = 1.7524 Å; standard deviation = 0.1718 Å; number of points = 100046



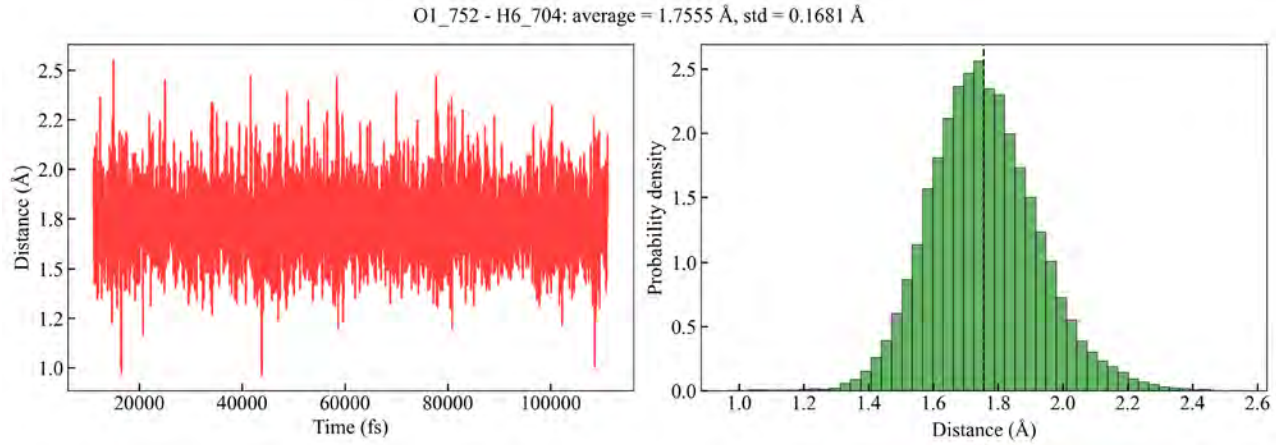
O1_751 - H6_703

Average distance = 1.7538 Å; standard deviation = 0.1626 Å; number of points = 100046



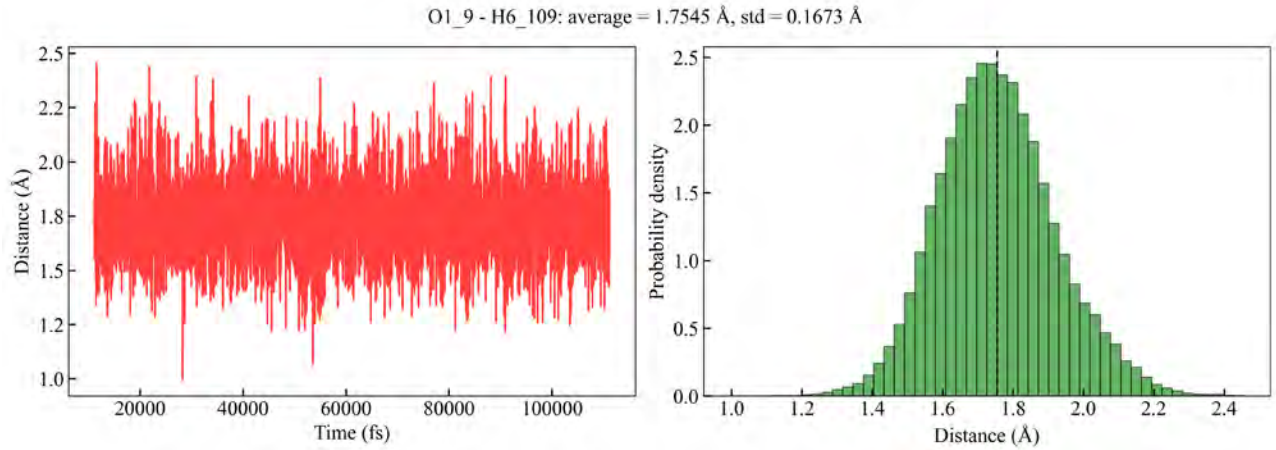
O1_752 - H6_704

Average distance = 1.7555 Å; standard deviation = 0.1681 Å; number of points = 100046



O1_9 - H6_109

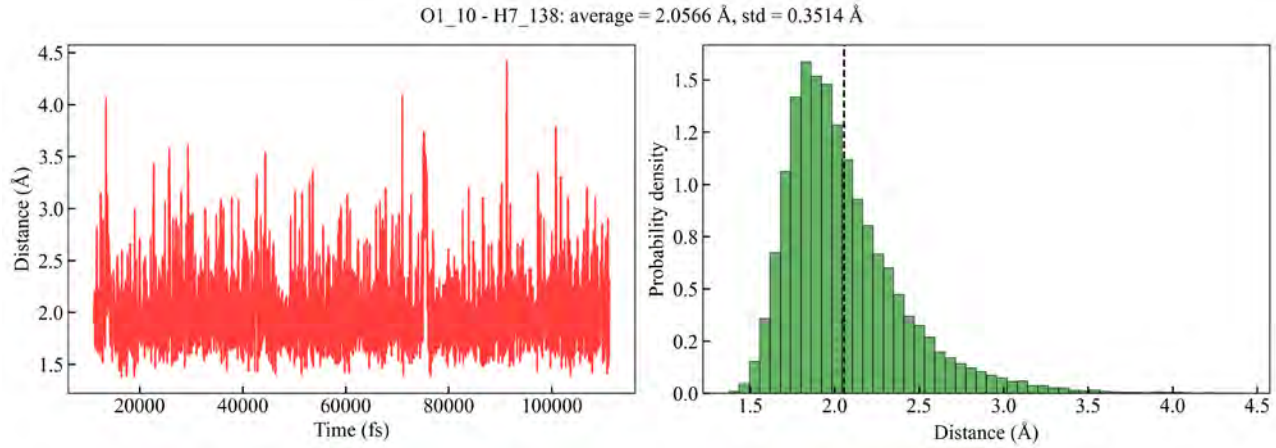
Average distance = 1.7545 Å; standard deviation = 0.1673 Å; number of points = 100046



O1 - H7

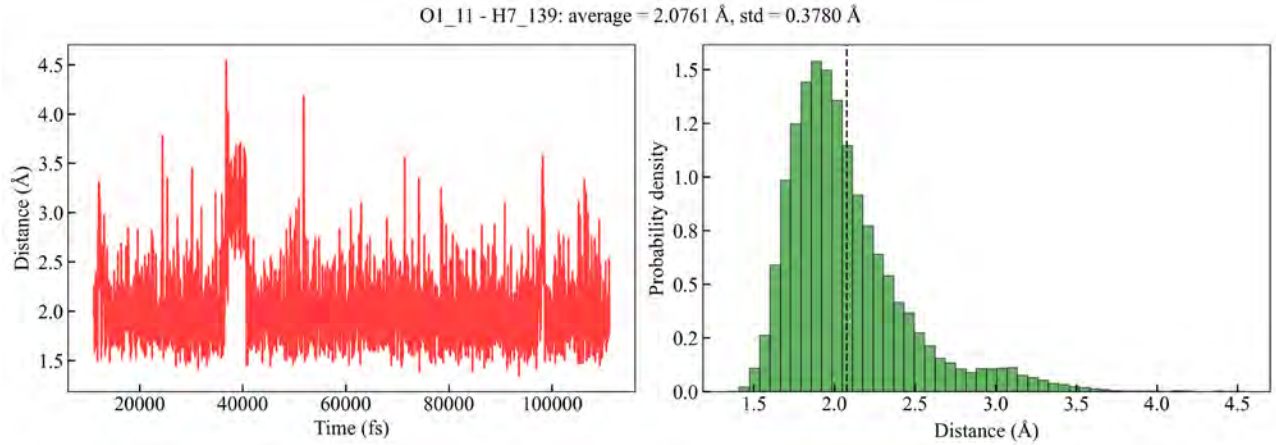
O1_10 - H7_138

Average distance = 2.0566 Å; standard deviation = 0.3514 Å; number of points = 100046



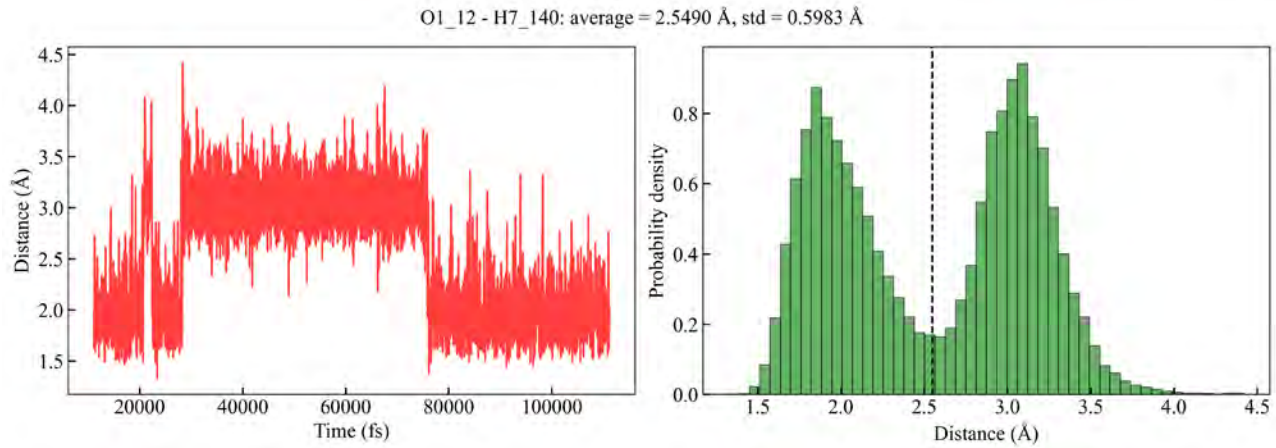
O1_11 - H7_139

Average distance = 2.0761 Å; standard deviation = 0.3780 Å; number of points = 100046



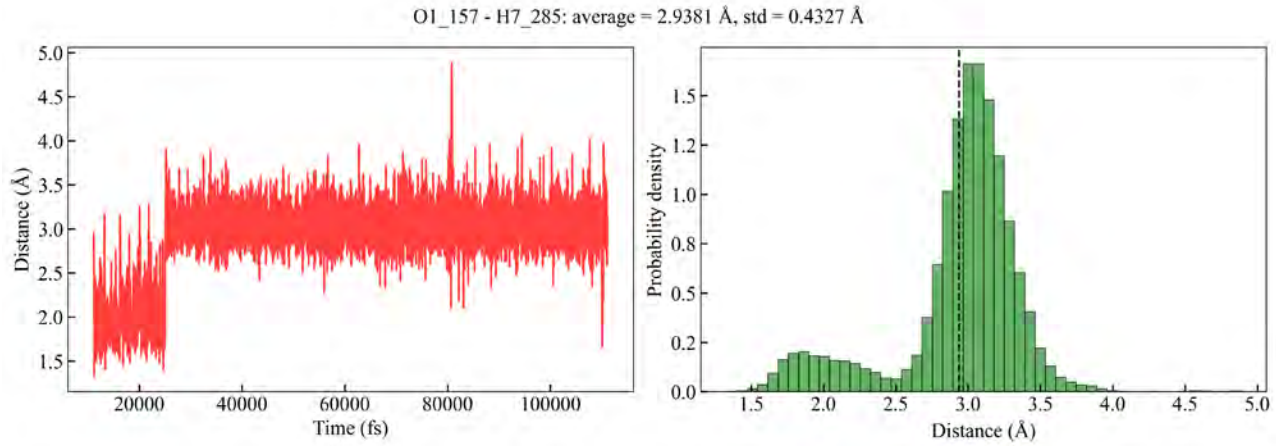
O1_12 - H7_140

Average distance = 2.5490 Å; standard deviation = 0.5983 Å; number of points = 100046



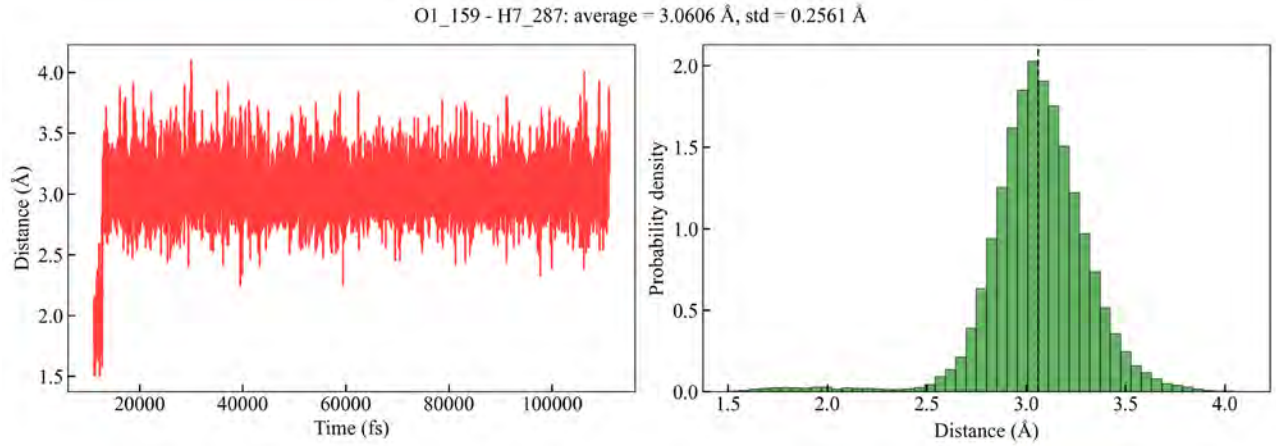
O1_157 - H7_285

Average distance = 2.9381 Å; standard deviation = 0.4327 Å; number of points = 100046



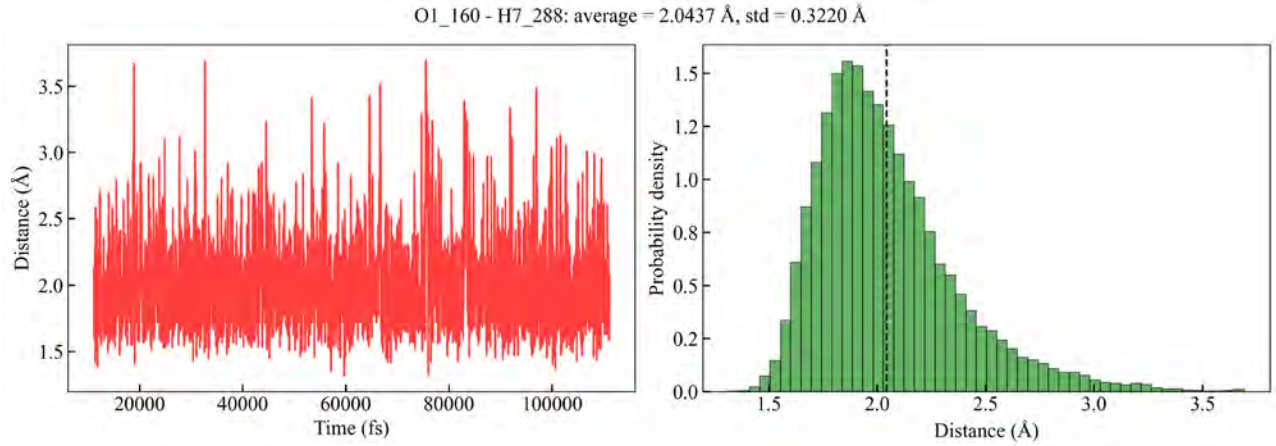
O1_159 - H7_287

Average distance = 3.0606 Å; standard deviation = 0.2561 Å; number of points = 100046



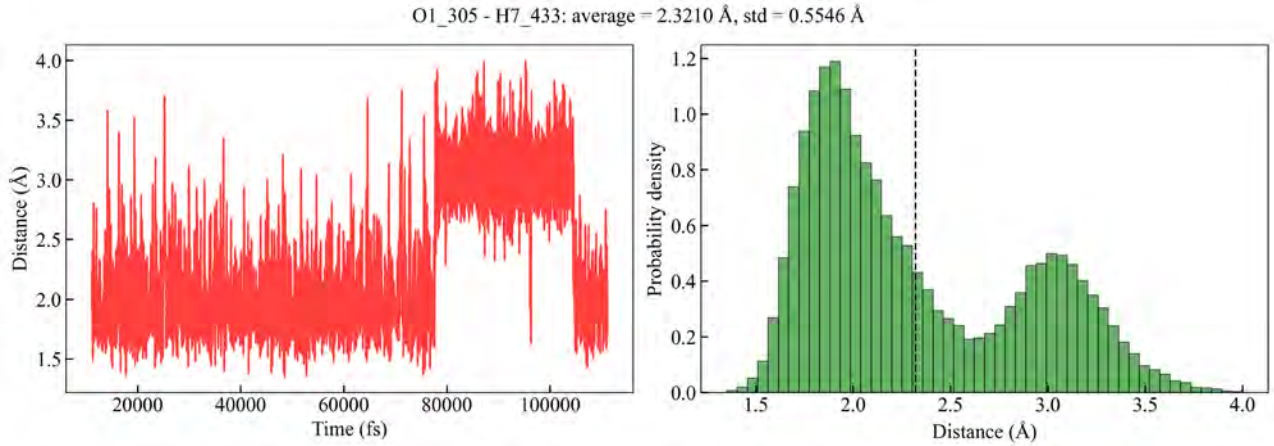
O1_160 - H7_288

Average distance = 2.0437 Å; standard deviation = 0.3220 Å; number of points = 100046



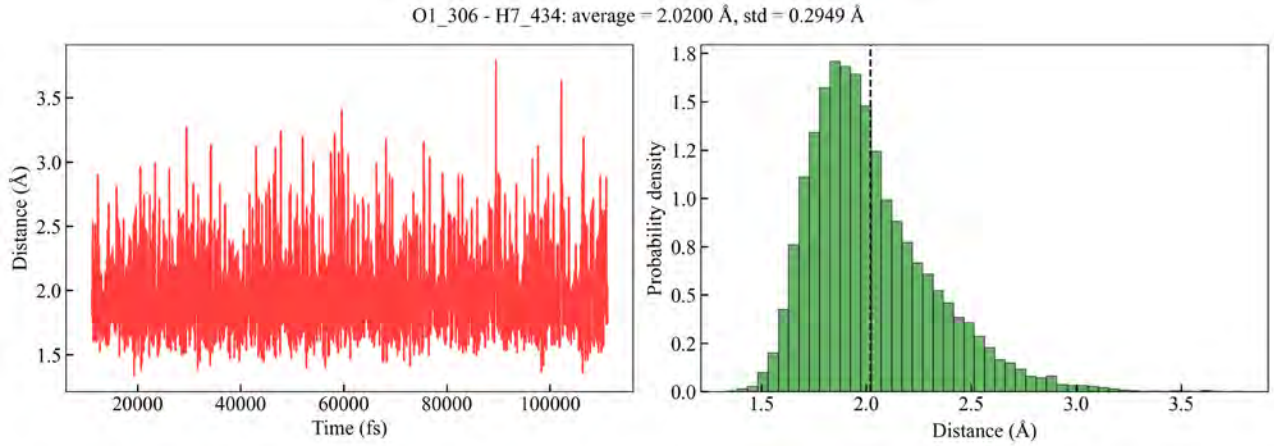
O1_305 - H7_433

Average distance = 2.3210 Å; standard deviation = 0.5546 Å; number of points = 100046



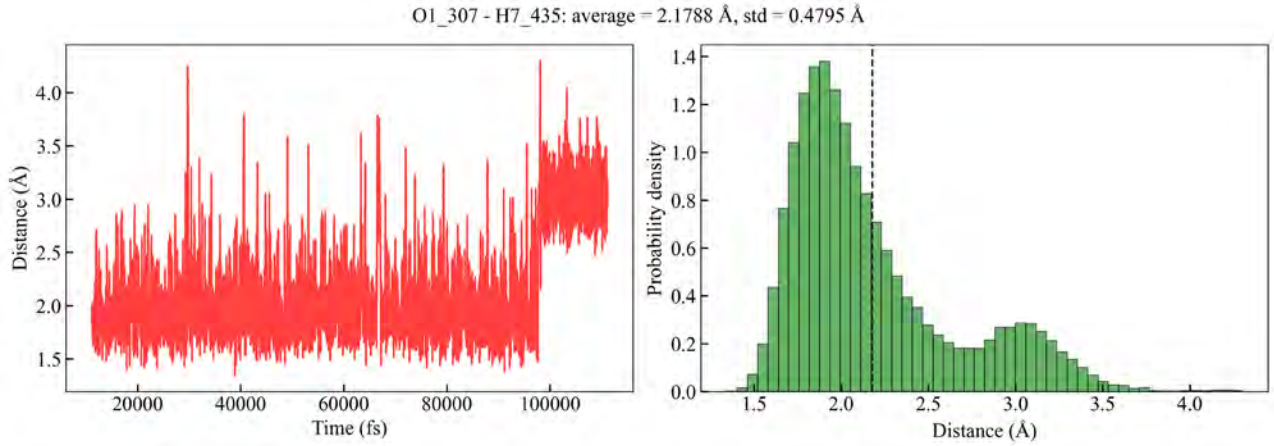
O1_306 - H7_434

Average distance = 2.0200 Å; standard deviation = 0.2949 Å; number of points = 100046



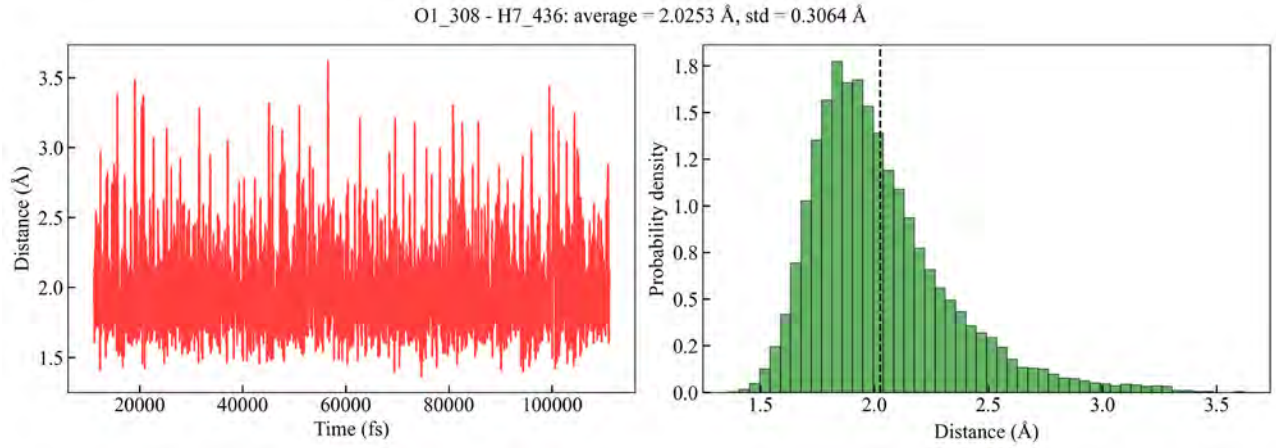
O1_307 - H7_435

Average distance = 2.1788 Å; standard deviation = 0.4795 Å; number of points = 100046



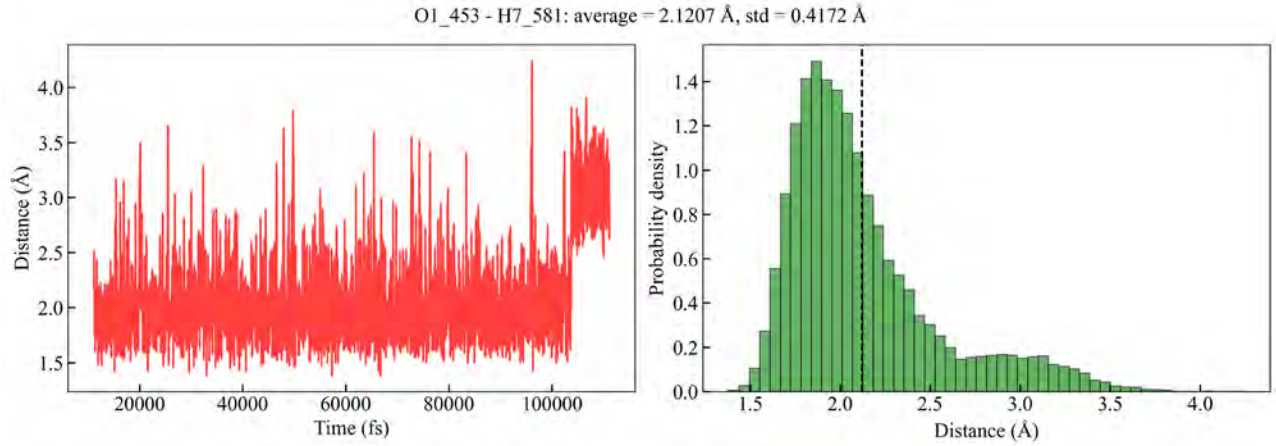
O1_308 - H7_436

Average distance = 2.0253 Å; standard deviation = 0.3064 Å; number of points = 100046



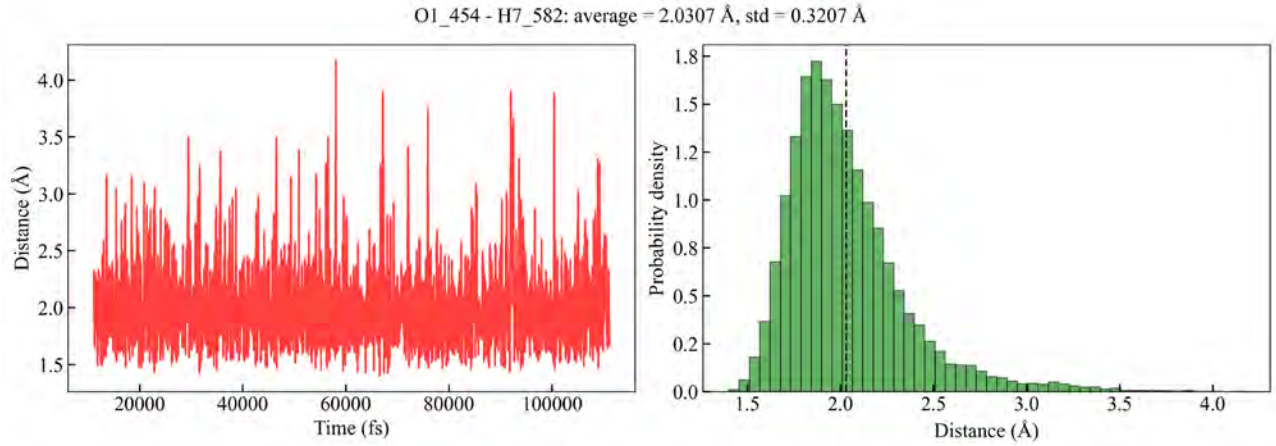
O1_453 - H7_581

Average distance = 2.1207 Å; standard deviation = 0.4172 Å; number of points = 100046



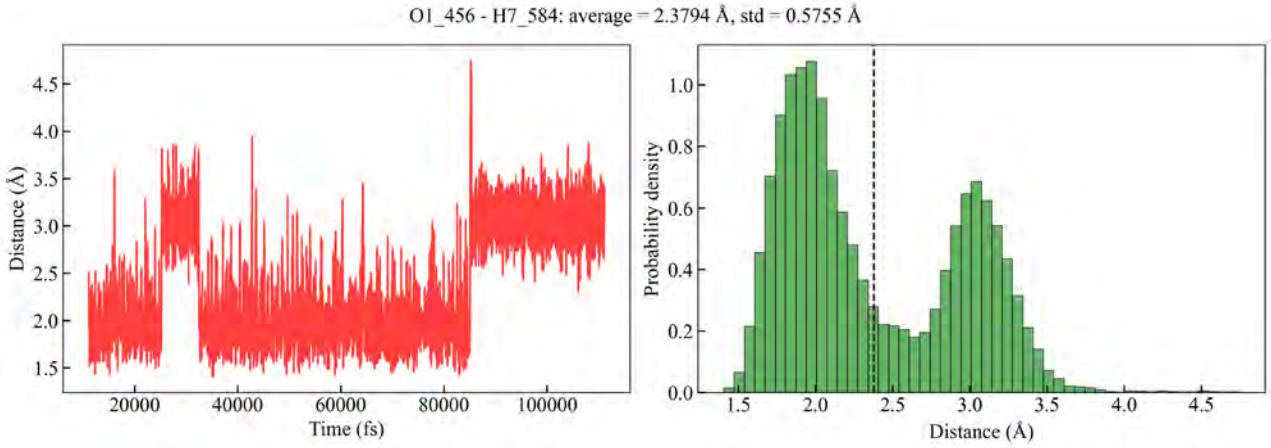
O1_454 - H7_582

Average distance = 2.0307 Å; standard deviation = 0.3207 Å; number of points = 100046



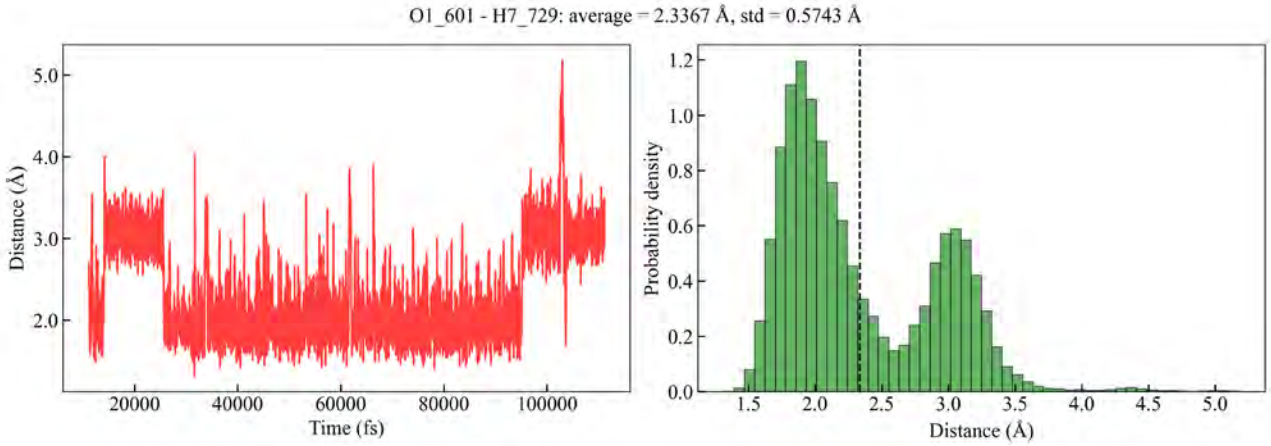
O1_456 - H7_584

Average distance = 2.3794 Å; standard deviation = 0.5755 Å; number of points = 100046



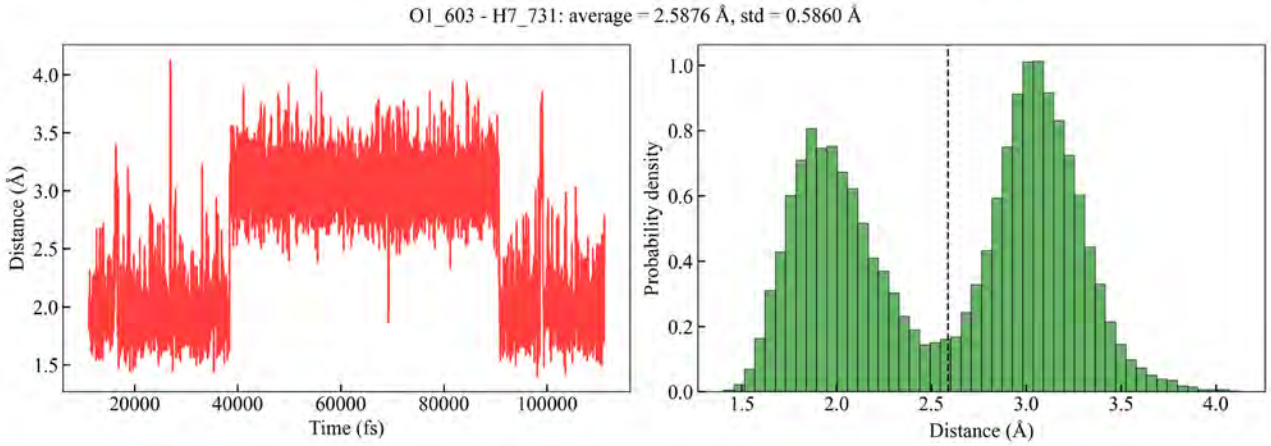
O1_601 - H7_729

Average distance = 2.3367 Å; standard deviation = 0.5743 Å; number of points = 100046



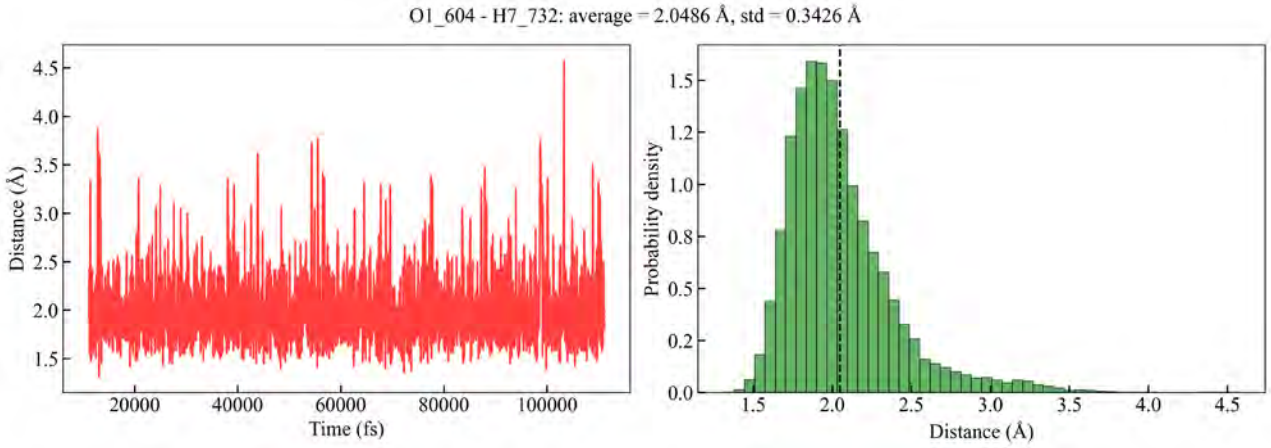
O1_603 - H7_731

Average distance = 2.5876 Å; standard deviation = 0.5860 Å; number of points = 100046



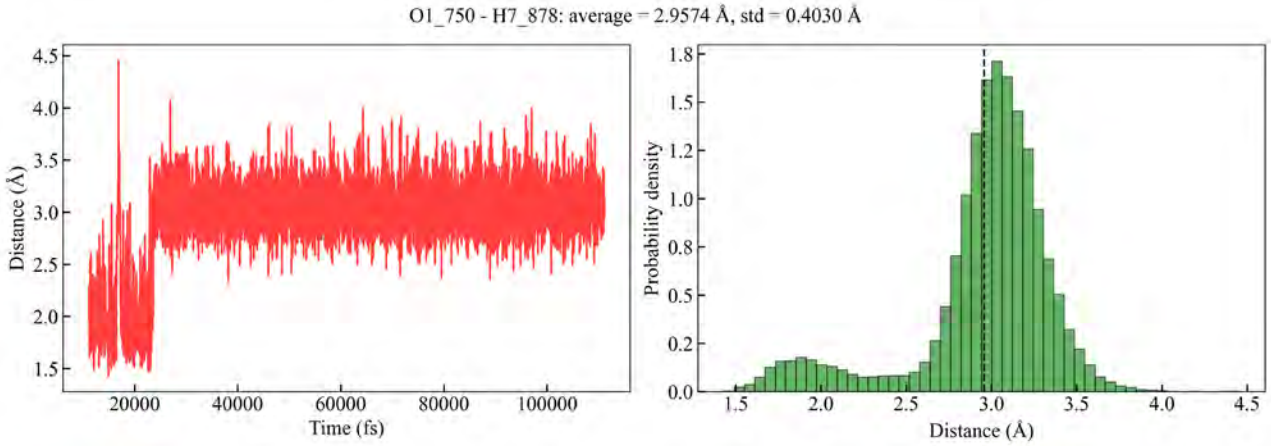
O1_604 - H7_732

Average distance = 2.0486 Å; standard deviation = 0.3426 Å; number of points = 100046



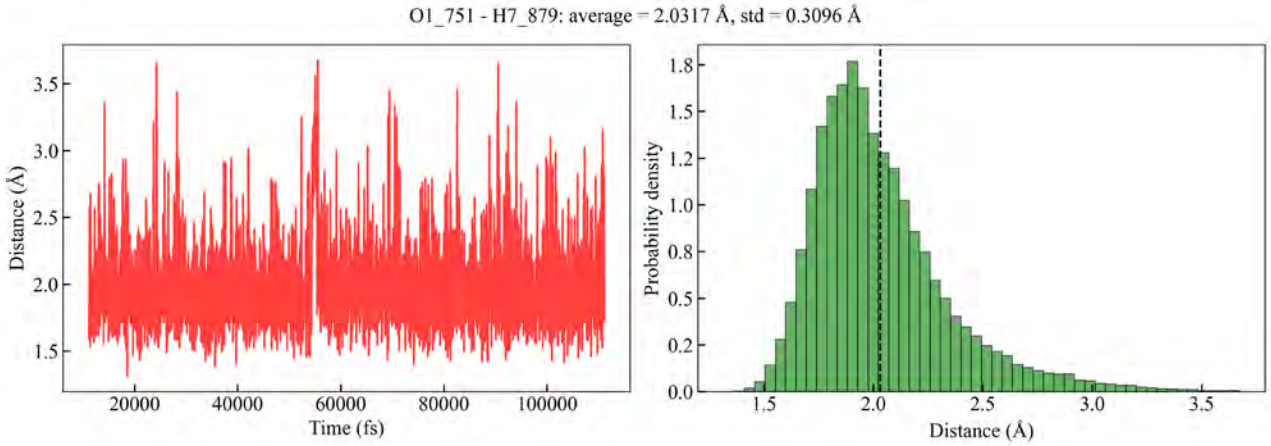
O1_750 - H7_878

Average distance = 2.9574 Å; standard deviation = 0.4030 Å; number of points = 100046



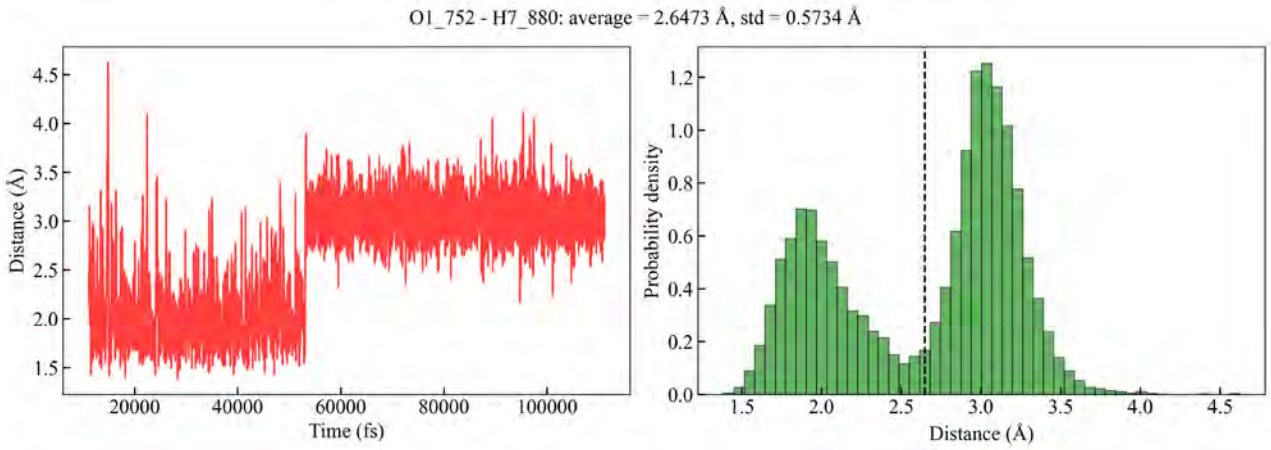
O1_751 - H7_879

Average distance = 2.0317 Å; standard deviation = 0.3096 Å; number of points = 100046



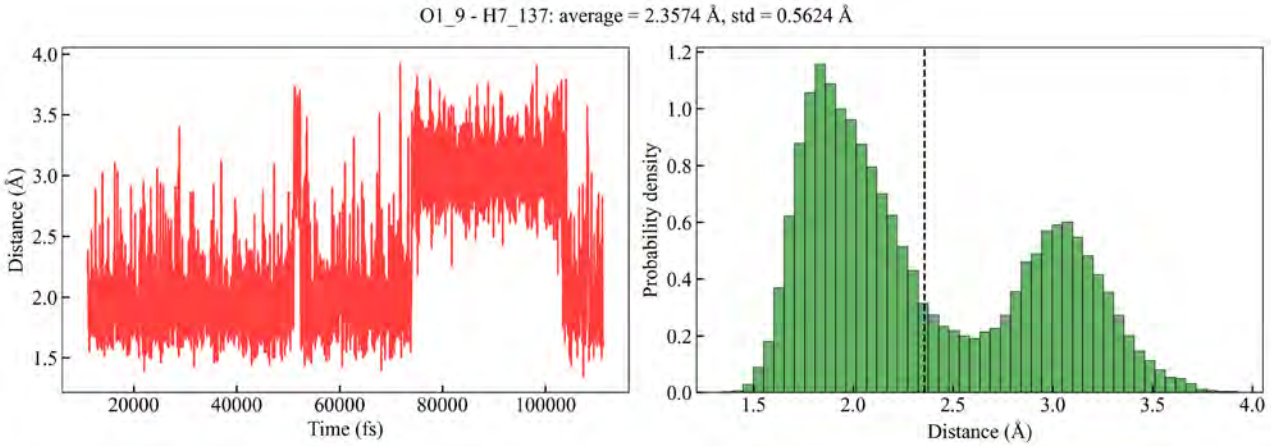
O1_752 - H7_880

Average distance = 2.6473 Å; standard deviation = 0.5734 Å; number of points = 100046



O1_9 - H7_137

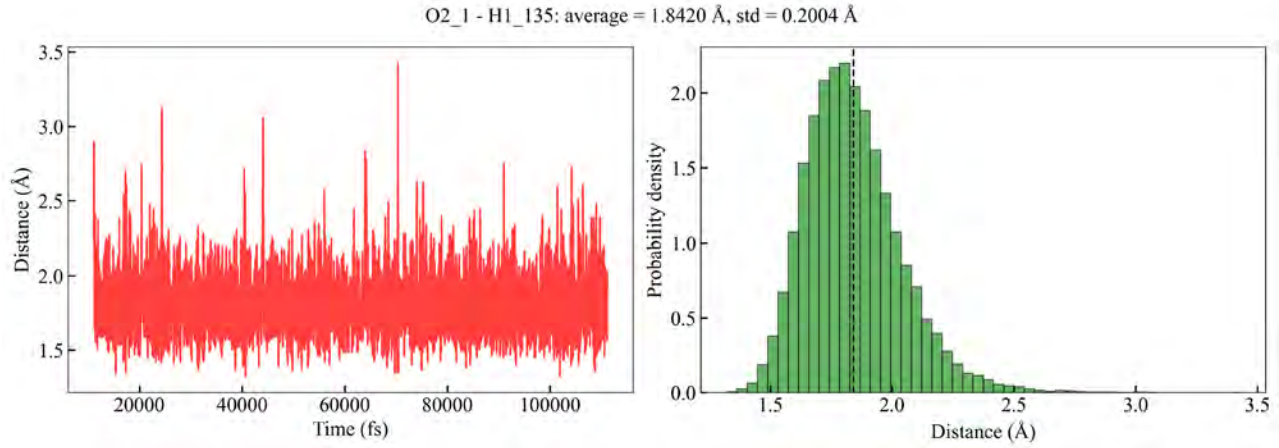
Average distance = 2.3574 Å; standard deviation = 0.5624 Å; number of points = 100046



O2 - H1

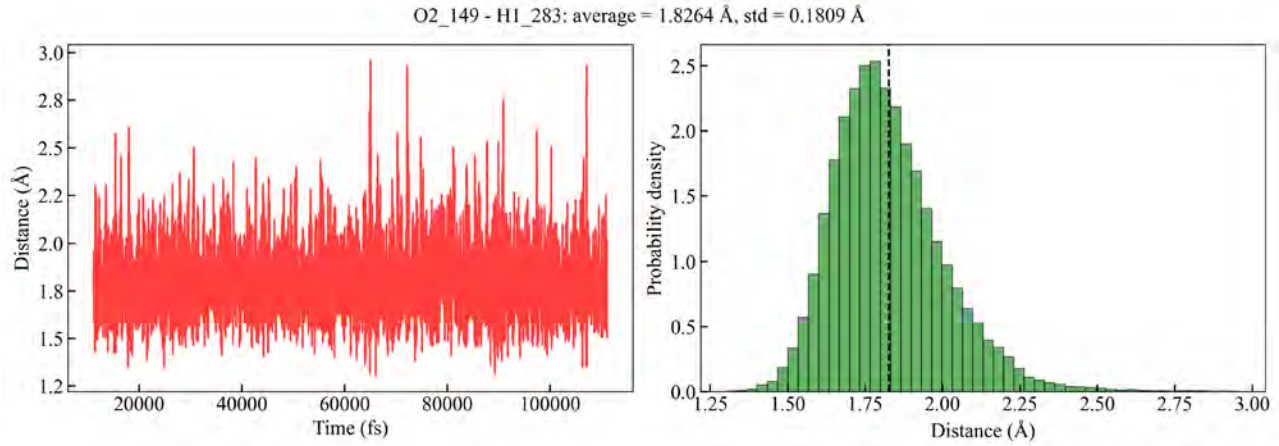
O2_1 - H1_135

Average distance = 1.8420 Å; standard deviation = 0.2004 Å; number of points = 100046



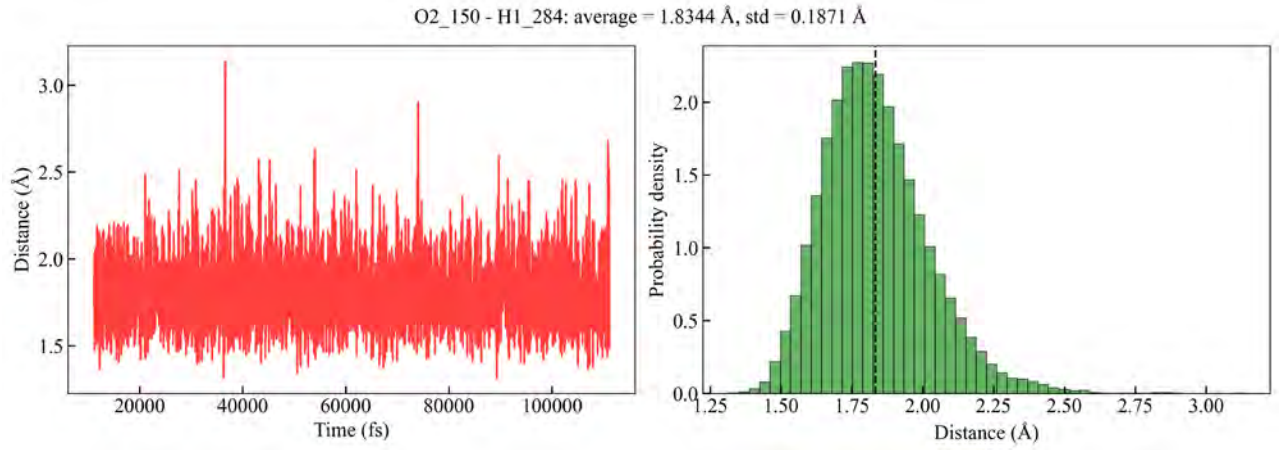
O2_149 - H1_283

Average distance = 1.8264 Å; standard deviation = 0.1809 Å; number of points = 100046



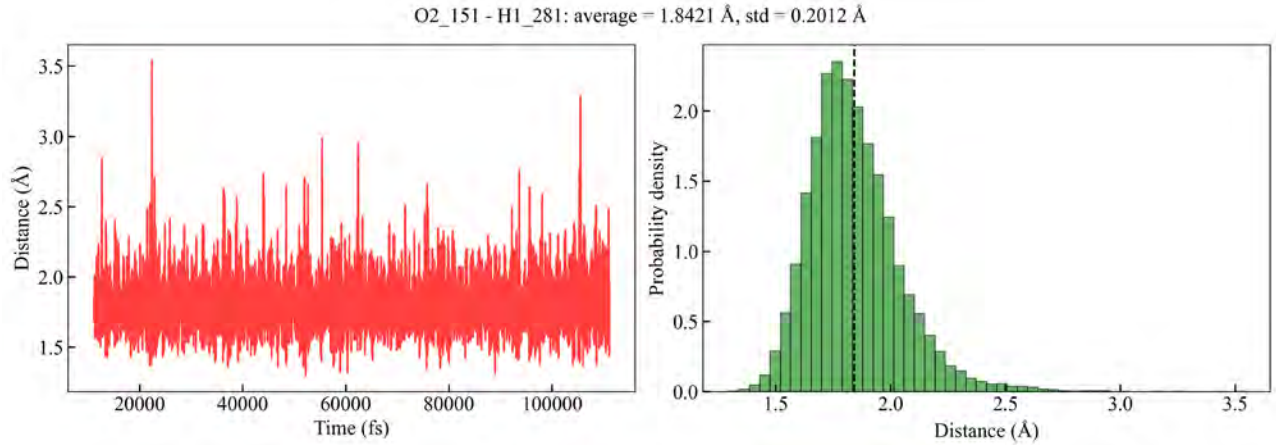
O2_150 - H1_284

Average distance = 1.8344 Å; standard deviation = 0.1871 Å; number of points = 100046



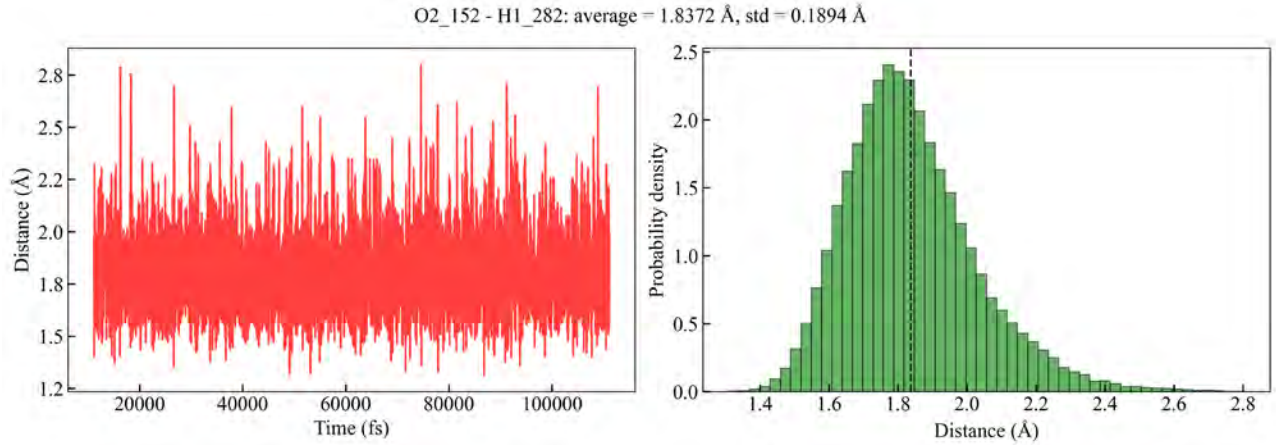
O2_151 - H1_281

Average distance = 1.8421 Å; standard deviation = 0.2012 Å; number of points = 100046



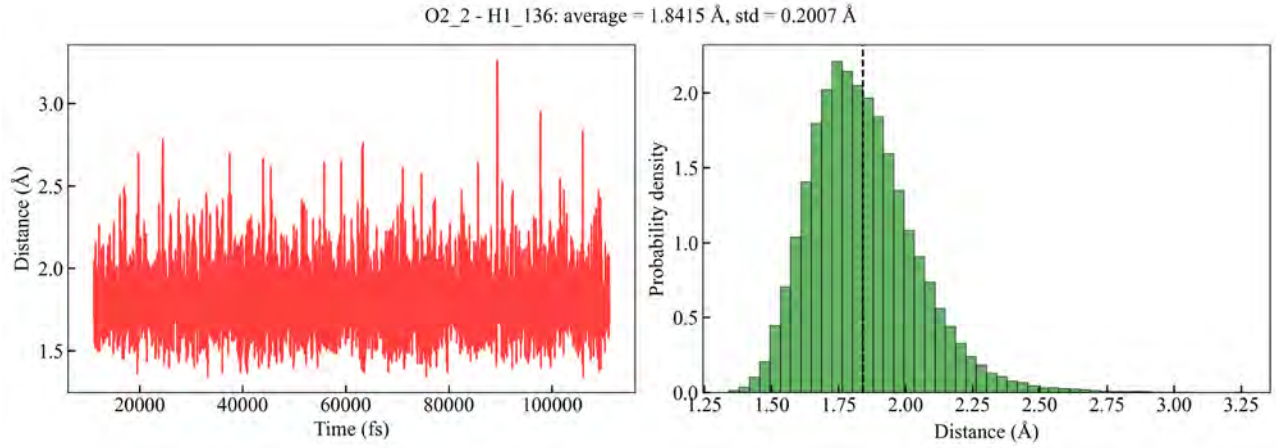
O2_152 - H1_282

Average distance = 1.8372 Å; standard deviation = 0.1894 Å; number of points = 100046



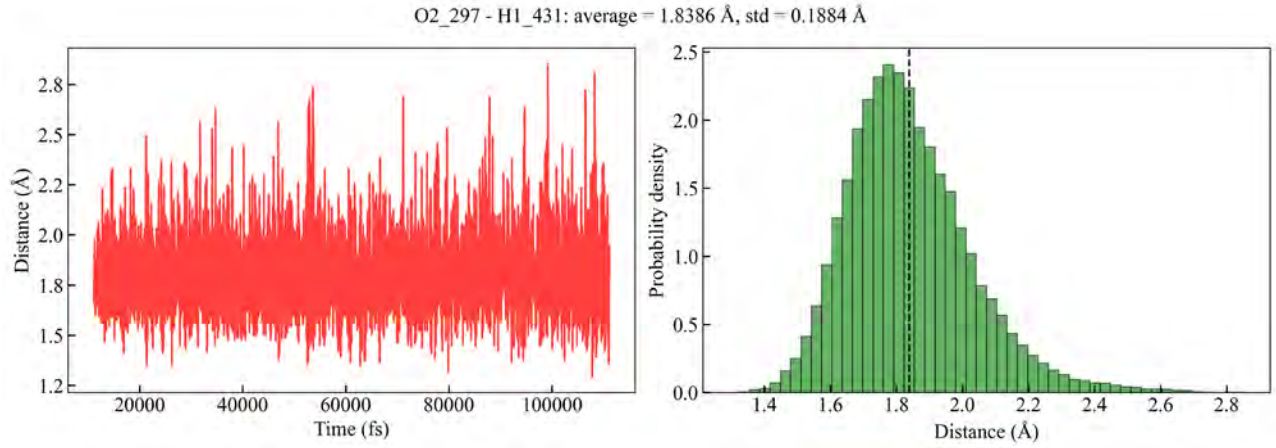
O2_2 - H1_136

Average distance = 1.8415 Å; standard deviation = 0.2007 Å; number of points = 100046



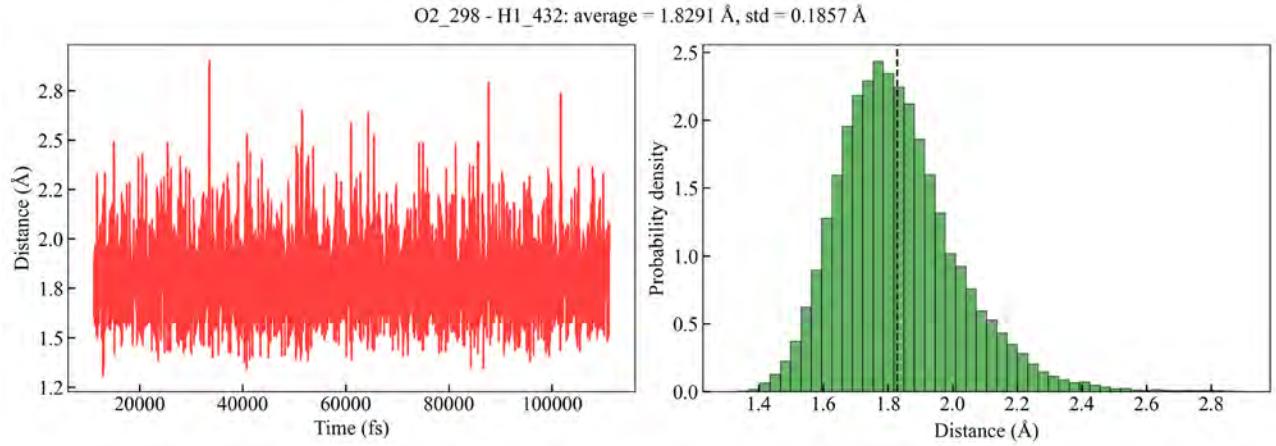
O2_297 - H1_431

Average distance = 1.8386 Å; standard deviation = 0.1884 Å; number of points = 100046



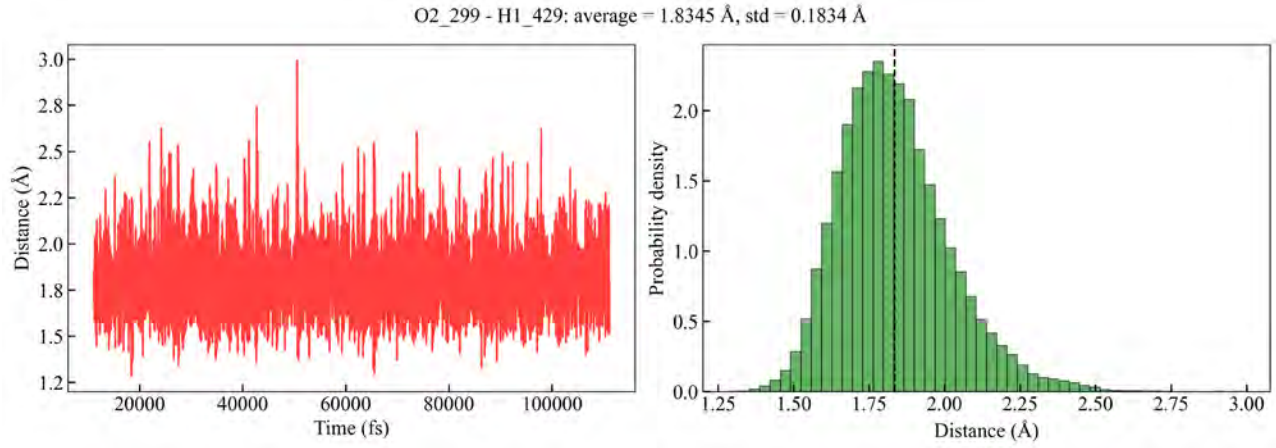
O2_298 - H1_432

Average distance = 1.8291 Å; standard deviation = 0.1857 Å; number of points = 100046



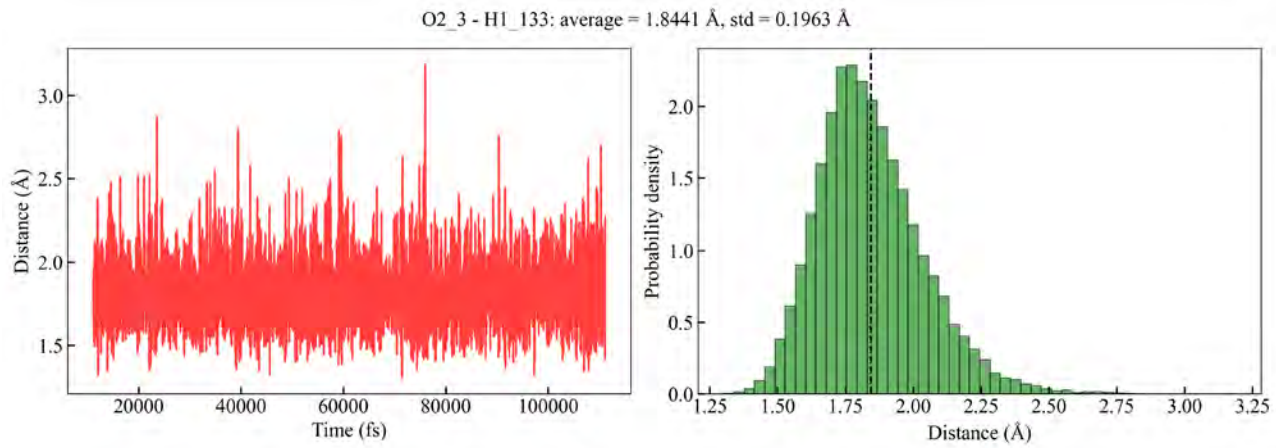
O2_299 - H1_429

Average distance = 1.8345 Å; standard deviation = 0.1834 Å; number of points = 100046



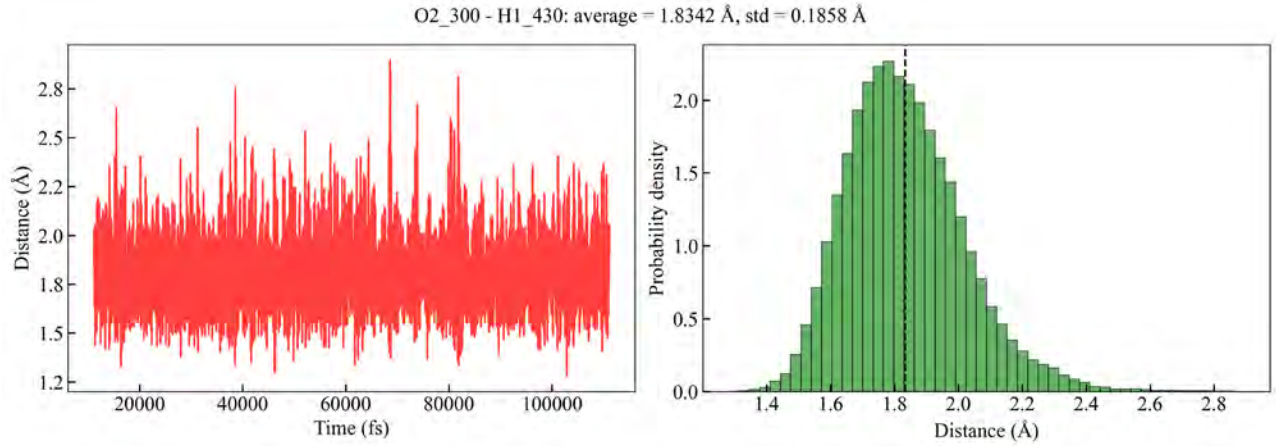
O2_3 - H1_133

Average distance = 1.8441 Å; standard deviation = 0.1963 Å; number of points = 100046



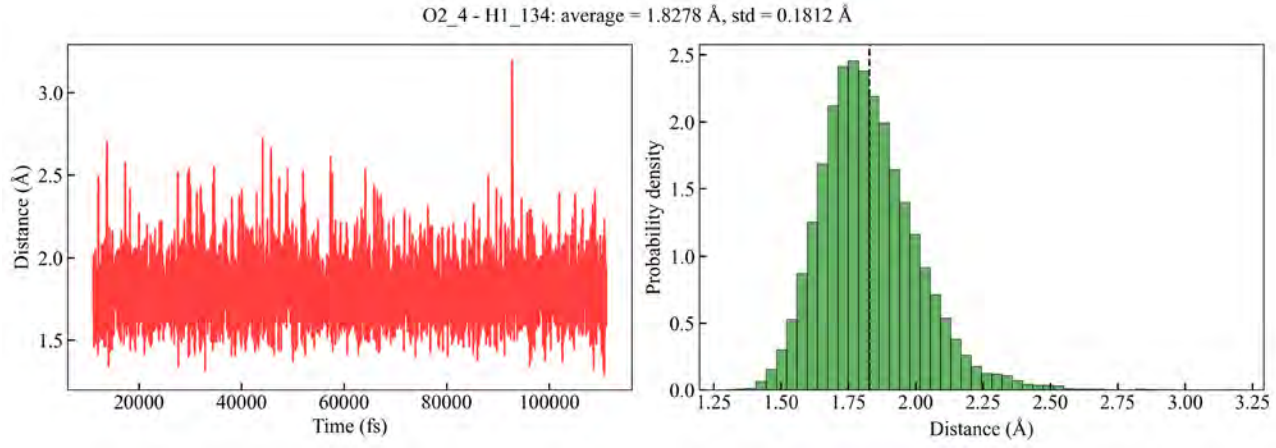
O2_300 - H1_430

Average distance = 1.8342 Å; standard deviation = 0.1858 Å; number of points = 100046



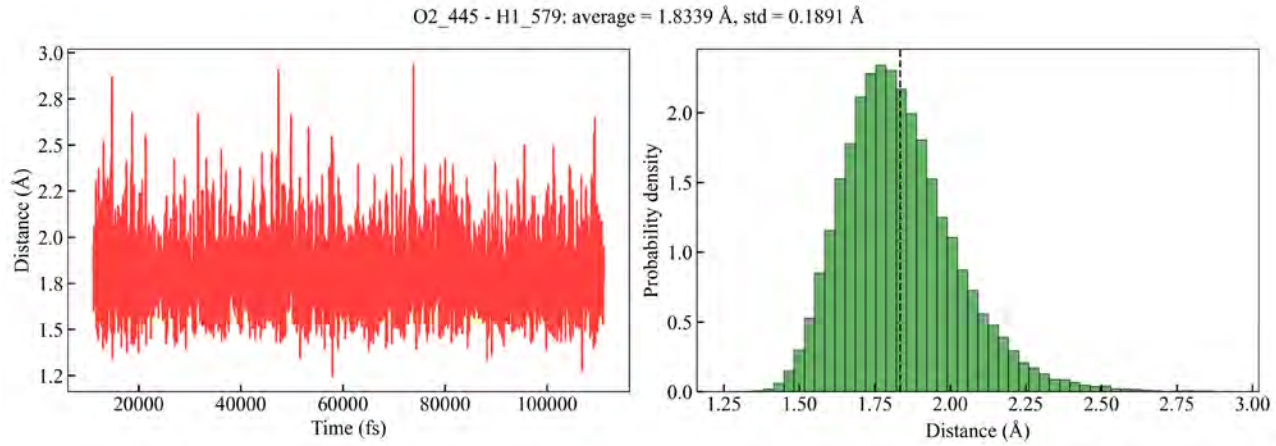
O2_4 - H1_134

Average distance = 1.8278 Å; standard deviation = 0.1812 Å; number of points = 100046



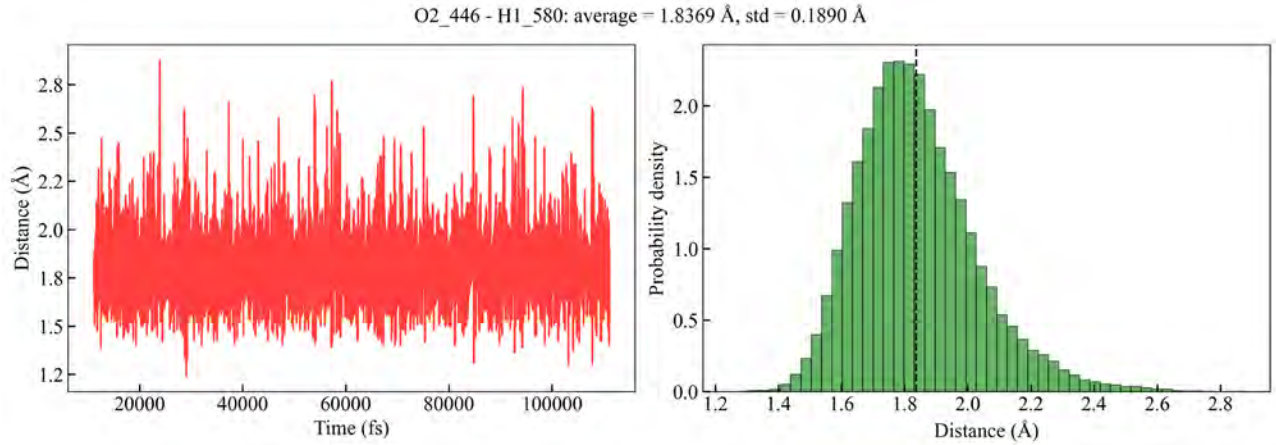
O2_445 - H1_579

Average distance = 1.8339 Å; standard deviation = 0.1891 Å; number of points = 100046



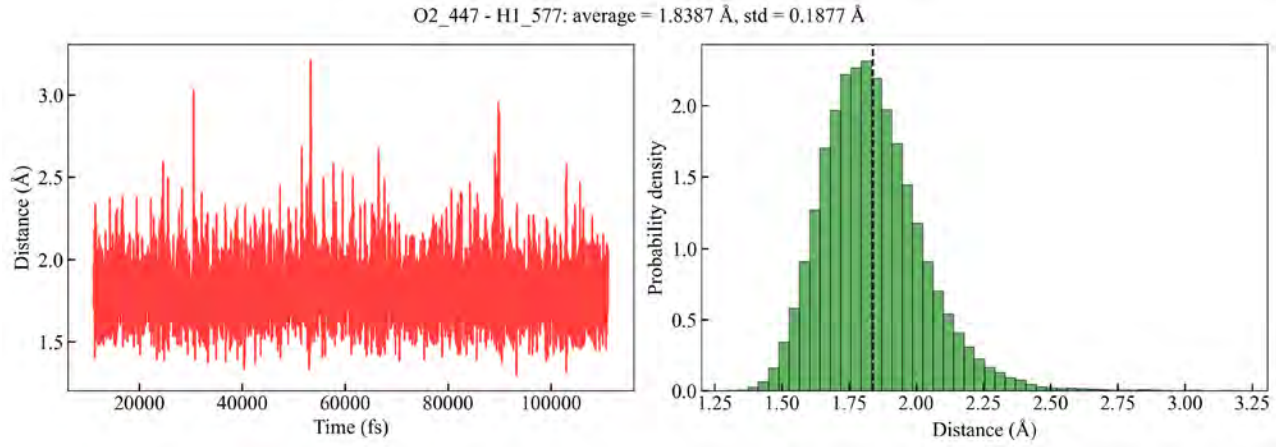
O2_446 - H1_580

Average distance = 1.8369 Å; standard deviation = 0.1890 Å; number of points = 100046



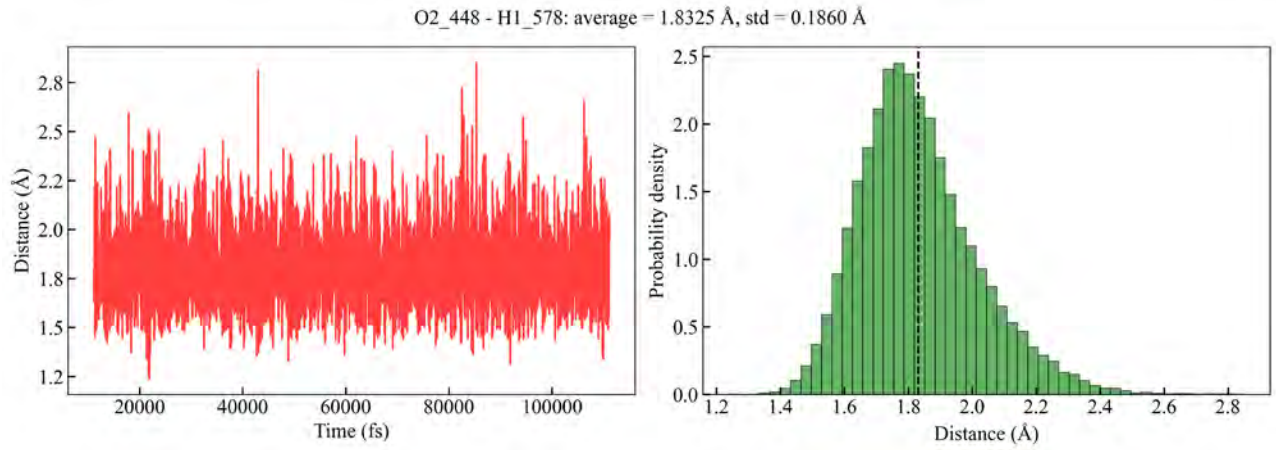
O2_447 - H1_577

Average distance = 1.8387 Å; standard deviation = 0.1877 Å; number of points = 100046



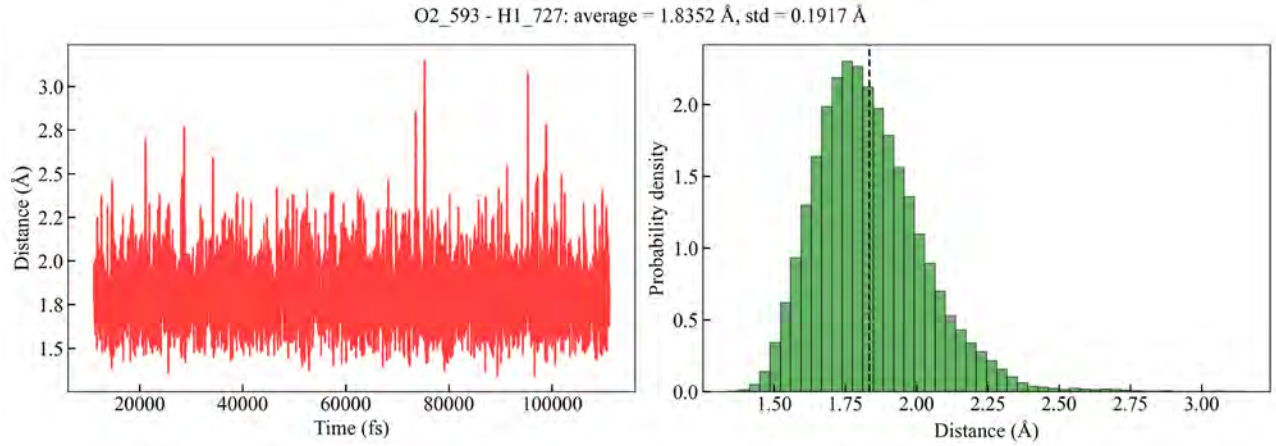
O2_448 - H1_578

Average distance = 1.8325 Å; standard deviation = 0.1860 Å; number of points = 100046



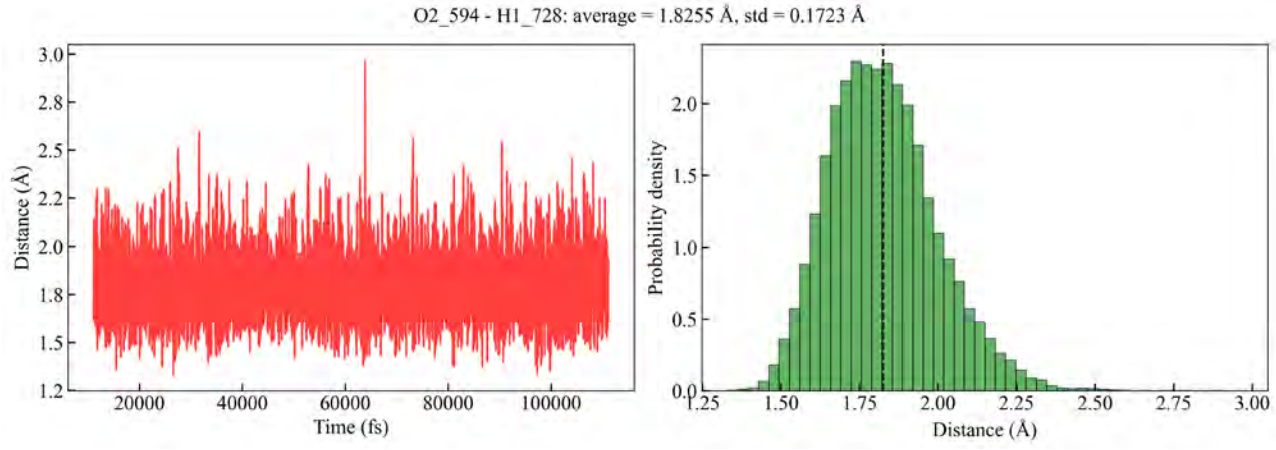
O2_593 - H1_727

Average distance = 1.8352 Å; standard deviation = 0.1917 Å; number of points = 100046



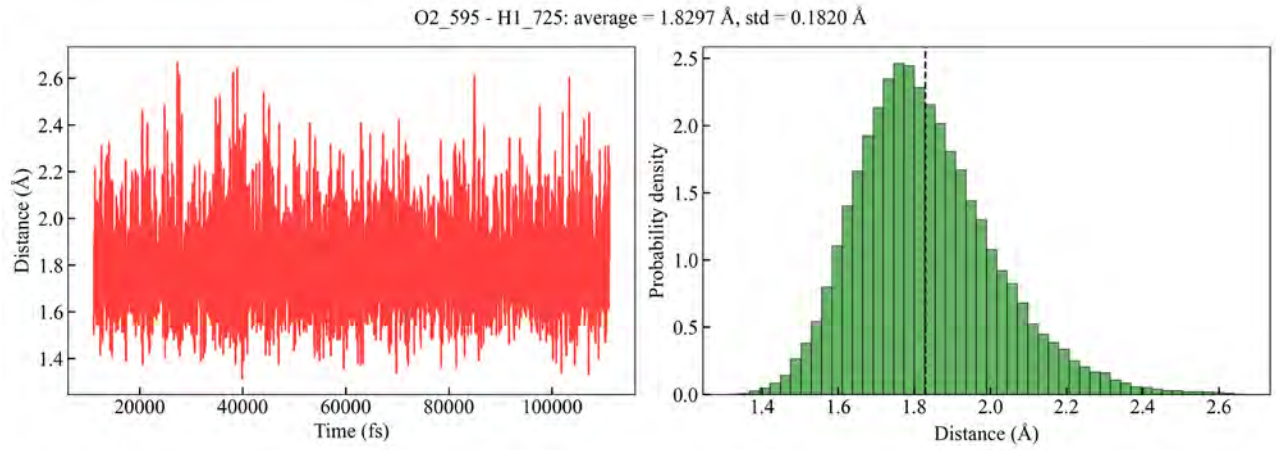
O2_594 - H1_728

Average distance = 1.8255 Å; standard deviation = 0.1723 Å; number of points = 100046



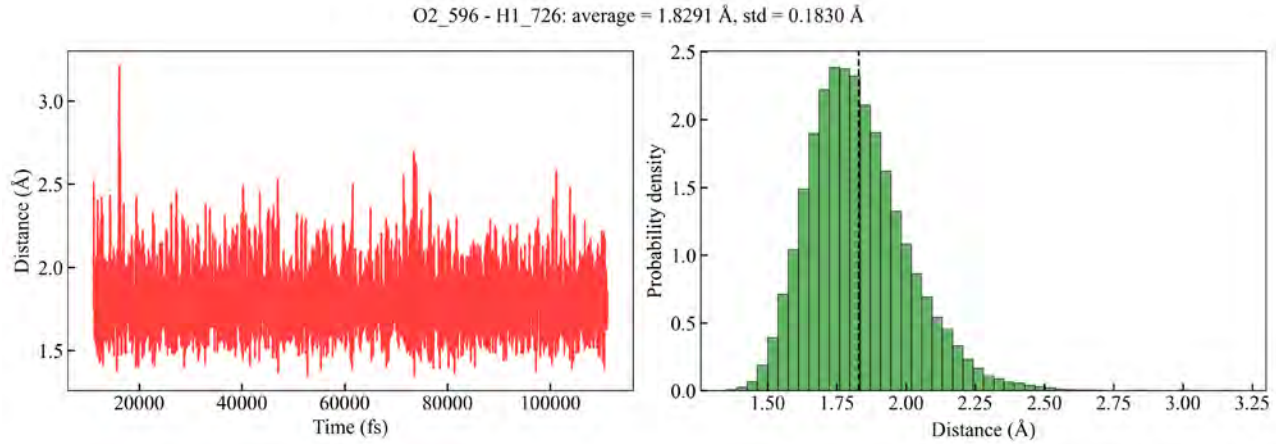
O2_595 - H1_725

Average distance = 1.8297 Å; standard deviation = 0.1820 Å; number of points = 100046



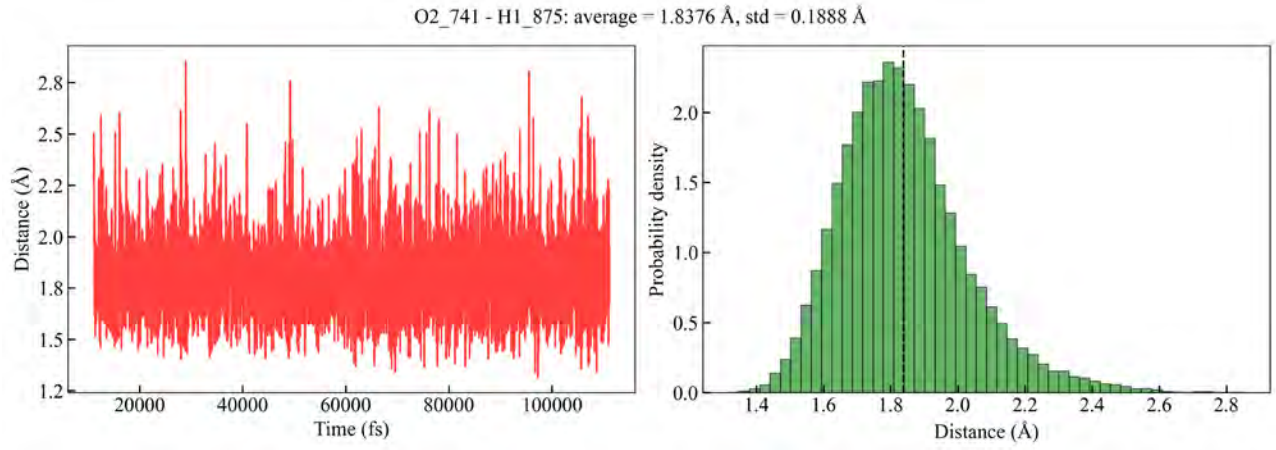
O2_596 - H1_726

Average distance = 1.8291 Å; standard deviation = 0.1830 Å; number of points = 100046



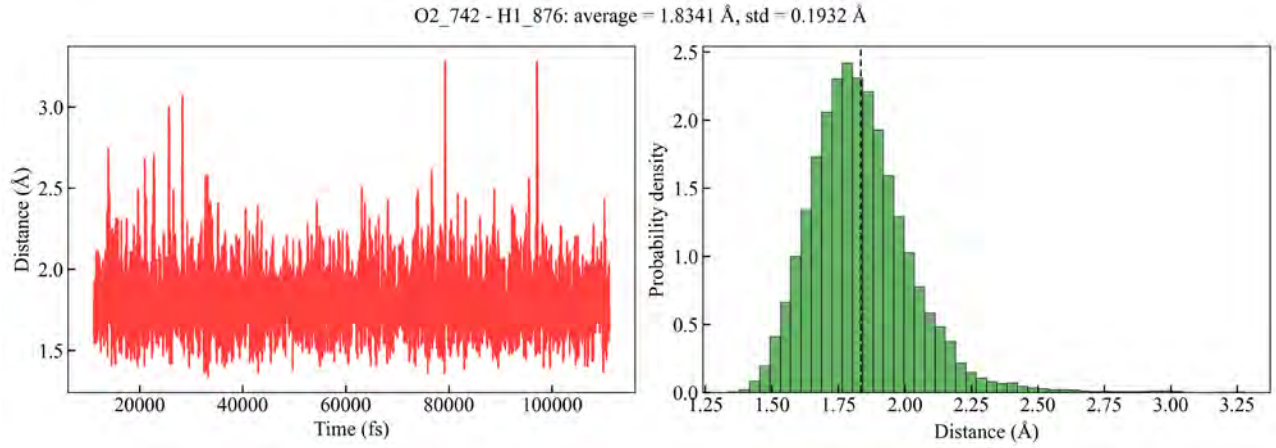
O2_741 - H1_875

Average distance = 1.8376 Å; standard deviation = 0.1888 Å; number of points = 100046



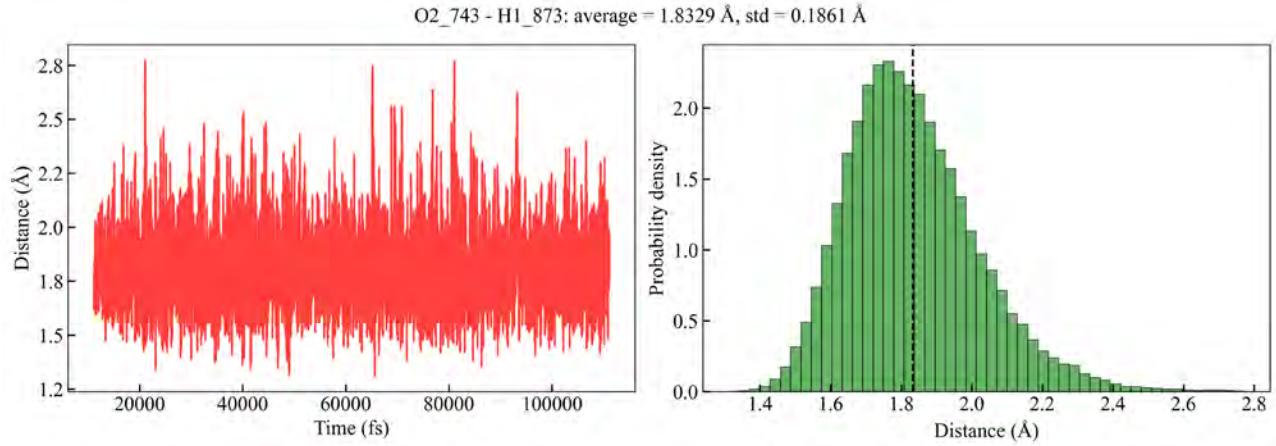
O2_742 - H1_876

Average distance = 1.8341 Å; standard deviation = 0.1932 Å; number of points = 100046



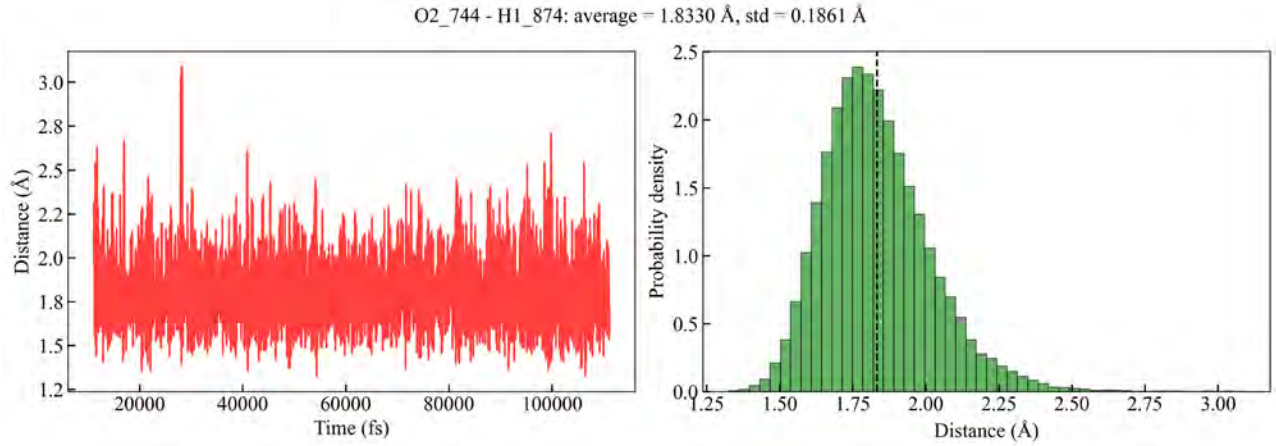
O2_743 - H1_873

Average distance = 1.8329 Å; standard deviation = 0.1861 Å; number of points = 100046



O2_744 - H1_874

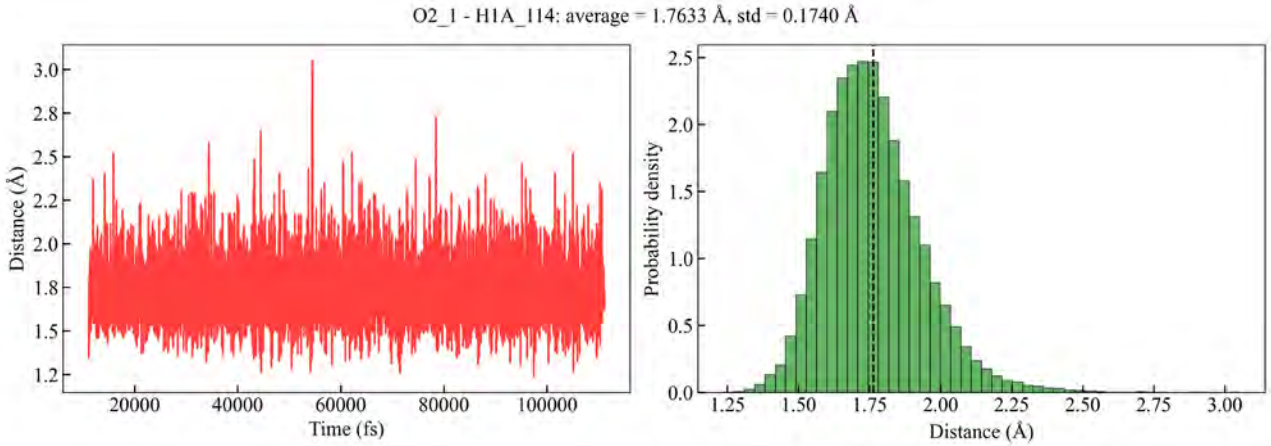
Average distance = 1.8330 Å; standard deviation = 0.1861 Å; number of points = 100046



O2 - H1A

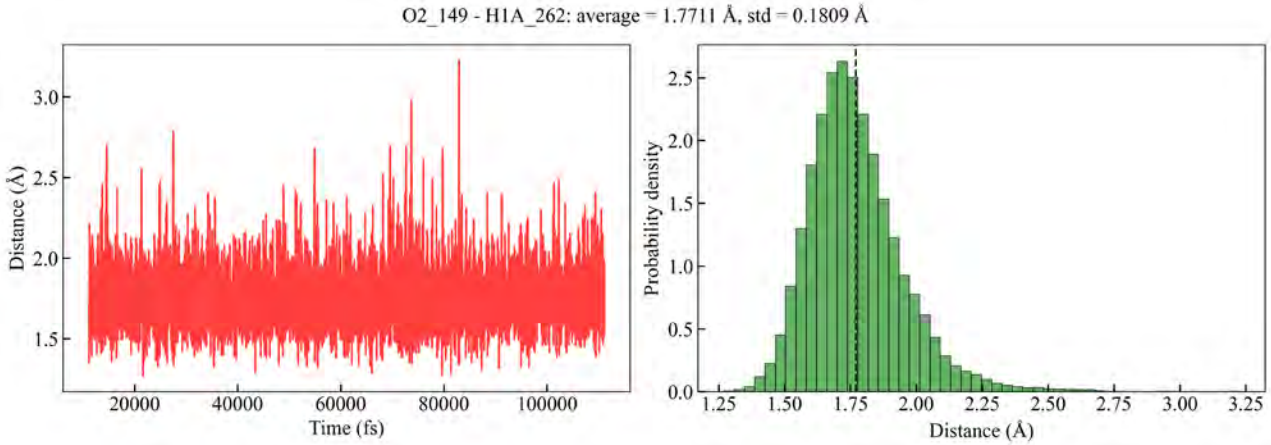
O2_1 - H1A_114

Average distance = 1.7633 Å; standard deviation = 0.1740 Å; number of points = 100046



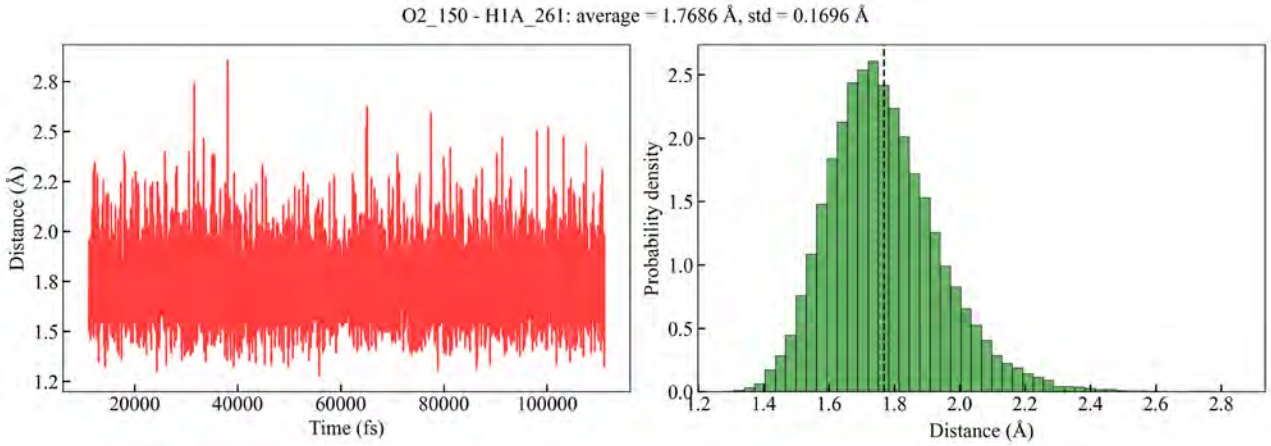
O2_149 - H1A_262

Average distance = 1.7711 Å; standard deviation = 0.1809 Å; number of points = 100046



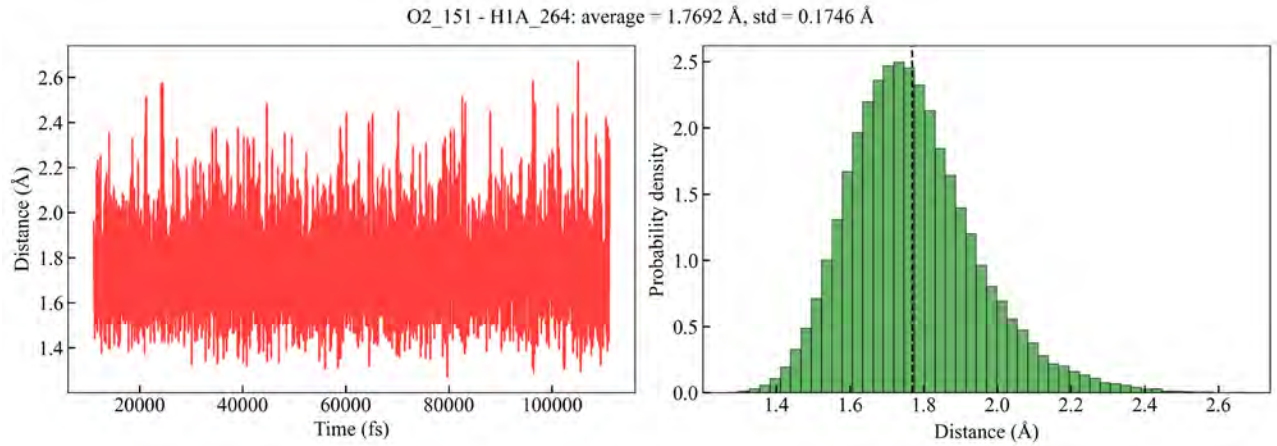
O2_150 - H1A_261

Average distance = 1.7686 Å; standard deviation = 0.1696 Å; number of points = 100046



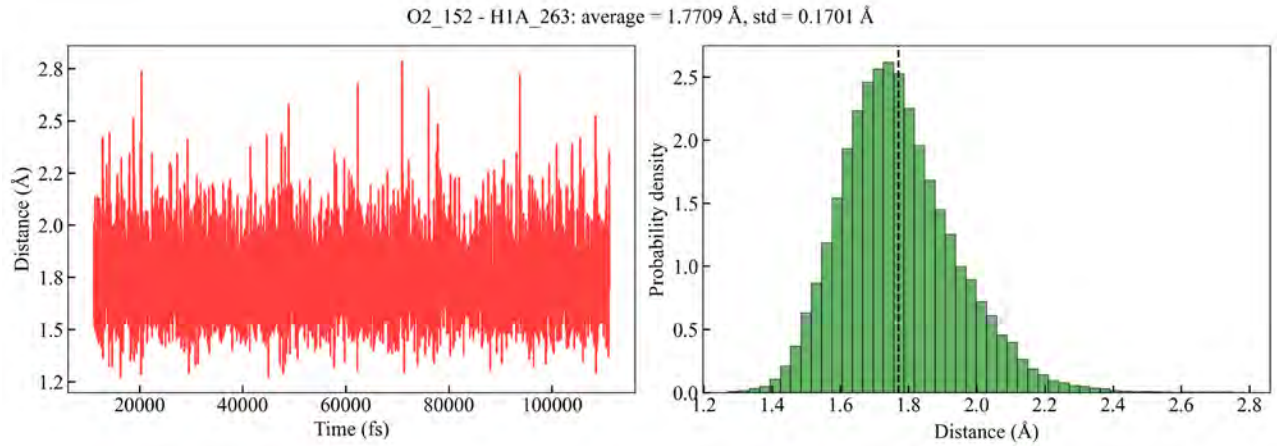
O2_151 - H1A_264

Average distance = 1.7692 Å; standard deviation = 0.1746 Å; number of points = 100046



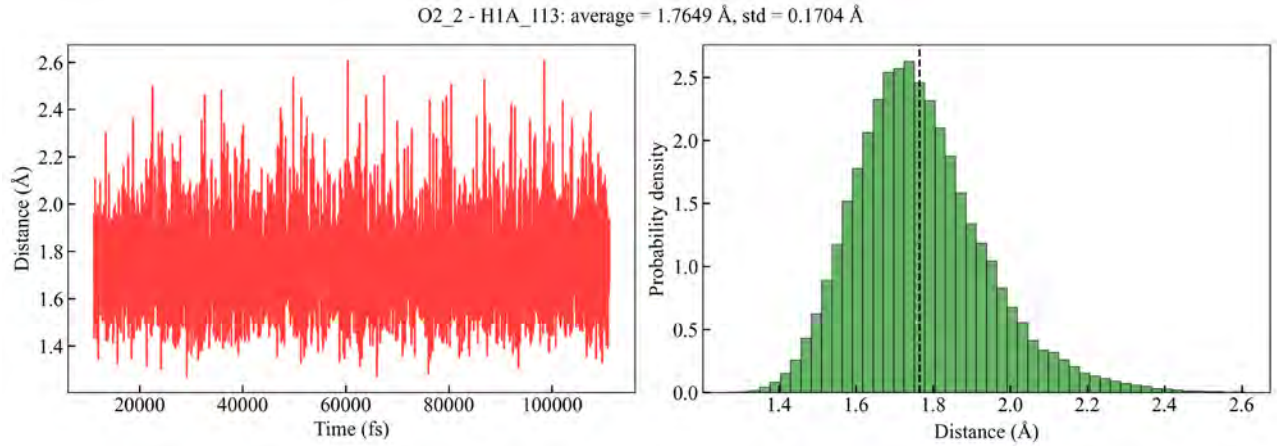
O2_152 - H1A_263

Average distance = 1.7709 Å; standard deviation = 0.1701 Å; number of points = 100046



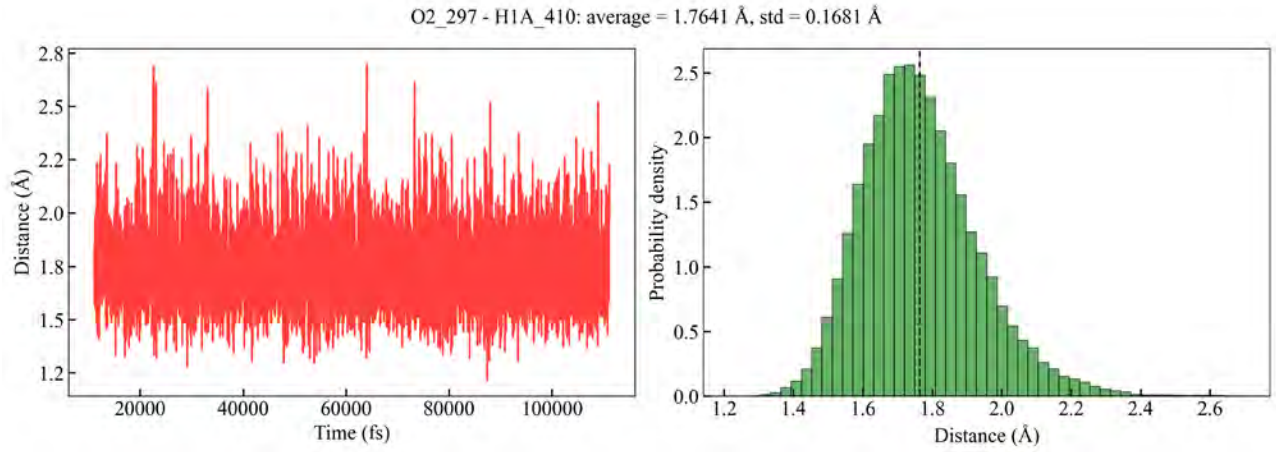
O2_2 - H1A_113

Average distance = 1.7649 Å; standard deviation = 0.1704 Å; number of points = 100046



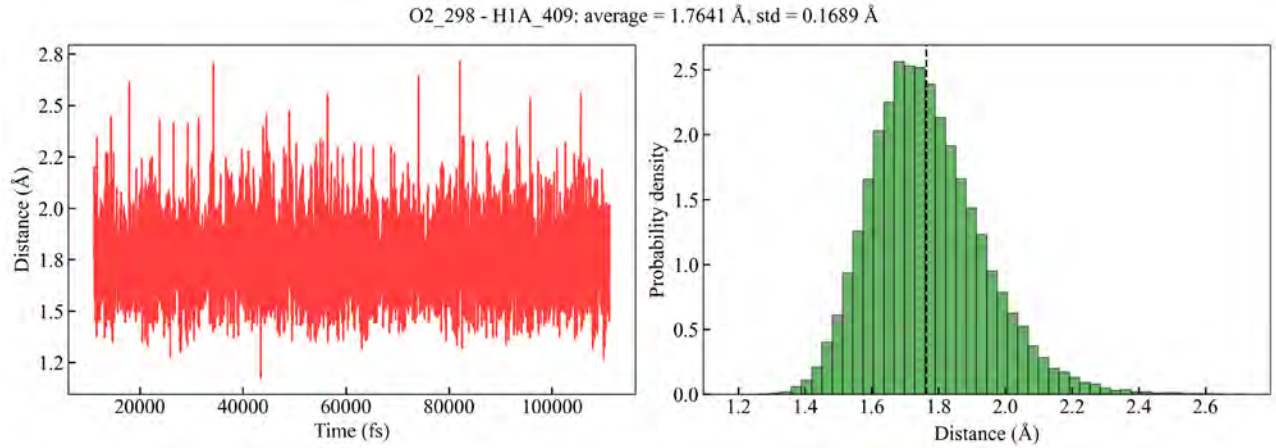
O2_297 - H1A_410

Average distance = 1.7641 Å; standard deviation = 0.1681 Å; number of points = 100046



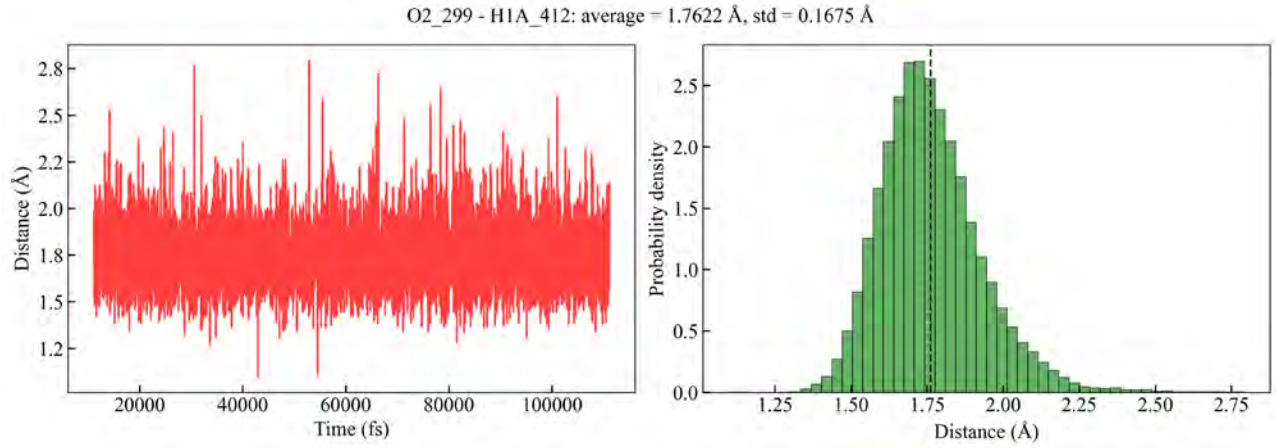
O2_298 - H1A_409

Average distance = 1.7641 Å; standard deviation = 0.1689 Å; number of points = 100046



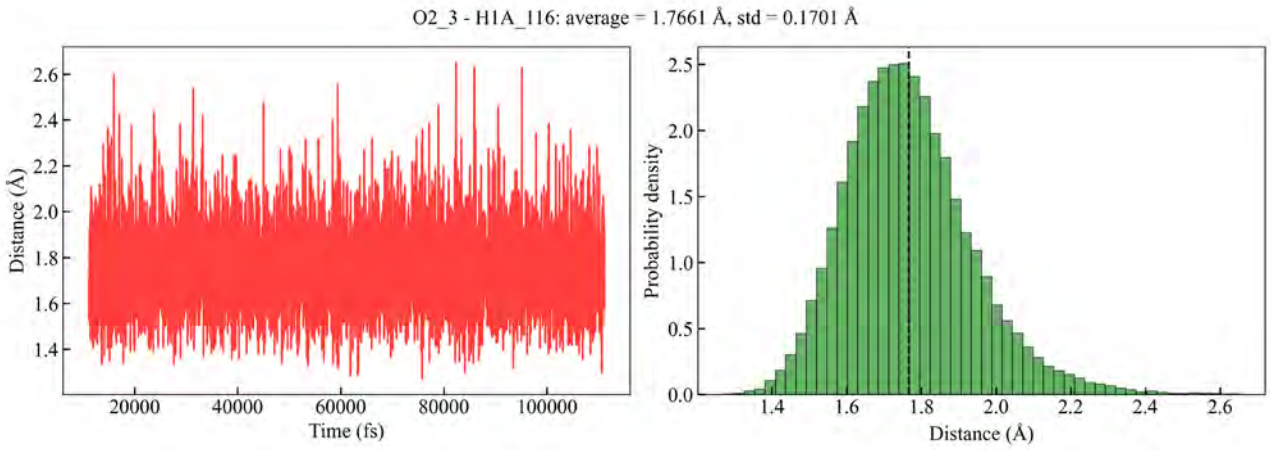
O2_299 - H1A_412

Average distance = 1.7622 Å; standard deviation = 0.1675 Å; number of points = 100046



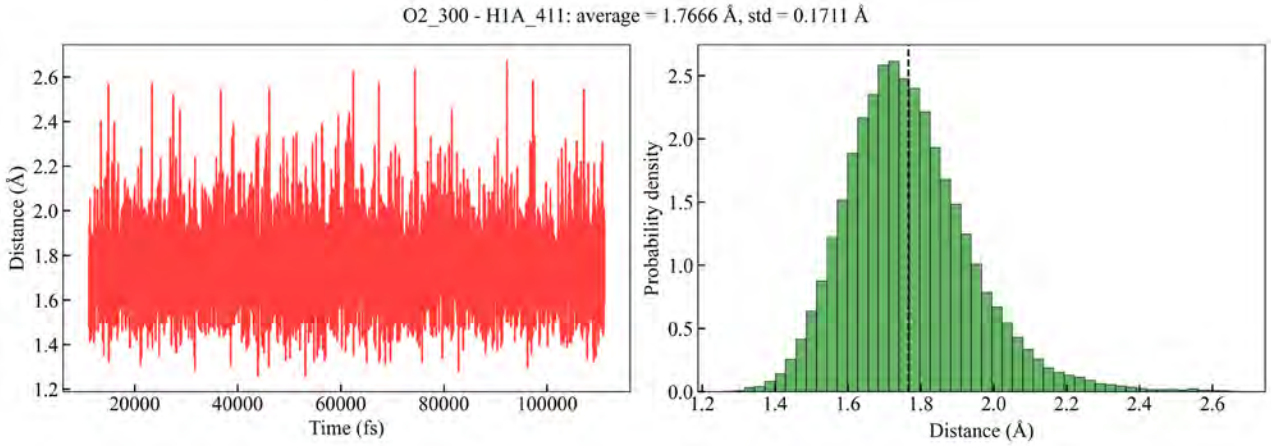
O2_3 - H1A_116

Average distance = 1.7661 Å; standard deviation = 0.1701 Å; number of points = 100046



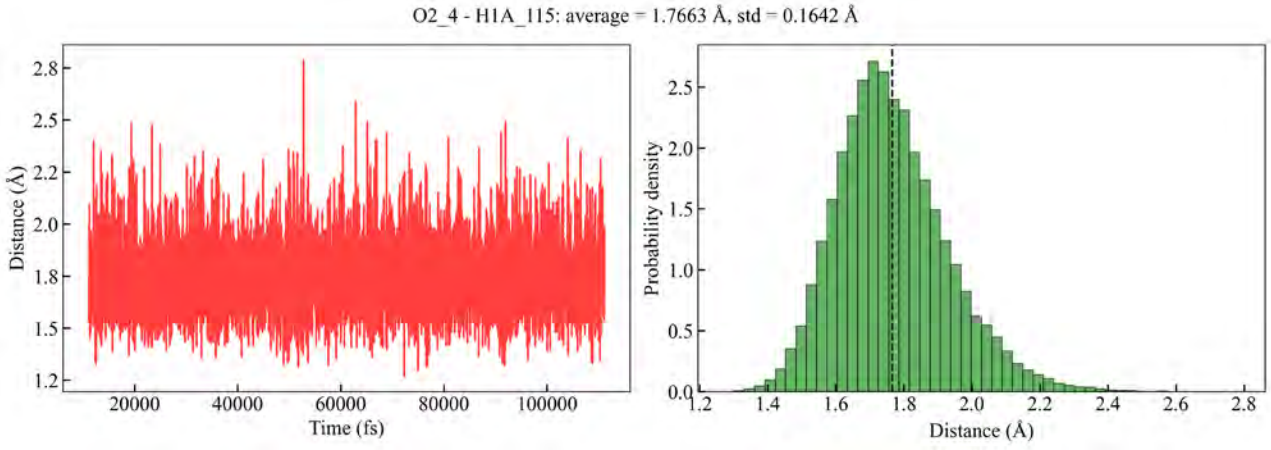
O2_300 - H1A_411

Average distance = 1.7666 Å; standard deviation = 0.1711 Å; number of points = 100046



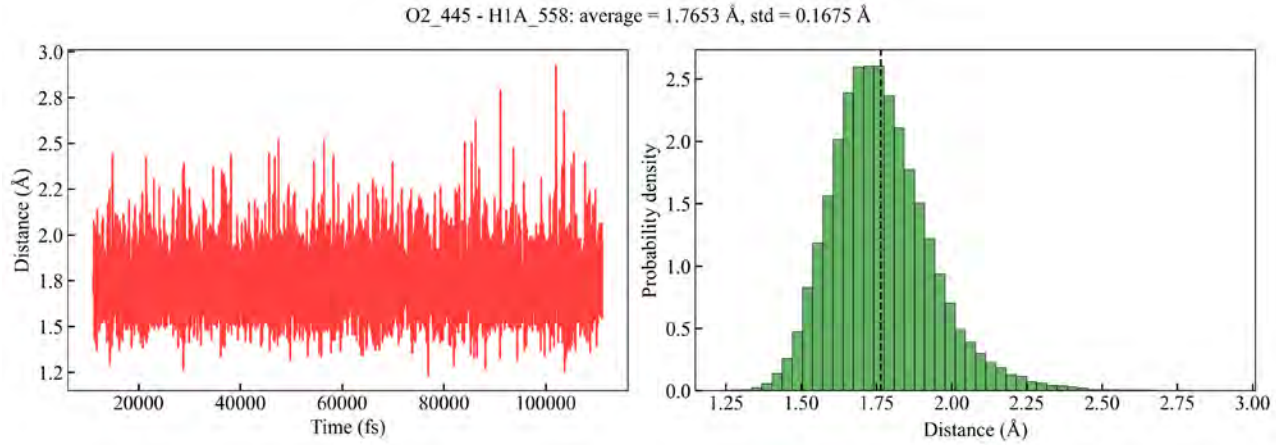
O2_4 - H1A_115

Average distance = 1.7663 Å; standard deviation = 0.1642 Å; number of points = 100046



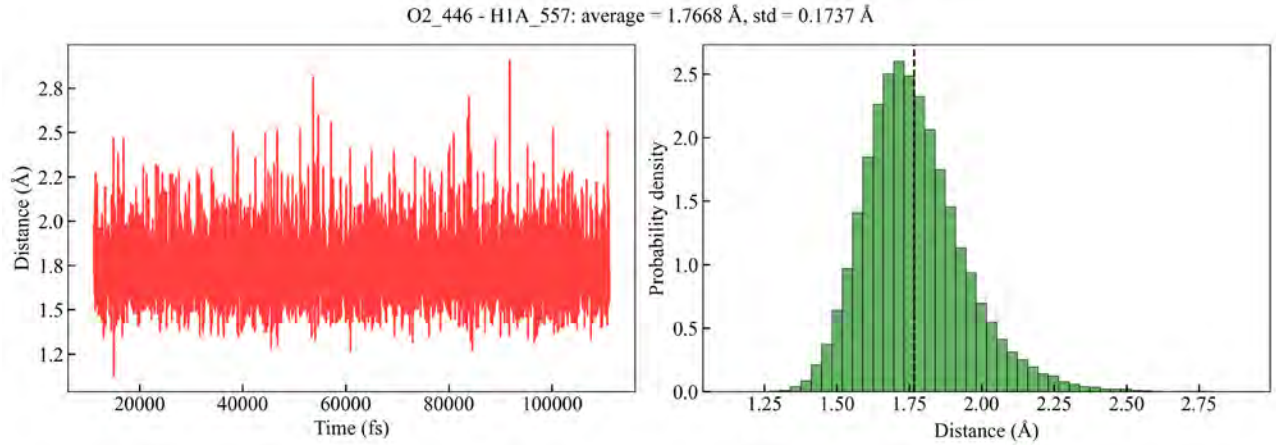
O2_445 - H1A_558

Average distance = 1.7653 Å; standard deviation = 0.1675 Å; number of points = 100046



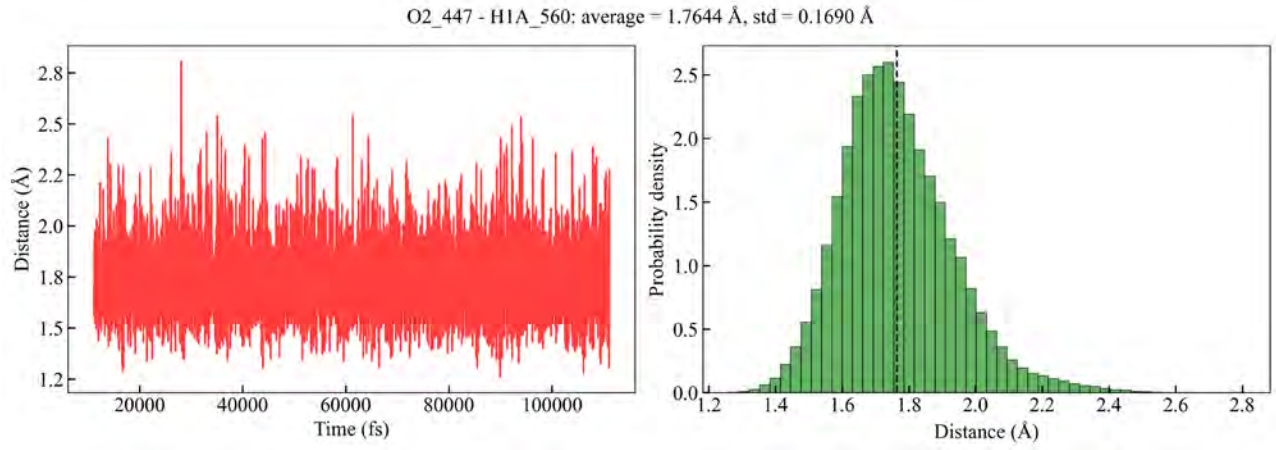
O2_446 - H1A_557

Average distance = 1.7668 Å; standard deviation = 0.1737 Å; number of points = 100046



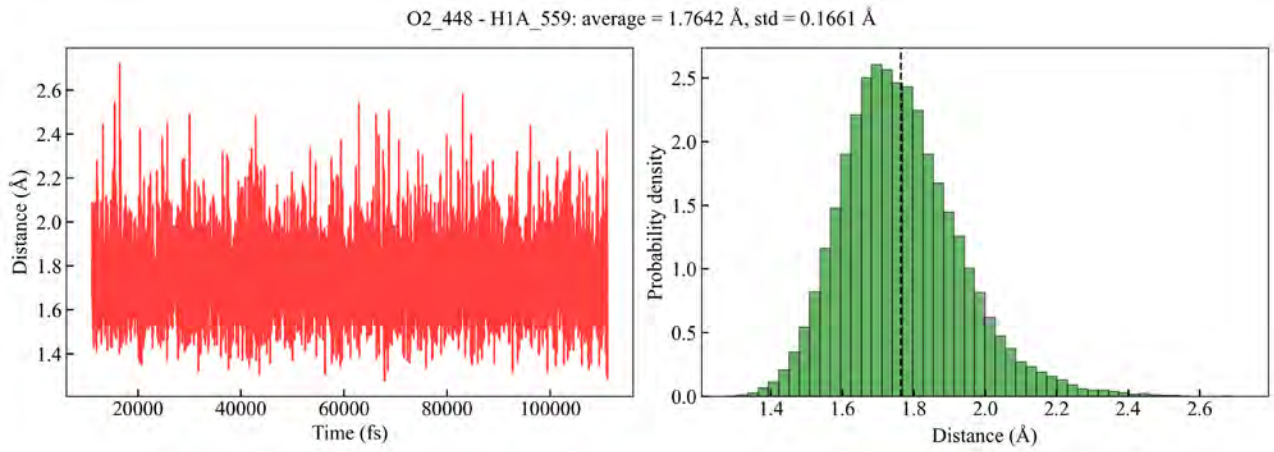
O2_447 - H1A_560

Average distance = 1.7644 Å; standard deviation = 0.1690 Å; number of points = 100046



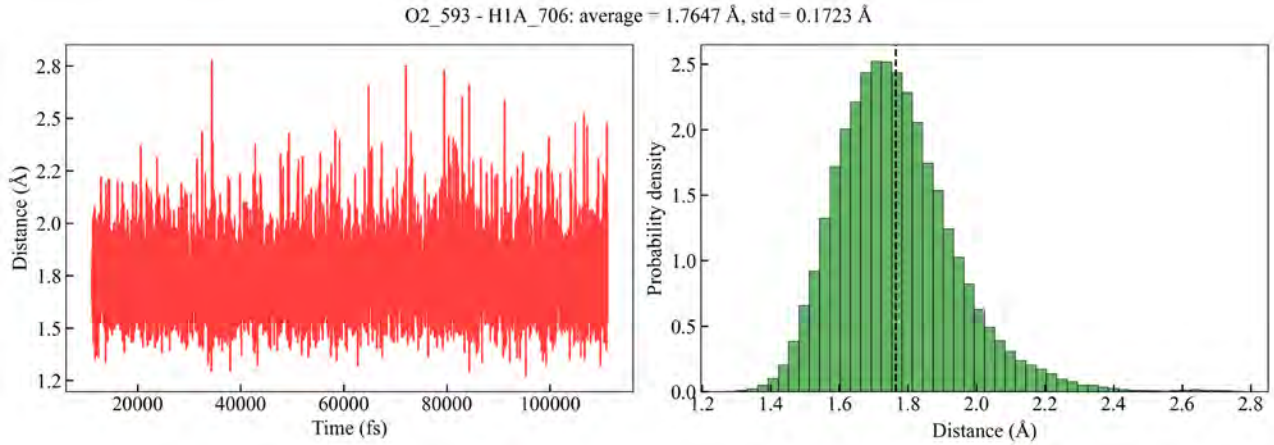
O2_448 - H1A_559

Average distance = 1.7642 Å; standard deviation = 0.1661 Å; number of points = 100046



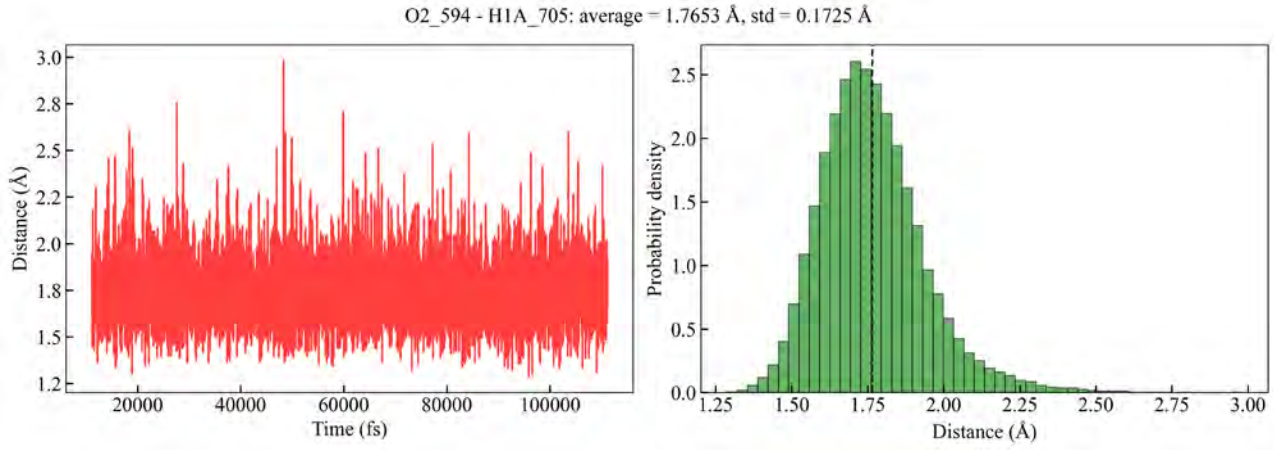
O2_593 - H1A_706

Average distance = 1.7647 Å; standard deviation = 0.1723 Å; number of points = 100046



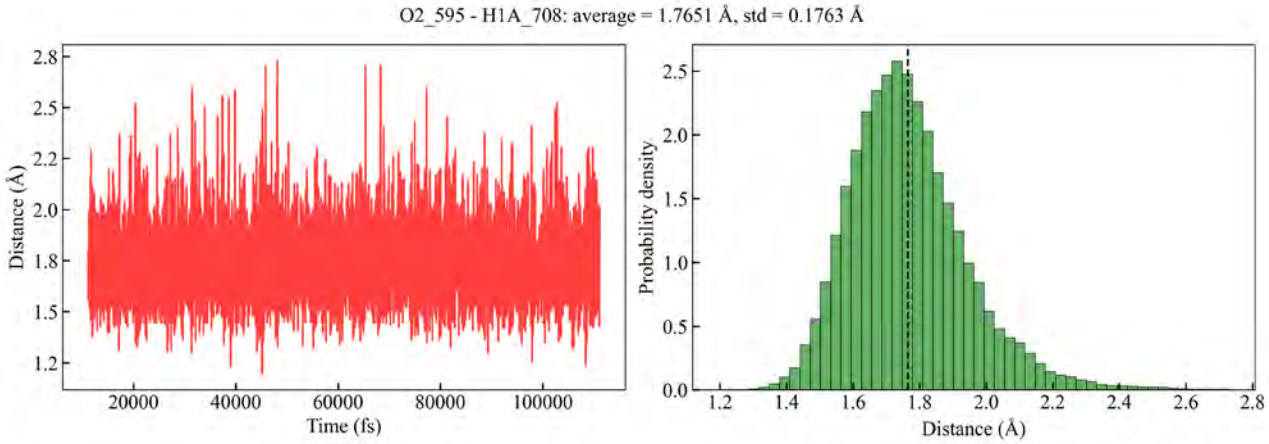
O2_594 - H1A_705

Average distance = 1.7653 Å; standard deviation = 0.1725 Å; number of points = 100046



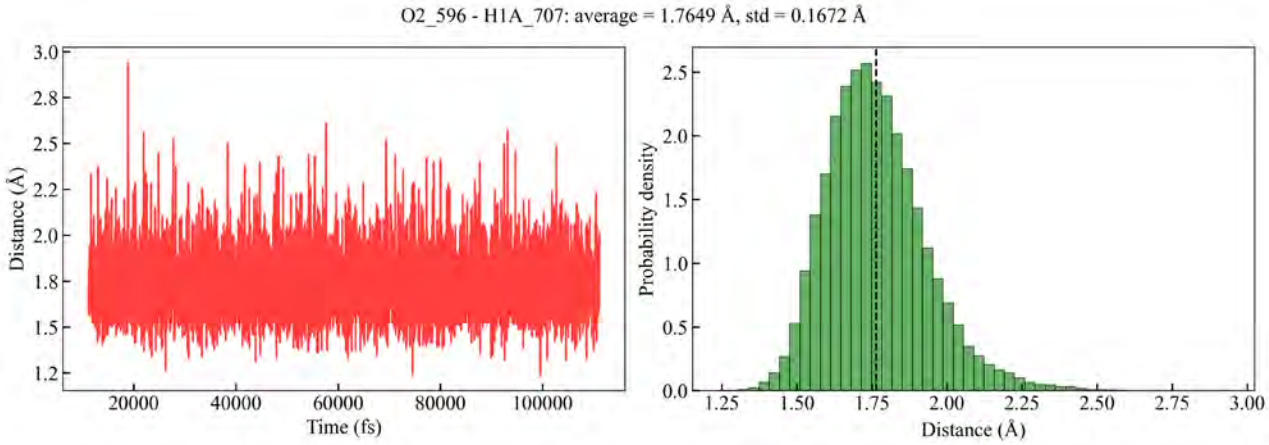
O2_595 - H1A_708

Average distance = 1.7651 Å; standard deviation = 0.1763 Å; number of points = 100046



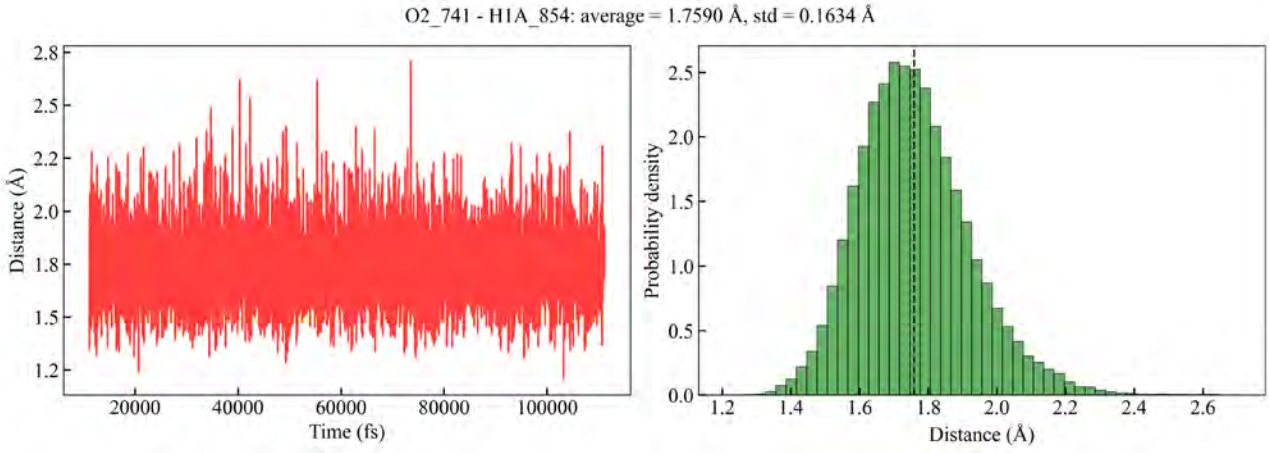
O2_596 - H1A_707

Average distance = 1.7649 Å; standard deviation = 0.1672 Å; number of points = 100046



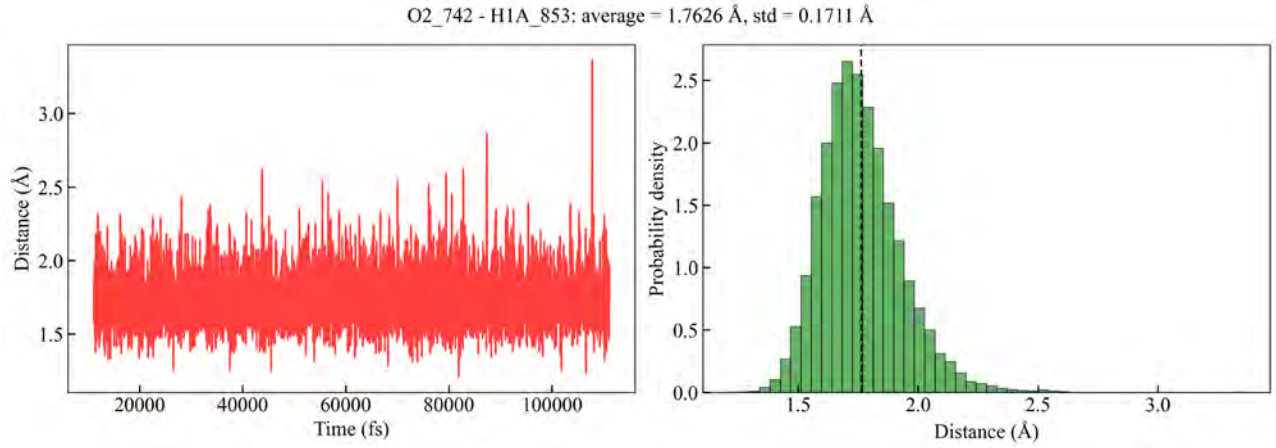
O2_741 - H1A_854

Average distance = 1.7590 Å; standard deviation = 0.1634 Å; number of points = 100046



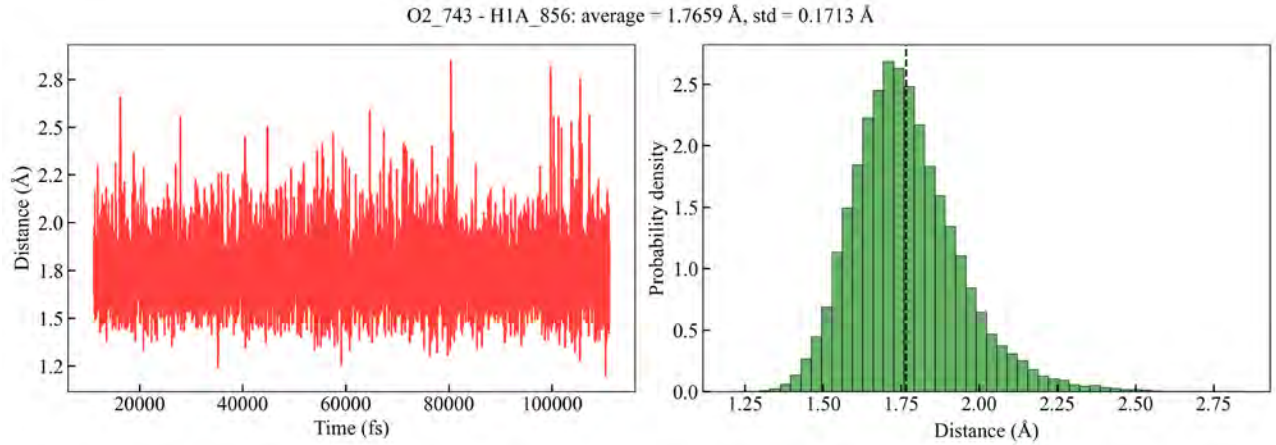
O2_742 - H1A_853

Average distance = 1.7626 Å; standard deviation = 0.1711 Å; number of points = 100046



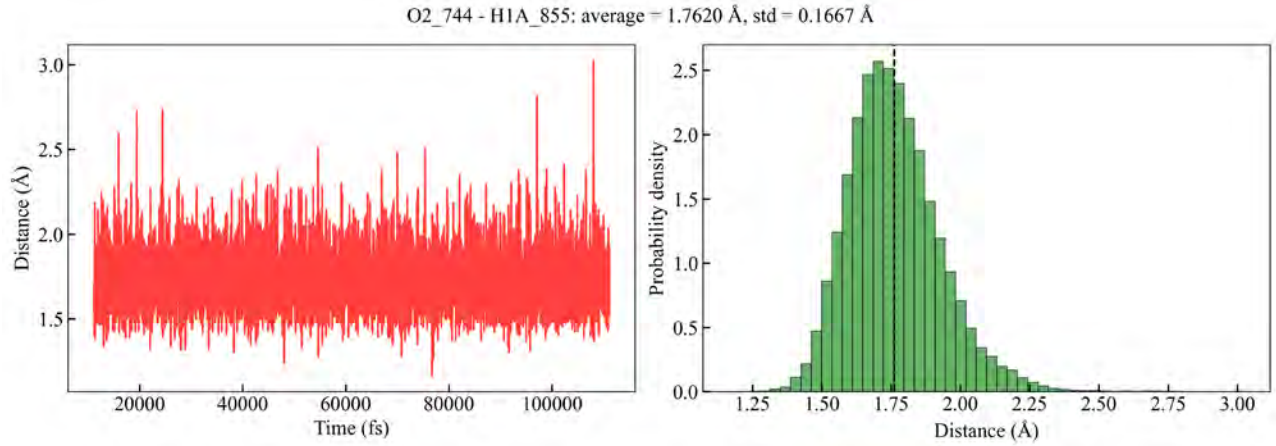
O2_743 - H1A_856

Average distance = 1.7659 Å; standard deviation = 0.1713 Å; number of points = 100046



O2_744 - H1A_855

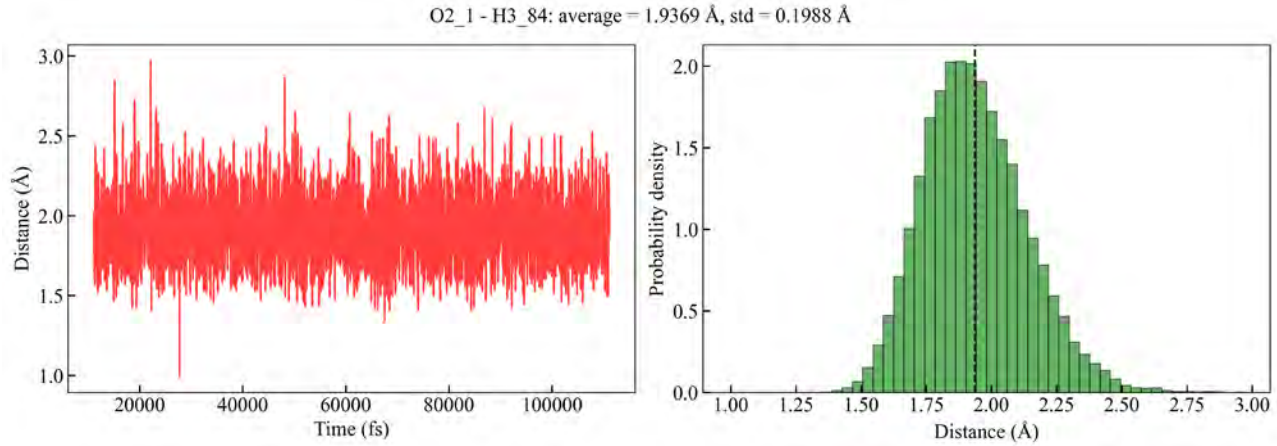
Average distance = 1.7620 Å; standard deviation = 0.1667 Å; number of points = 100046



O2 - H3

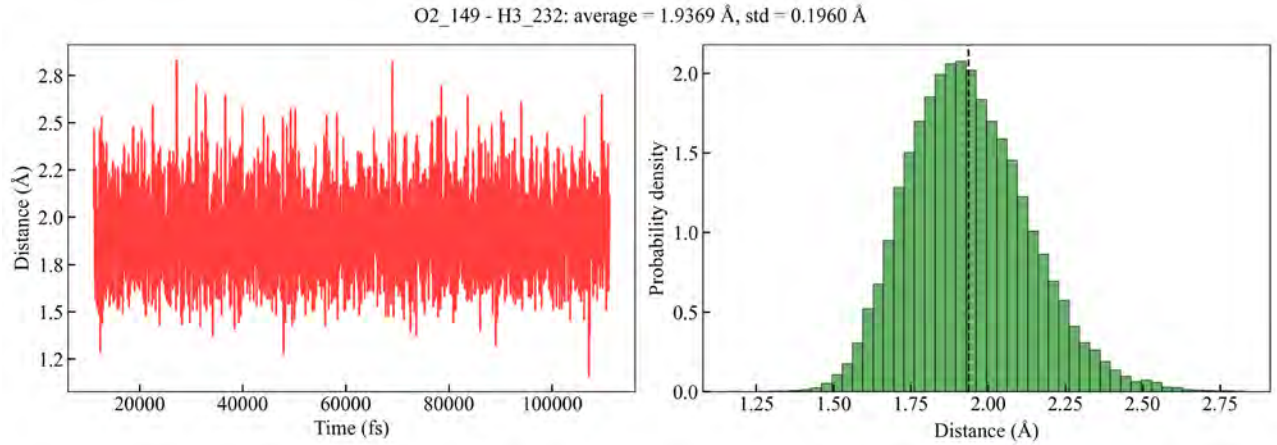
O2_1 - H3_84

Average distance = 1.9369 Å; standard deviation = 0.1988 Å; number of points = 100046



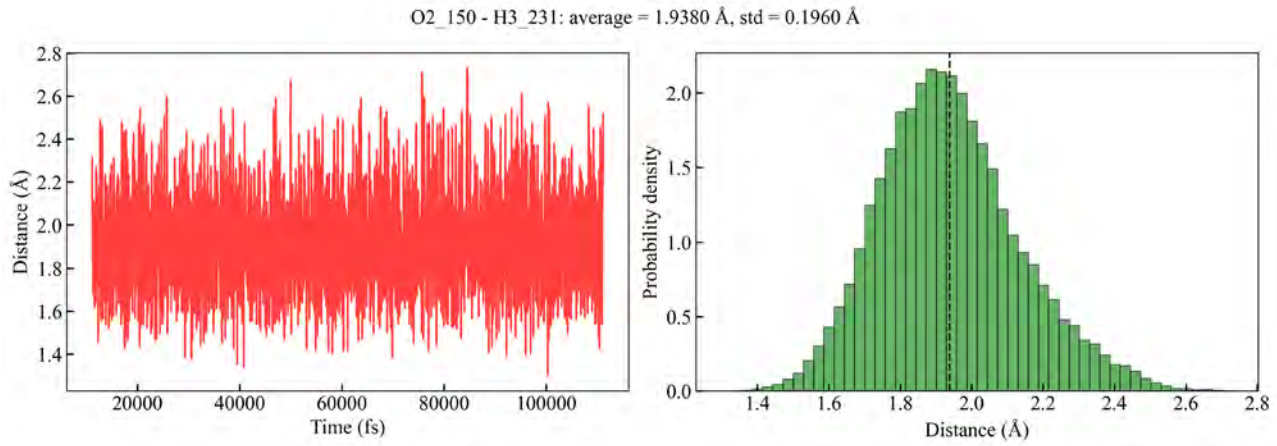
O2_149 - H3_232

Average distance = 1.9369 Å; standard deviation = 0.1960 Å; number of points = 100046



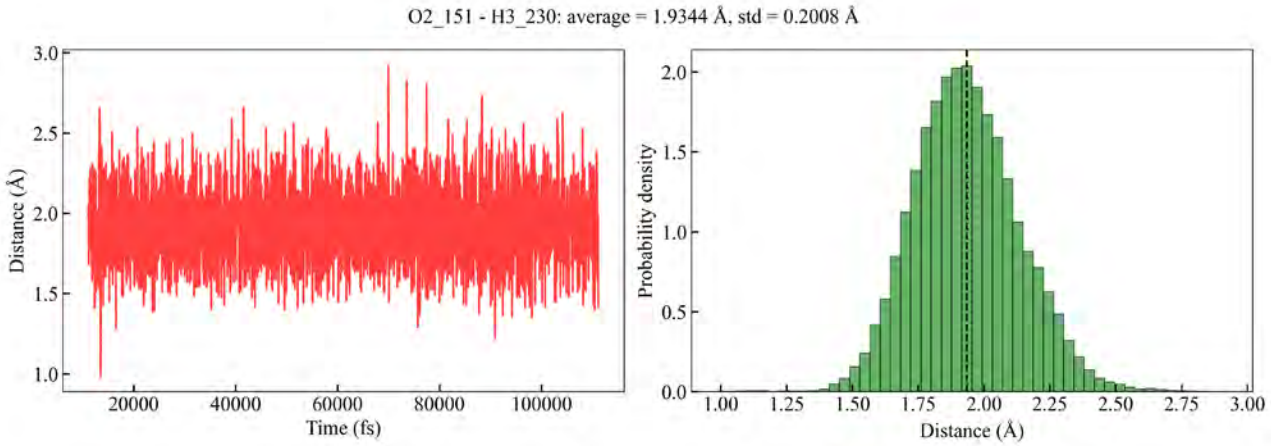
O2_150 - H3_231

Average distance = 1.9380 Å; standard deviation = 0.1960 Å; number of points = 100046



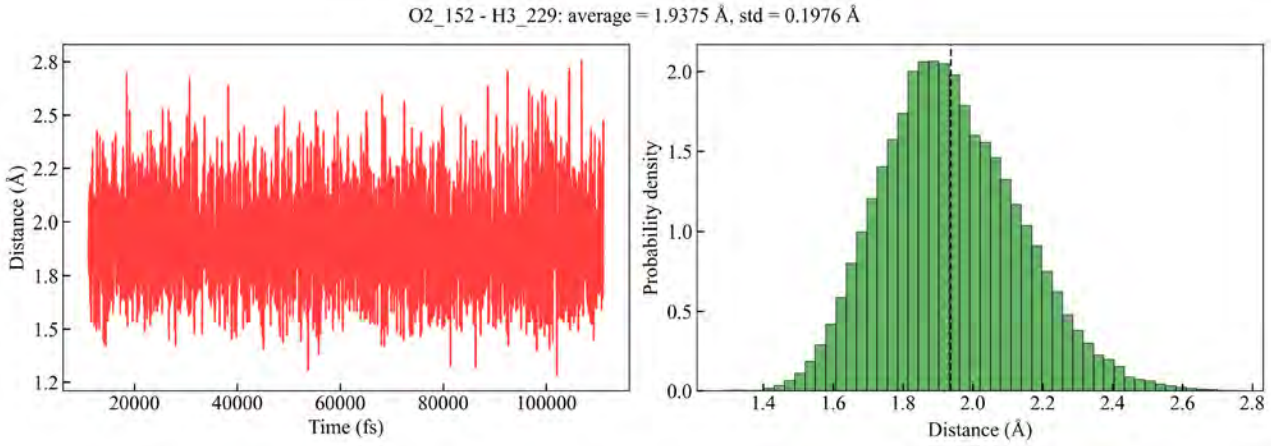
O2_151 - H3_230

Average distance = 1.9344 Å; standard deviation = 0.2008 Å; number of points = 100046



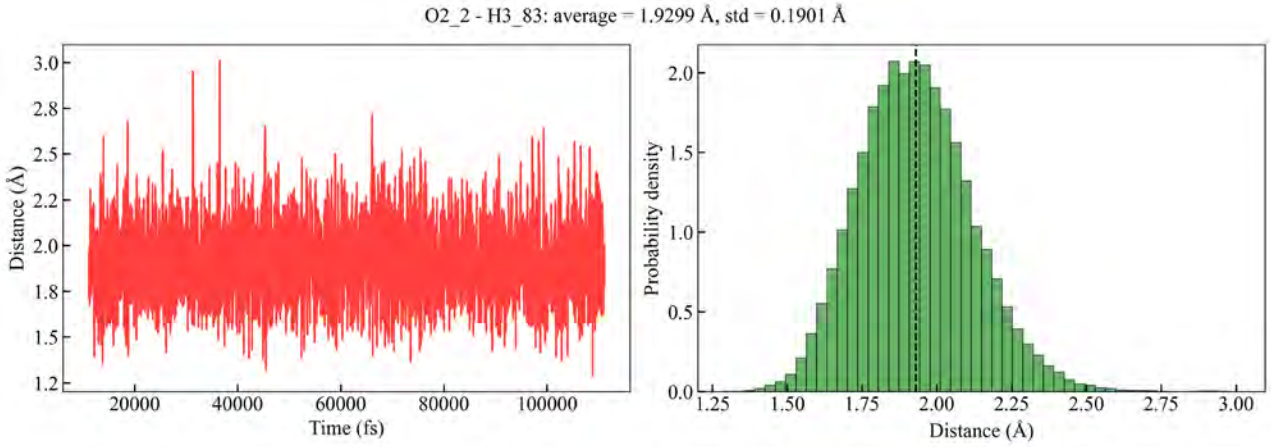
O2_152 - H3_229

Average distance = 1.9375 Å; standard deviation = 0.1976 Å; number of points = 100046



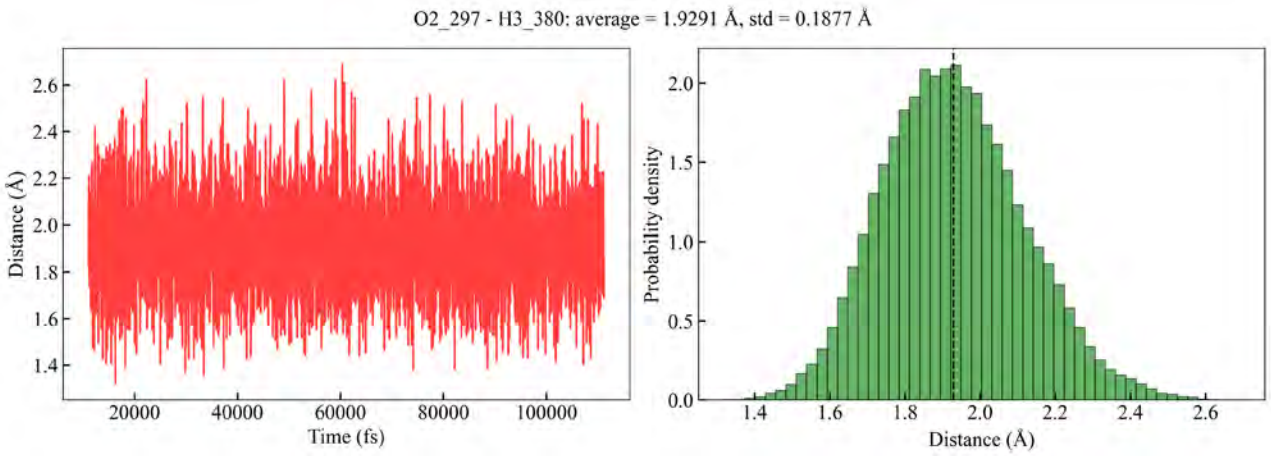
O2_2 - H3_83

Average distance = 1.9299 Å; standard deviation = 0.1901 Å; number of points = 100046



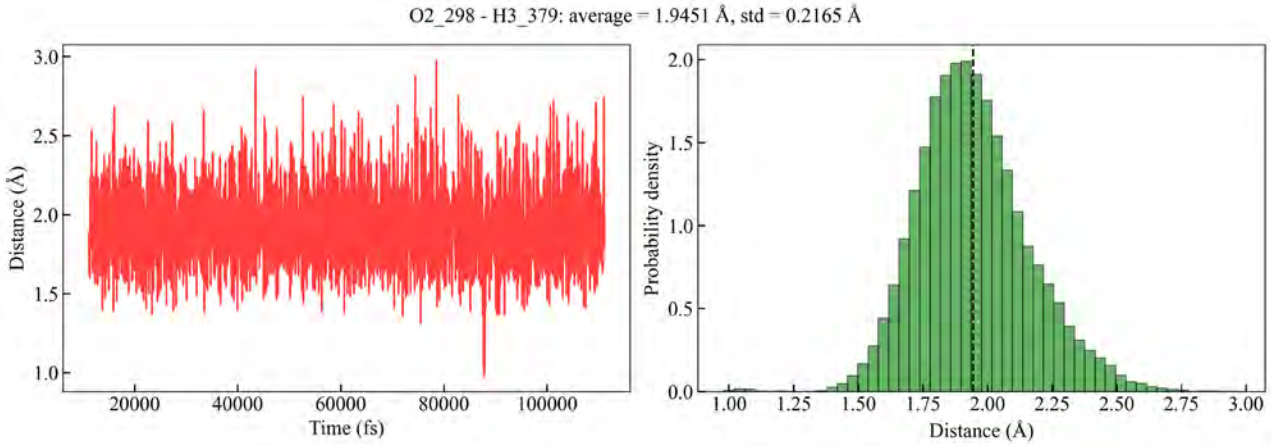
O2_297 - H3_380

Average distance = 1.9291 Å; standard deviation = 0.1877 Å; number of points = 100046



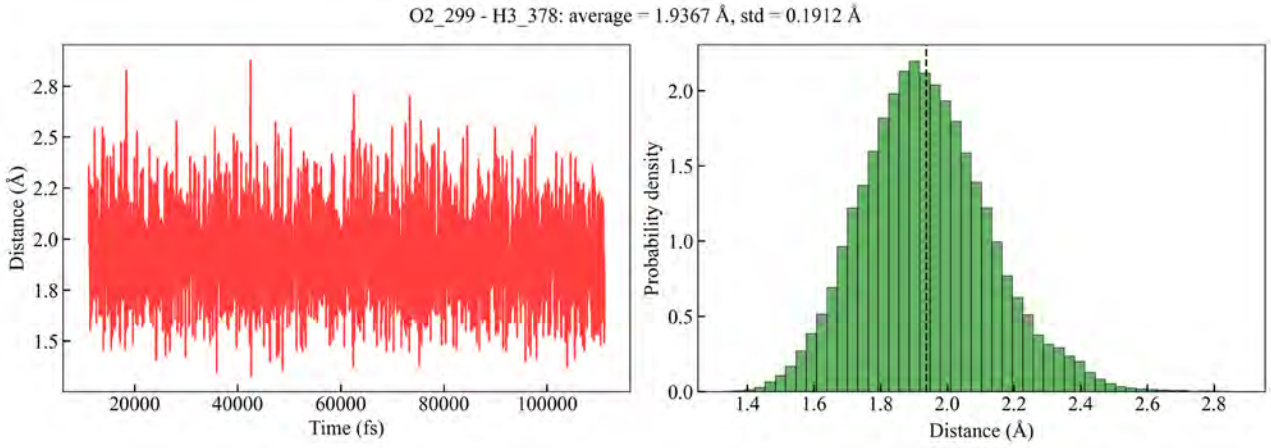
O2_298 - H3_379

Average distance = 1.9451 Å; standard deviation = 0.2165 Å; number of points = 100046



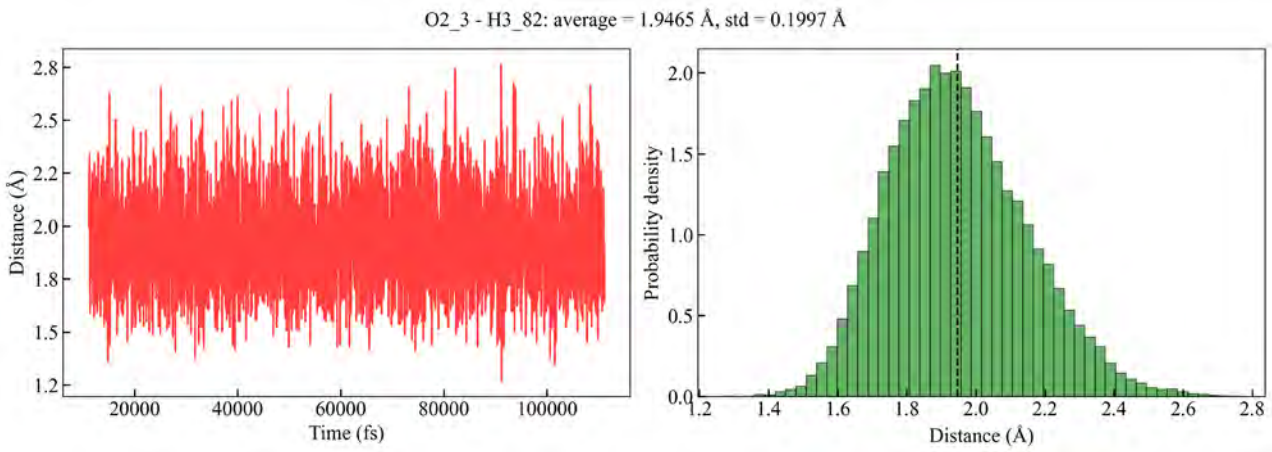
O2_299 - H3_378

Average distance = 1.9367 Å; standard deviation = 0.1912 Å; number of points = 100046



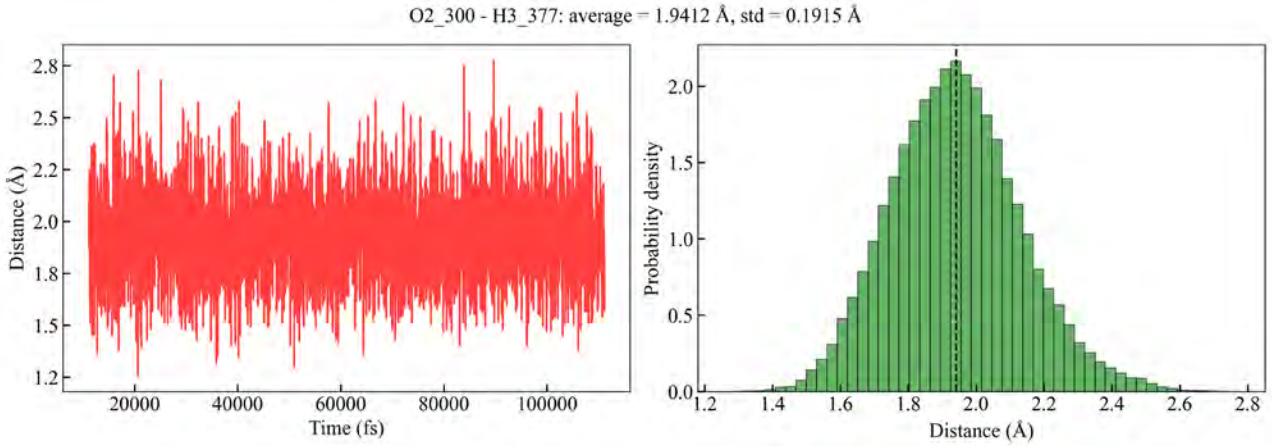
O2_3 - H3_82

Average distance = 1.9465 Å; standard deviation = 0.1997 Å; number of points = 100046



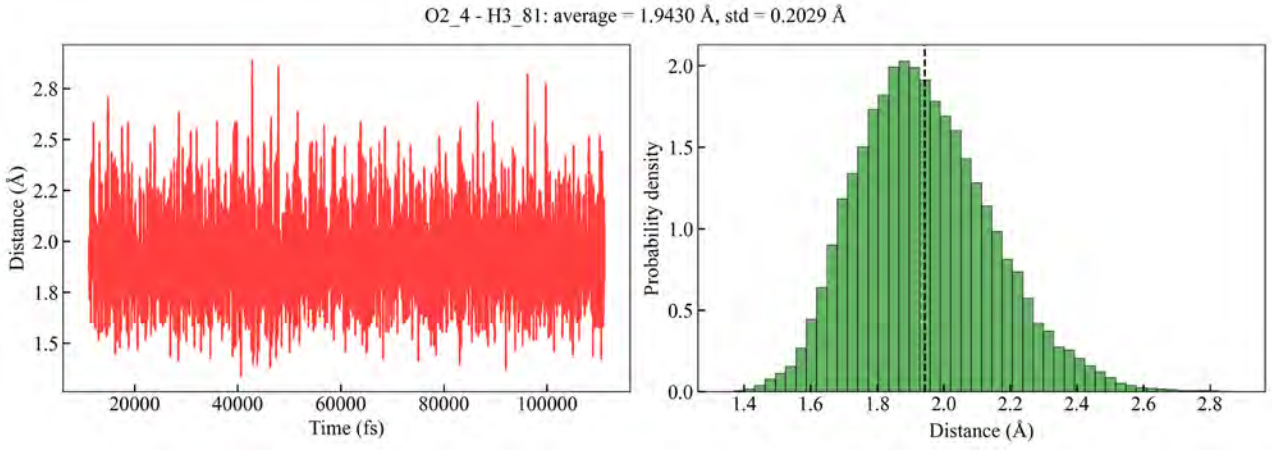
O2_300 - H3_377

Average distance = 1.9412 Å; standard deviation = 0.1915 Å; number of points = 100046



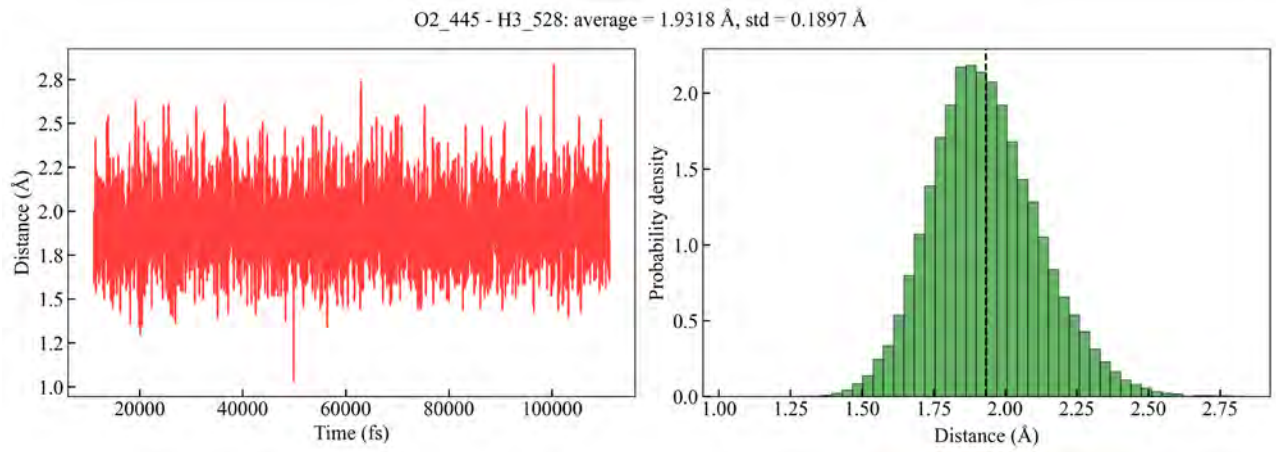
O2_4 - H3_81

Average distance = 1.9430 Å; standard deviation = 0.2029 Å; number of points = 100046



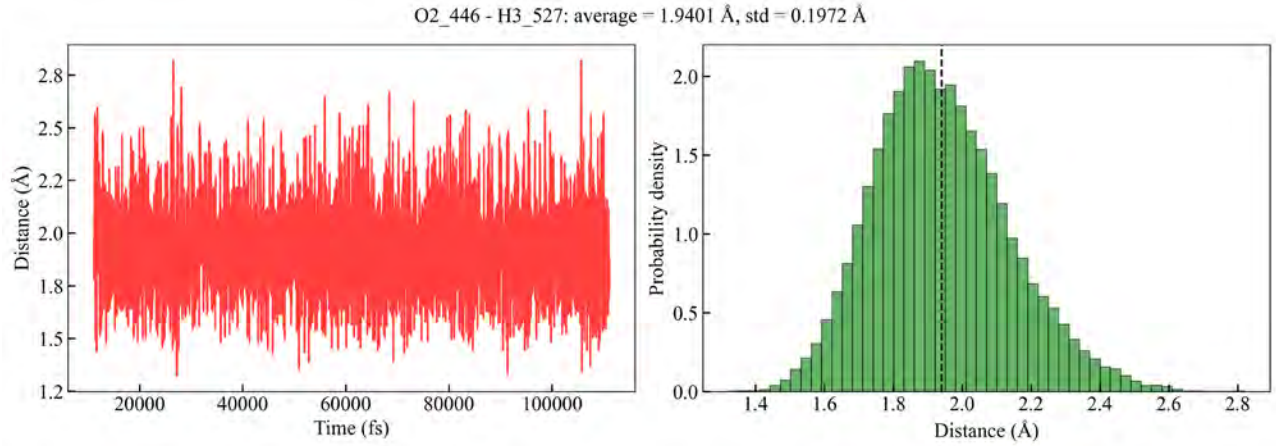
O2_445 - H3_528

Average distance = 1.9318 Å; standard deviation = 0.1897 Å; number of points = 100046



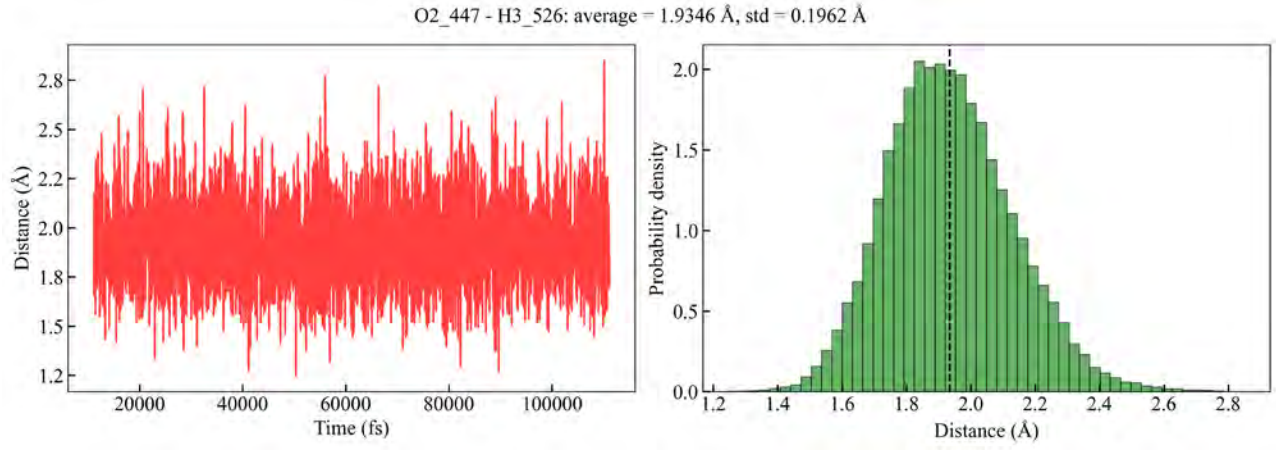
O2_446 - H3_527

Average distance = 1.9401 Å; standard deviation = 0.1972 Å; number of points = 100046



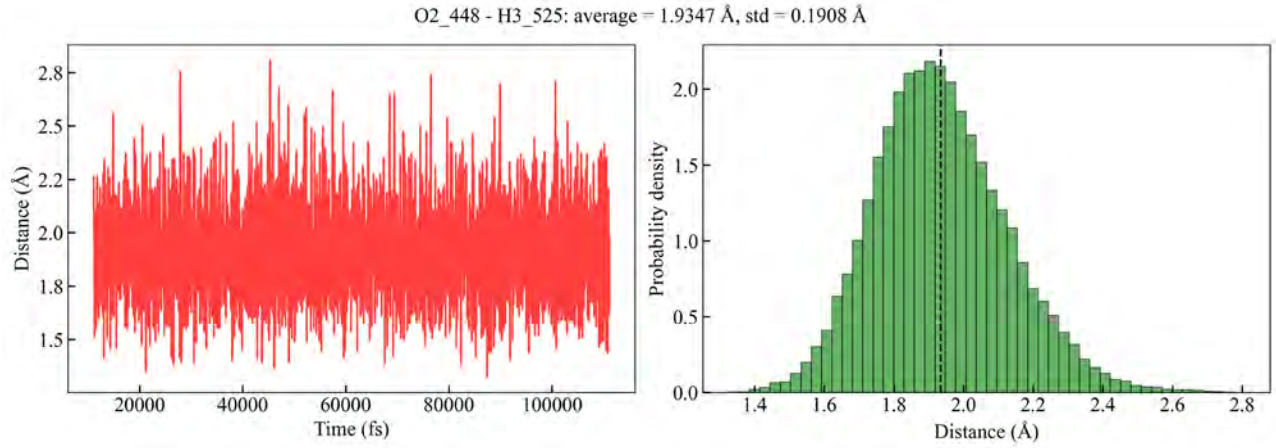
O2_447 - H3_526

Average distance = 1.9346 Å; standard deviation = 0.1962 Å; number of points = 100046



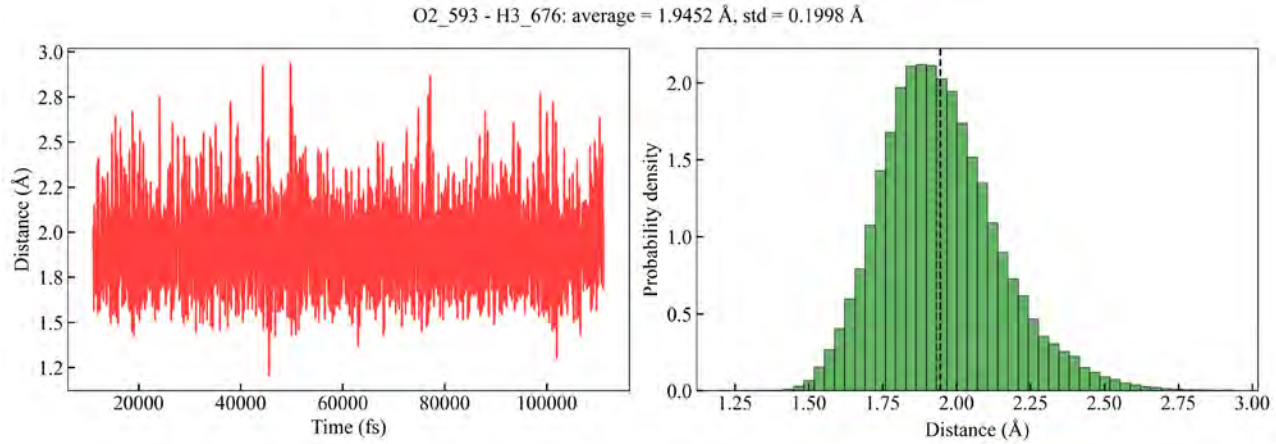
O2_448 - H3_525

Average distance = 1.9347 Å; standard deviation = 0.1908 Å; number of points = 100046



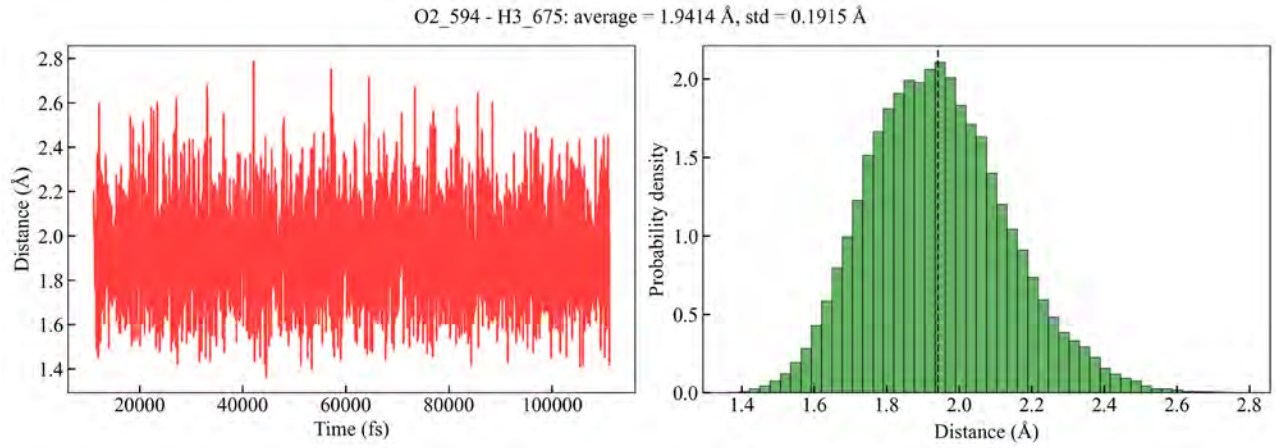
O2_593 - H3_676

Average distance = 1.9452 Å; standard deviation = 0.1998 Å; number of points = 100046



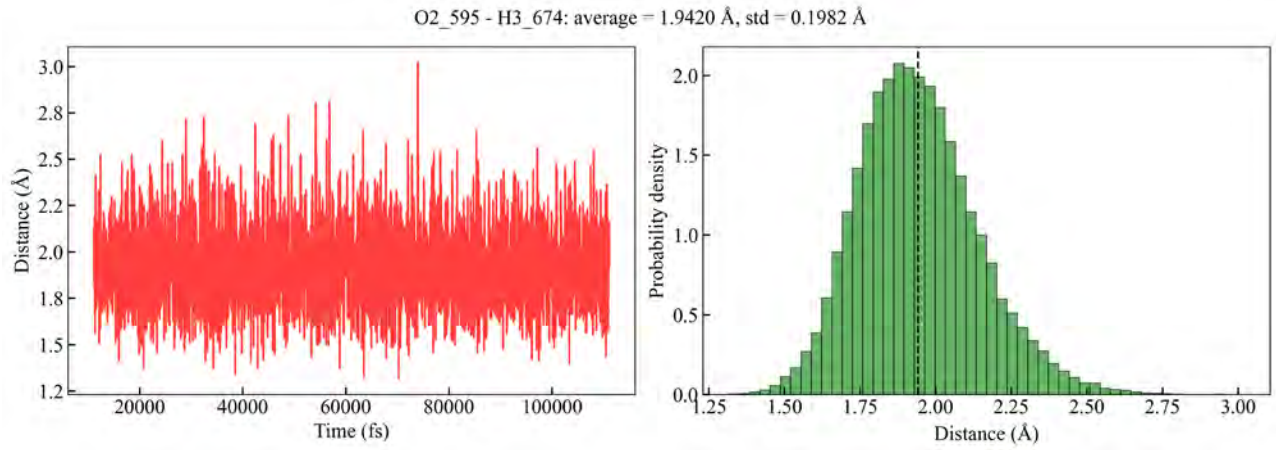
O2_594 - H3_675

Average distance = 1.9414 Å; standard deviation = 0.1915 Å; number of points = 100046



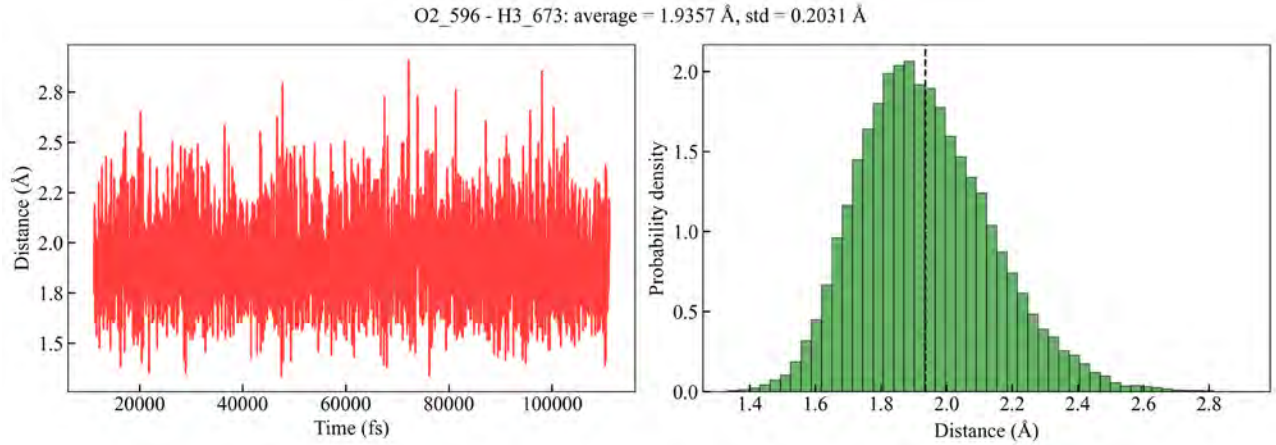
O2_595 - H3_674

Average distance = 1.9420 Å; standard deviation = 0.1982 Å; number of points = 100046



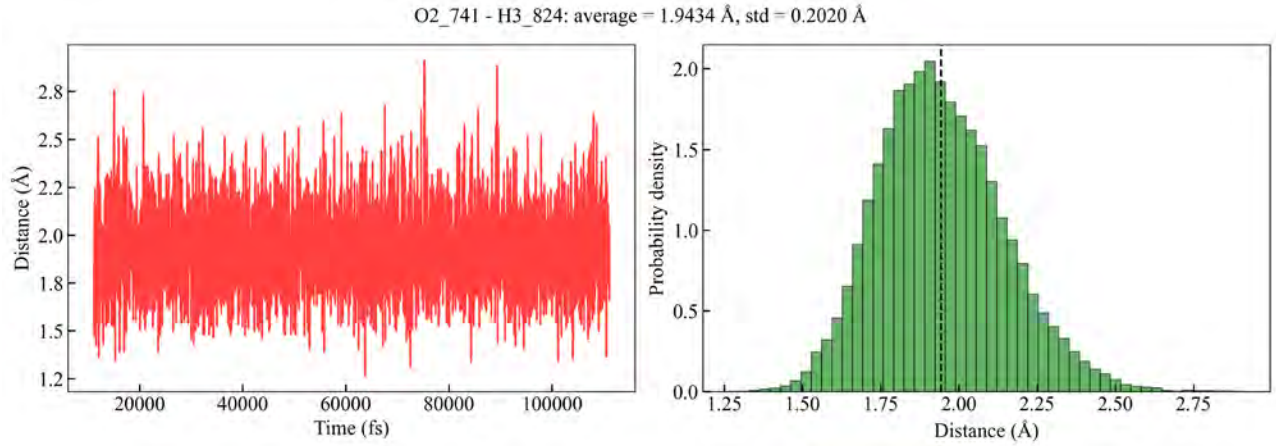
O2_596 - H3_673

Average distance = 1.9357 Å; standard deviation = 0.2031 Å; number of points = 100046



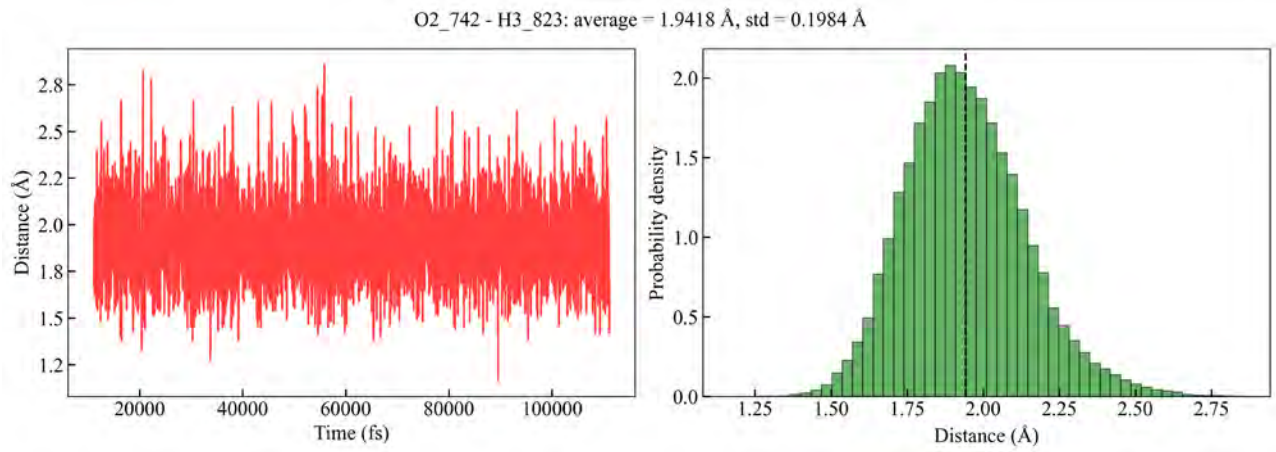
O2_741 - H3_824

Average distance = 1.9434 Å; standard deviation = 0.2020 Å; number of points = 100046



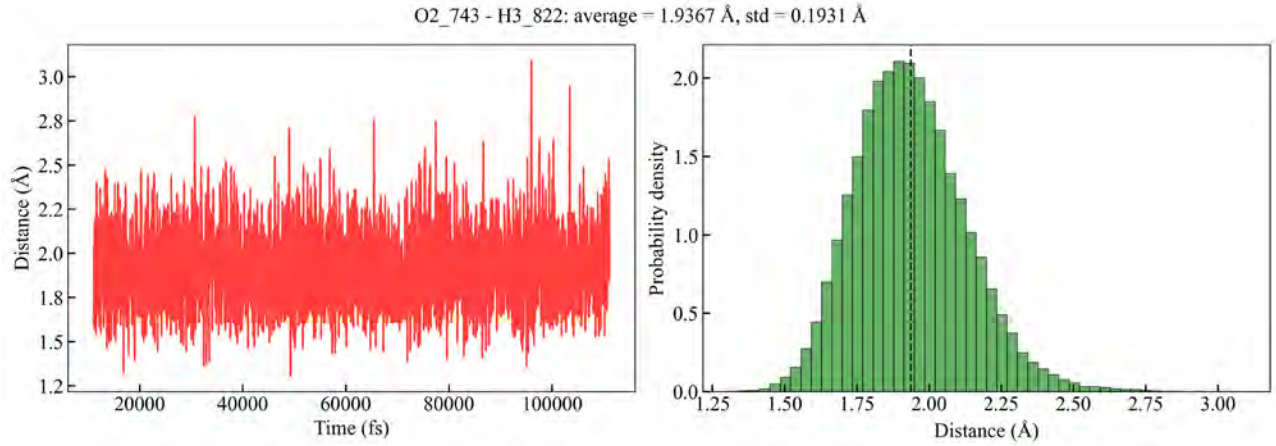
O2_742 - H3_823

Average distance = 1.9418 Å; standard deviation = 0.1984 Å; number of points = 100046



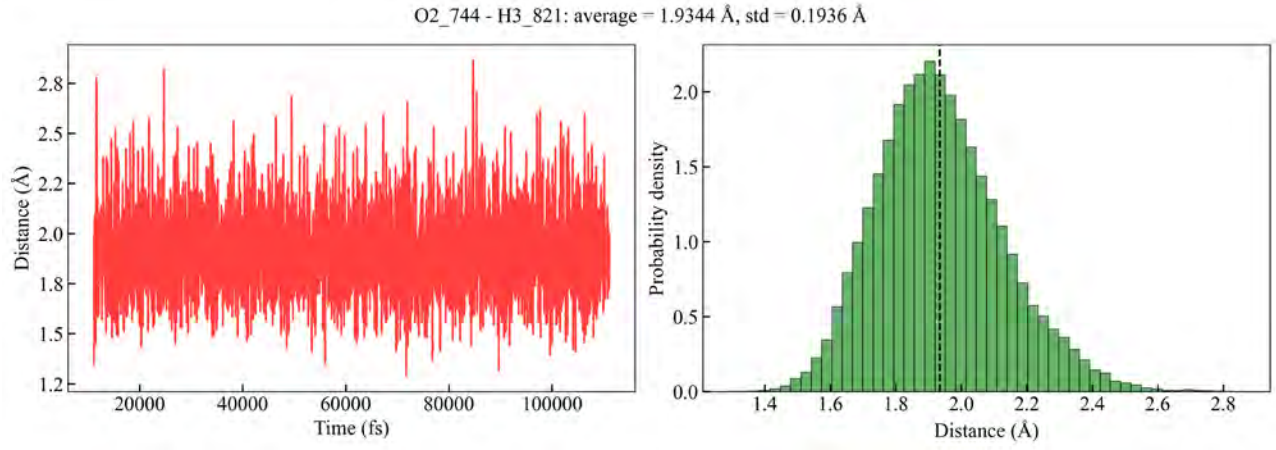
O2_743 - H3_822

Average distance = 1.9367 Å; standard deviation = 0.1931 Å; number of points = 100046



O2_744 - H3_821

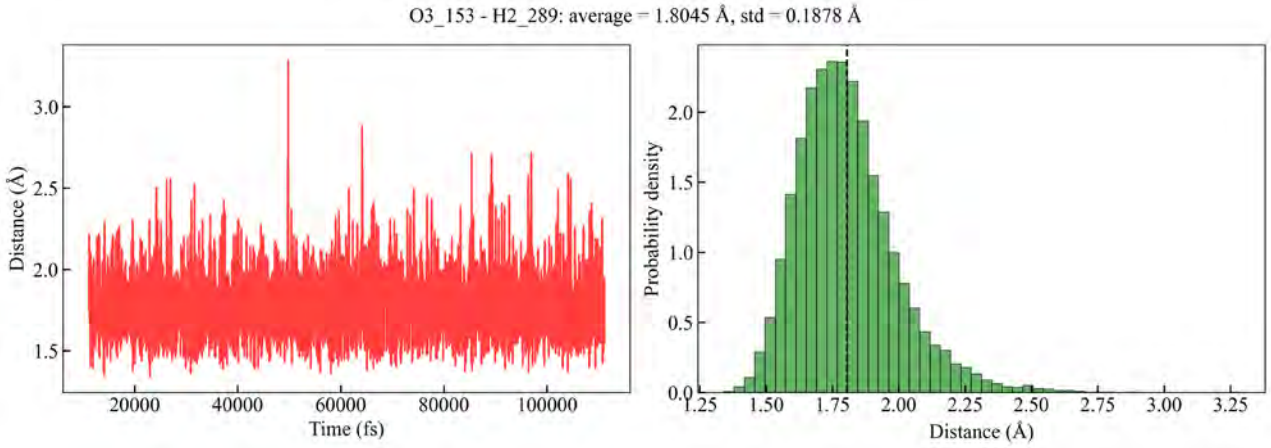
Average distance = 1.9344 Å; standard deviation = 0.1936 Å; number of points = 100046



O3 - H2

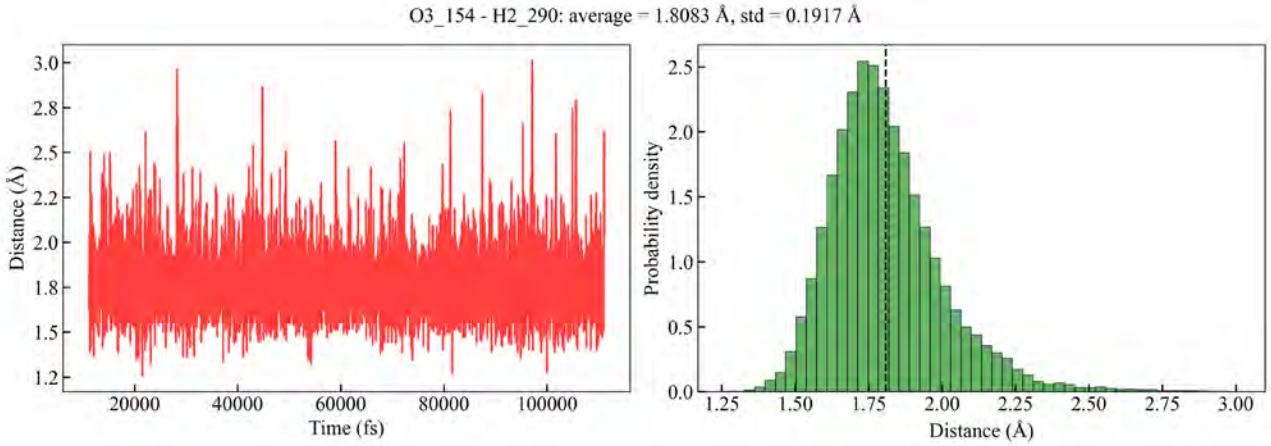
O3_153 - H2_289

Average distance = 1.8045 Å; standard deviation = 0.1878 Å; number of points = 100046



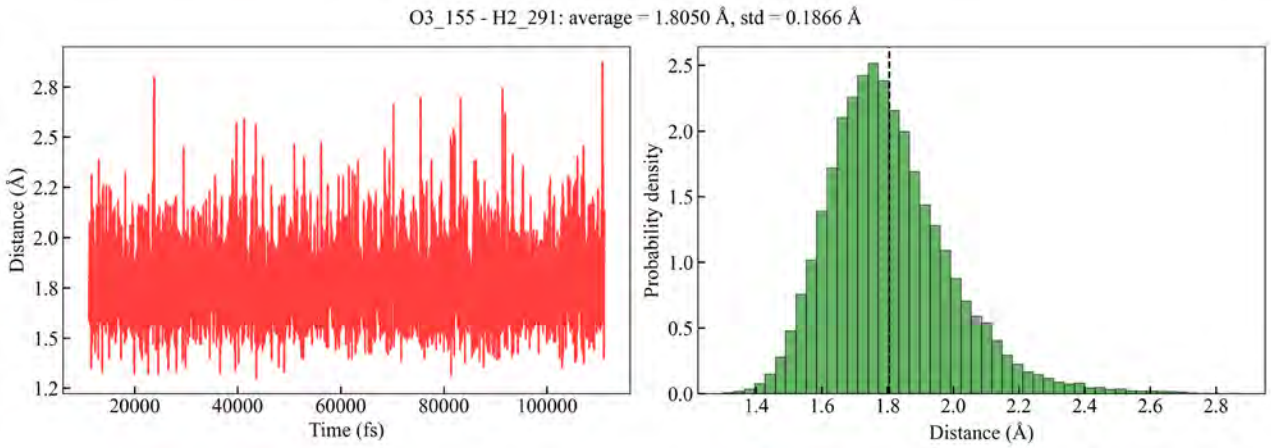
O3_154 - H2_290

Average distance = 1.8083 Å; standard deviation = 0.1917 Å; number of points = 100046



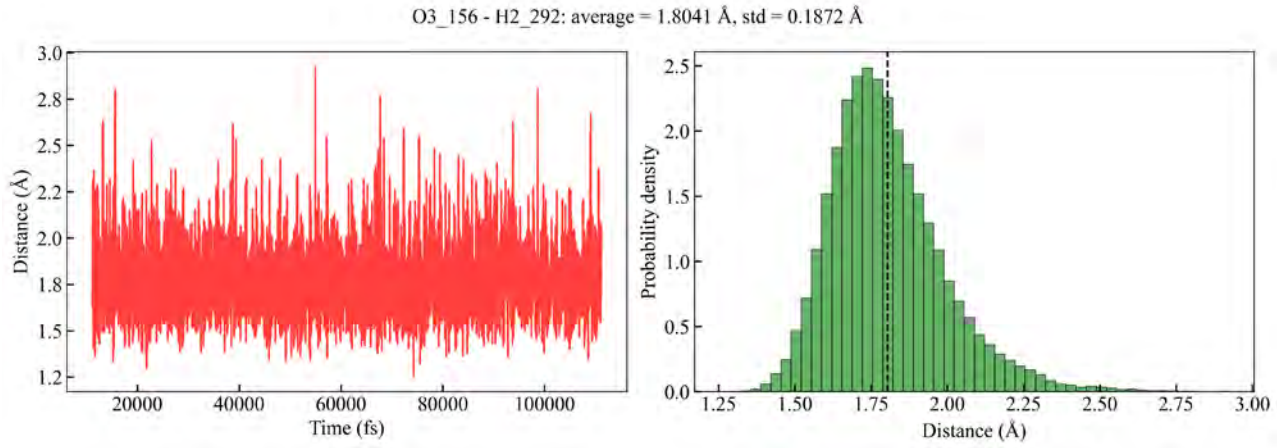
O3_155 - H2_291

Average distance = 1.8050 Å; standard deviation = 0.1866 Å; number of points = 100046



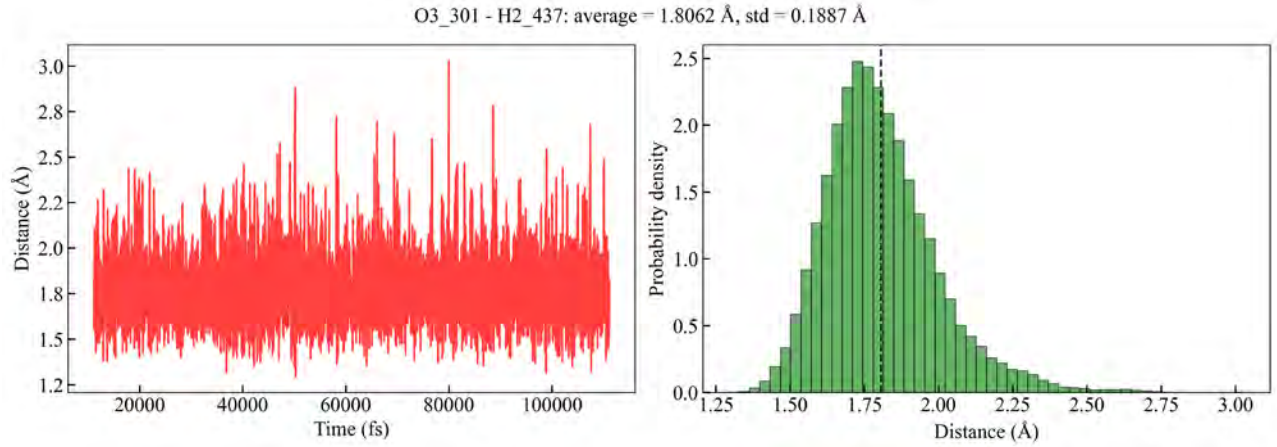
O3_156 - H2_292

Average distance = 1.8041 Å; standard deviation = 0.1872 Å; number of points = 100046



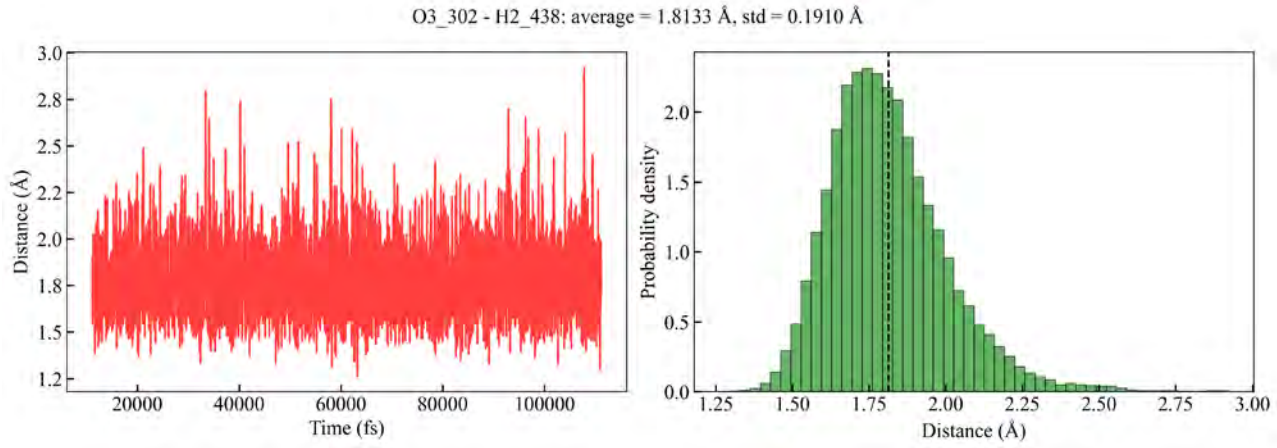
O3_301 - H2_437

Average distance = 1.8062 Å; standard deviation = 0.1887 Å; number of points = 100046



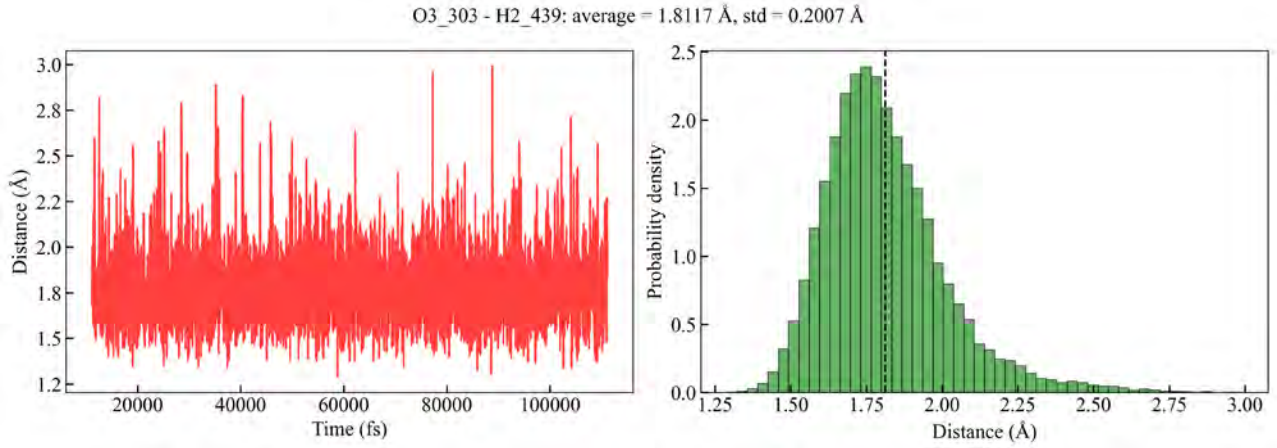
O3_302 - H2_438

Average distance = 1.8133 Å; standard deviation = 0.1910 Å; number of points = 100046



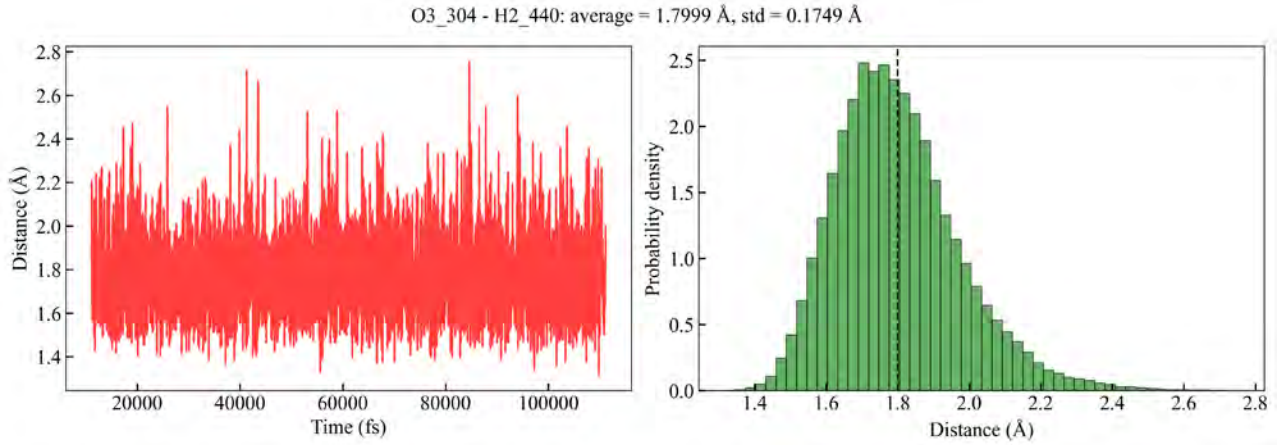
O3_303 - H2_439

Average distance = 1.8117 Å; standard deviation = 0.2007 Å; number of points = 100046



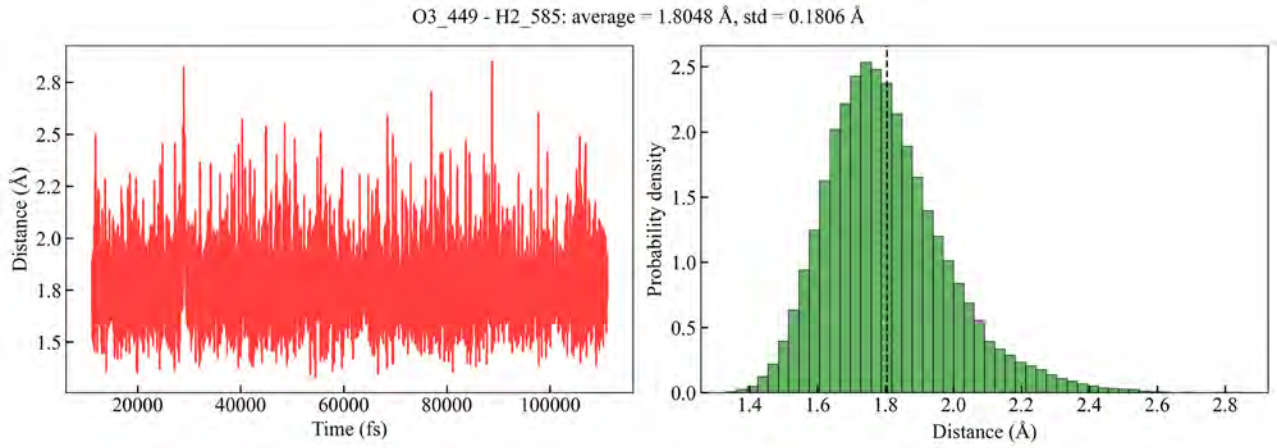
O3_304 - H2_440

Average distance = 1.7999 Å; standard deviation = 0.1749 Å; number of points = 100046



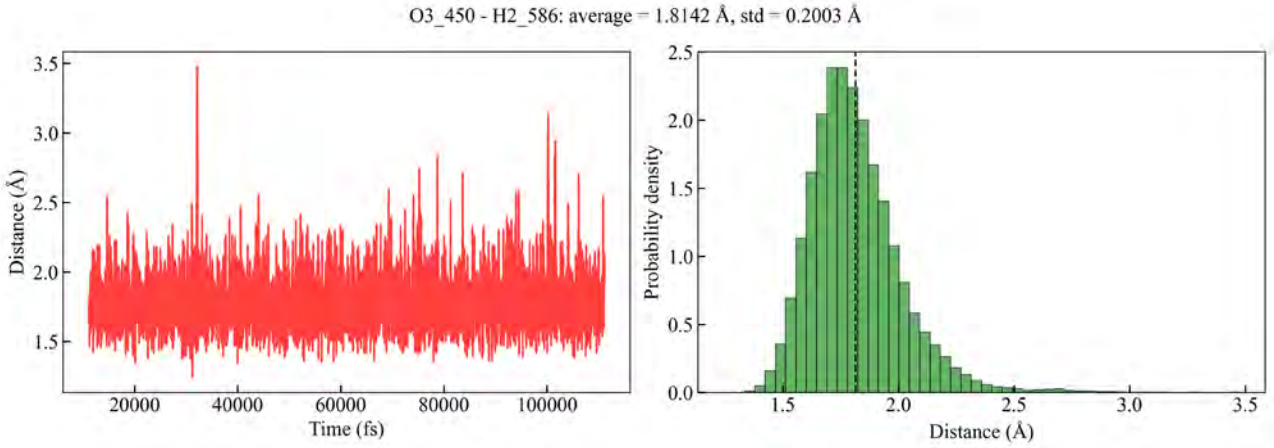
O3_449 - H2_585

Average distance = 1.8048 Å; standard deviation = 0.1806 Å; number of points = 100046



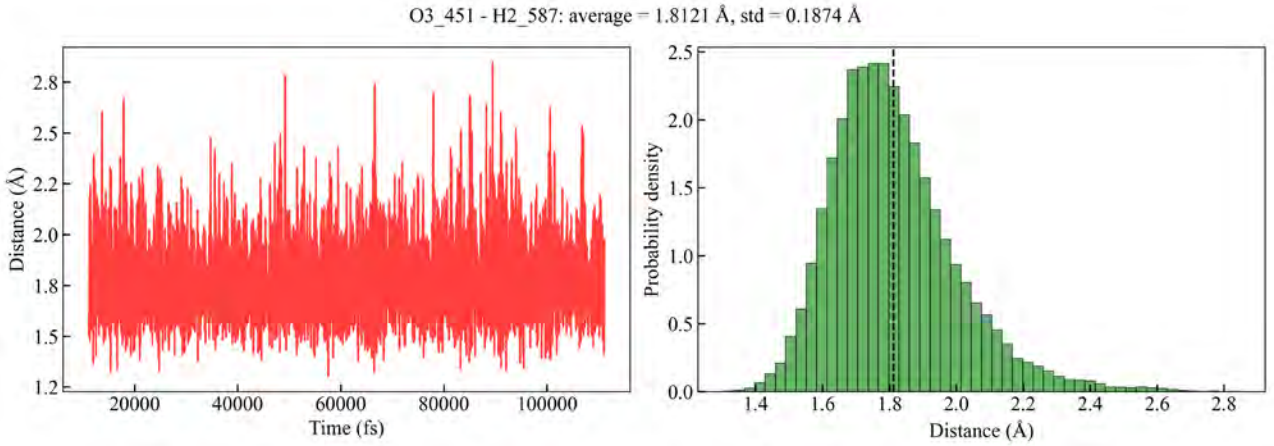
O3_450 - H2_586

Average distance = 1.8142 Å; standard deviation = 0.2003 Å; number of points = 100046



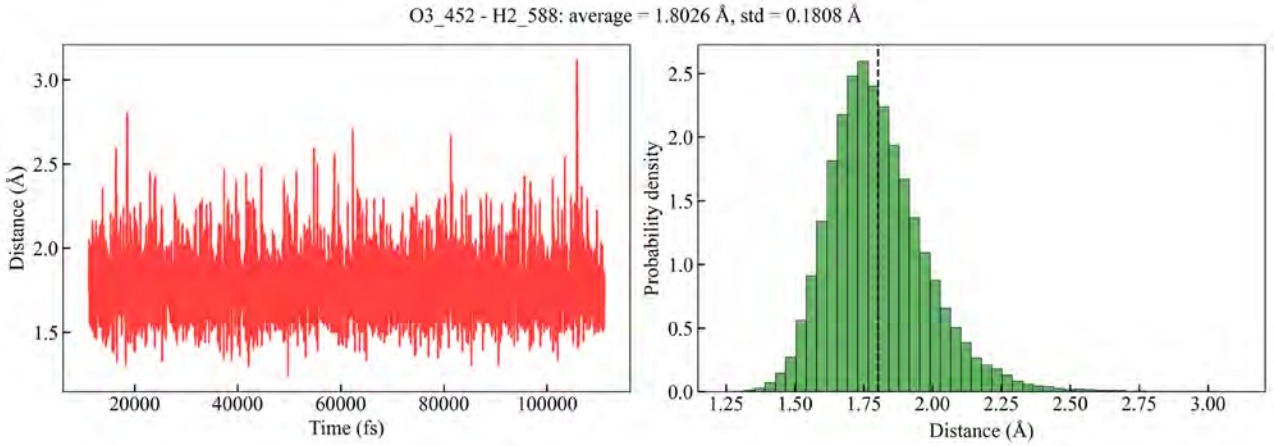
O3_451 - H2_587

Average distance = 1.8121 Å; standard deviation = 0.1874 Å; number of points = 100046



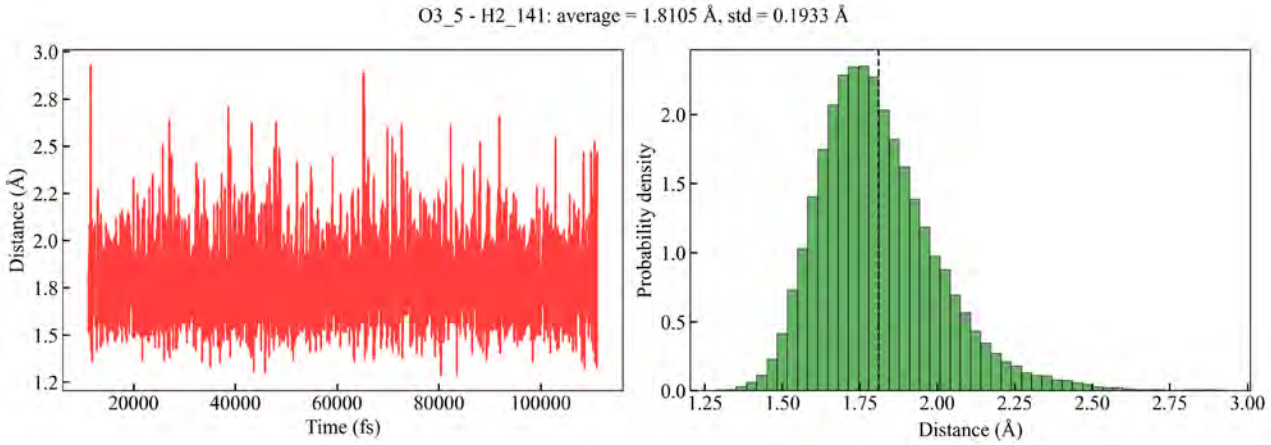
O3_452 - H2_588

Average distance = 1.8026 Å; standard deviation = 0.1808 Å; number of points = 100046



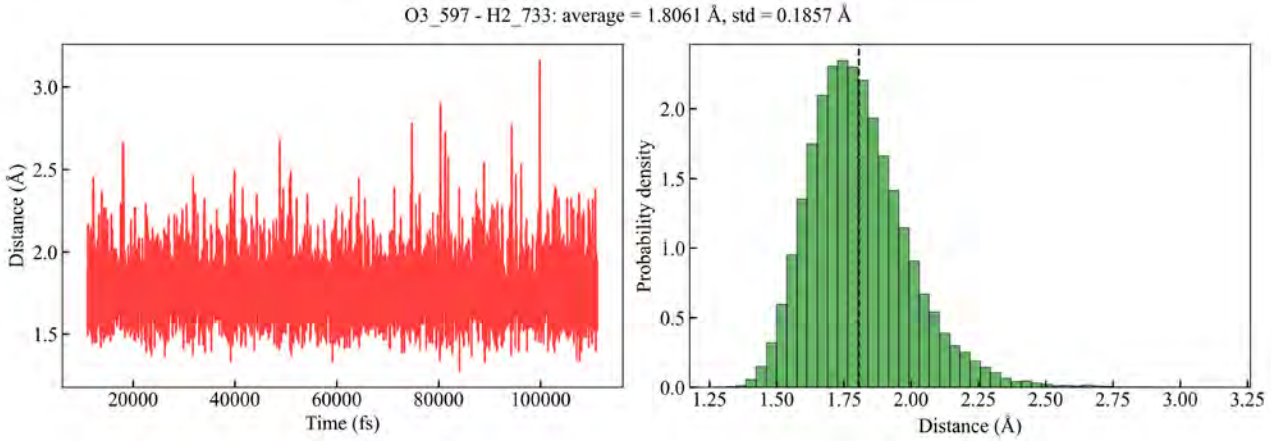
O3_5 - H2_141

Average distance = 1.8105 Å; standard deviation = 0.1933 Å; number of points = 100046



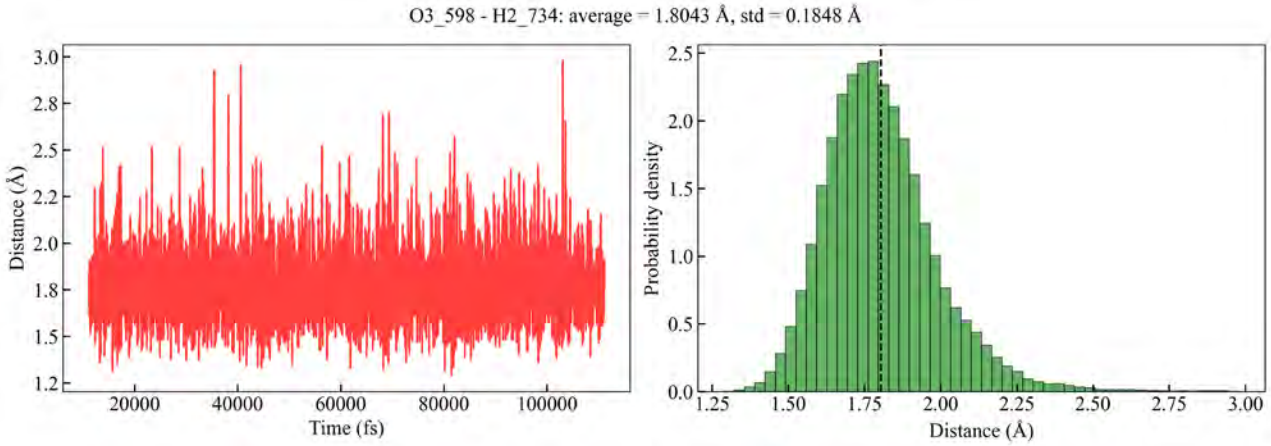
O3_597 - H2_733

Average distance = 1.8061 Å; standard deviation = 0.1857 Å; number of points = 100046



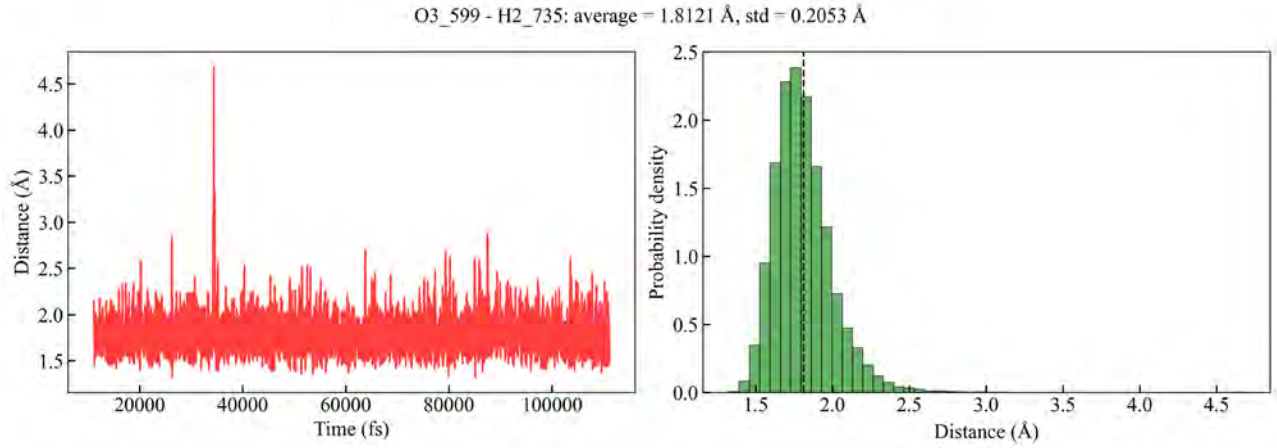
O3_598 - H2_734

Average distance = 1.8043 Å; standard deviation = 0.1848 Å; number of points = 100046



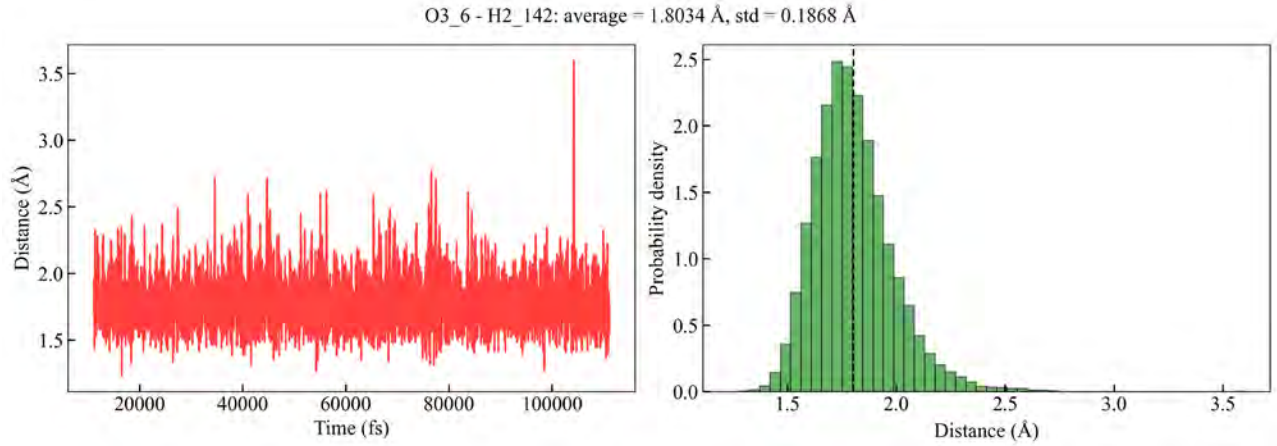
O3_599 - H2_735

Average distance = 1.8121 Å; standard deviation = 0.2053 Å; number of points = 100046



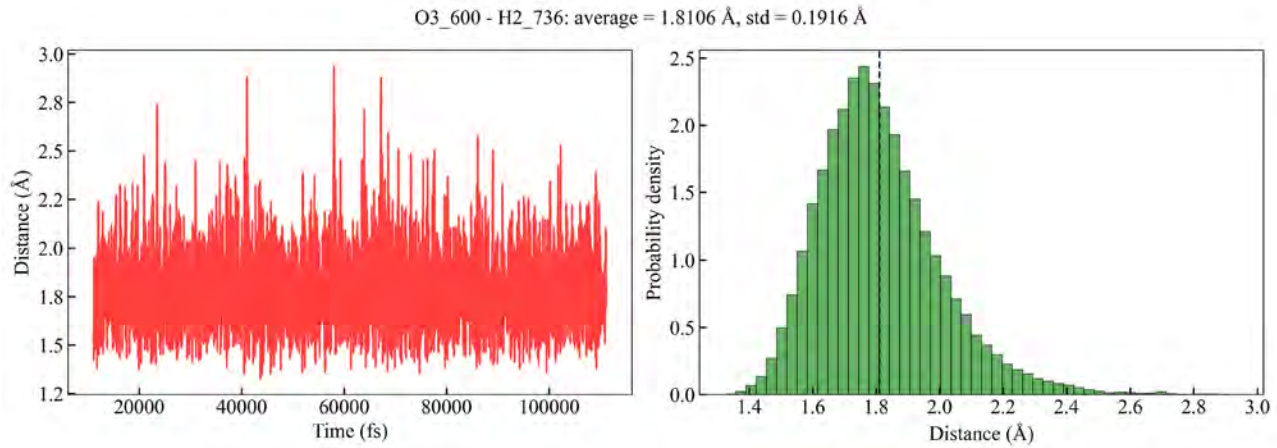
O3_6 - H2_142

Average distance = 1.8034 Å; standard deviation = 0.1868 Å; number of points = 100046



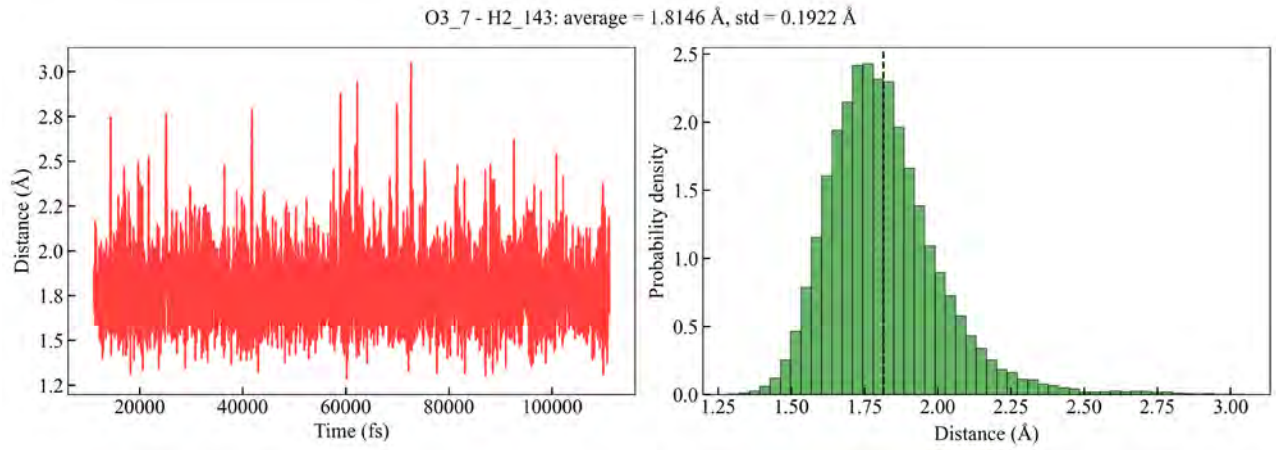
O3_600 - H2_736

Average distance = 1.8106 Å; standard deviation = 0.1916 Å; number of points = 100046



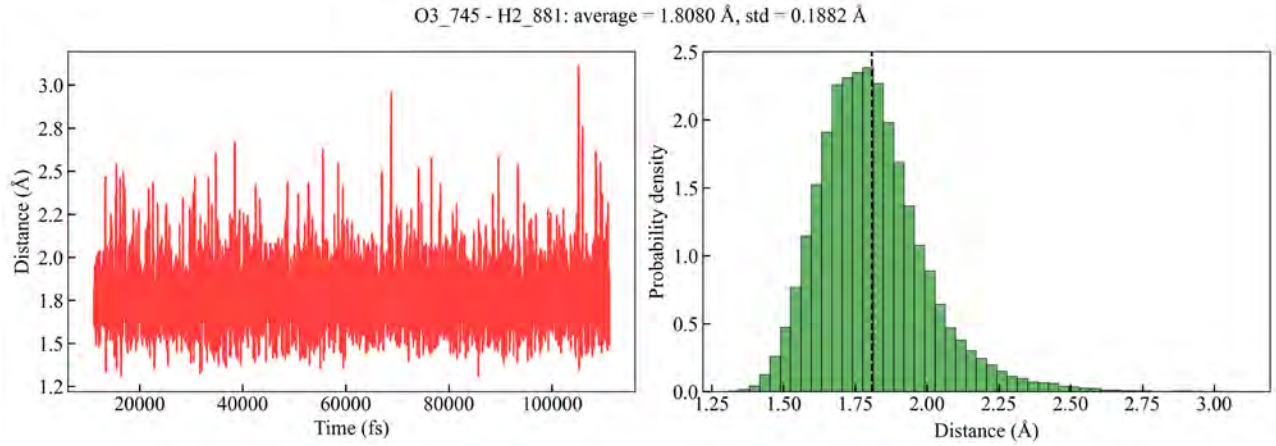
O3_7 - H2_143

Average distance = 1.8146 Å; standard deviation = 0.1922 Å; number of points = 100046



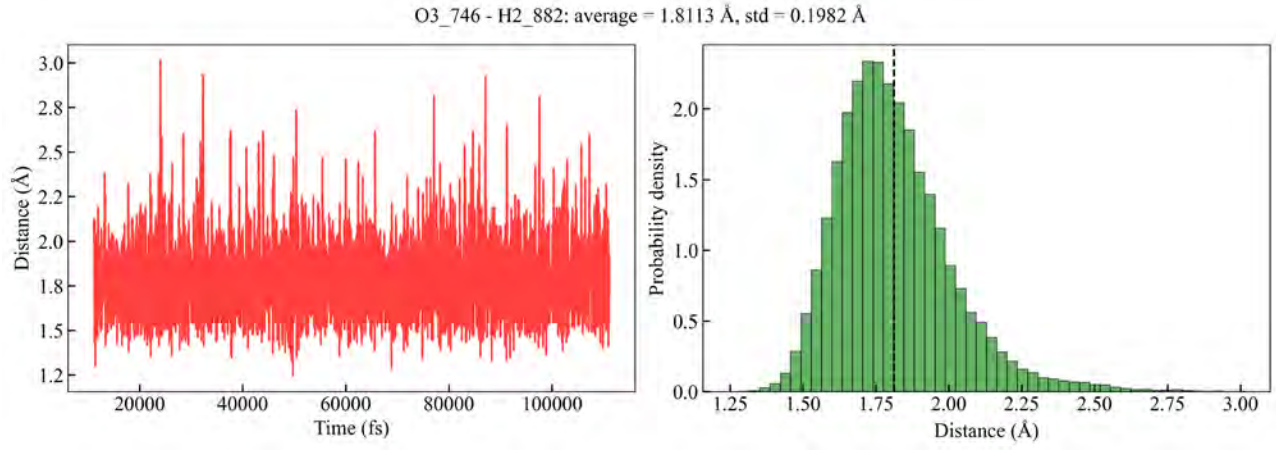
O3_745 - H2_881

Average distance = 1.8080 Å; standard deviation = 0.1882 Å; number of points = 100046



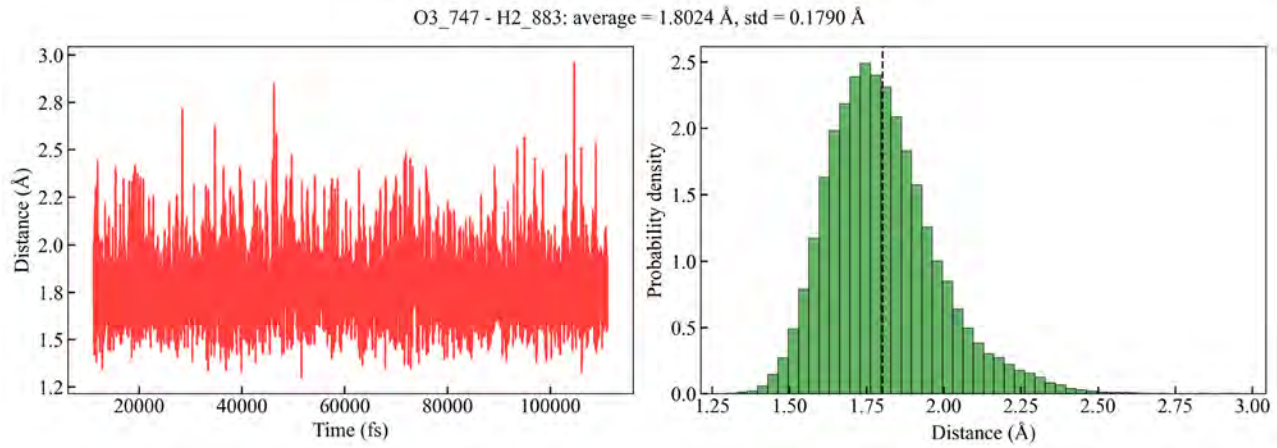
O3_746 - H2_882

Average distance = 1.8113 Å; standard deviation = 0.1982 Å; number of points = 100046



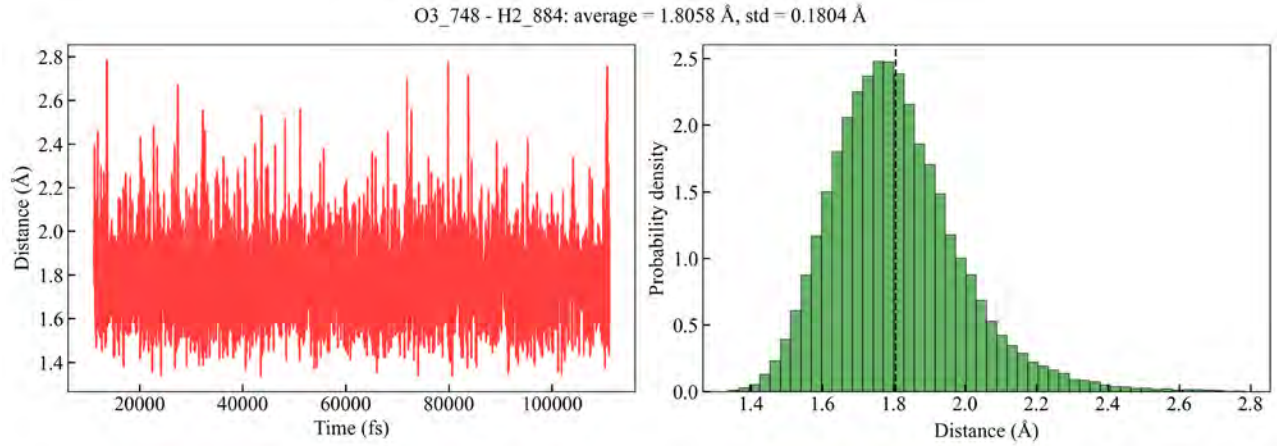
O3_747 - H2_883

Average distance = 1.8024 Å; standard deviation = 0.1790 Å; number of points = 100046



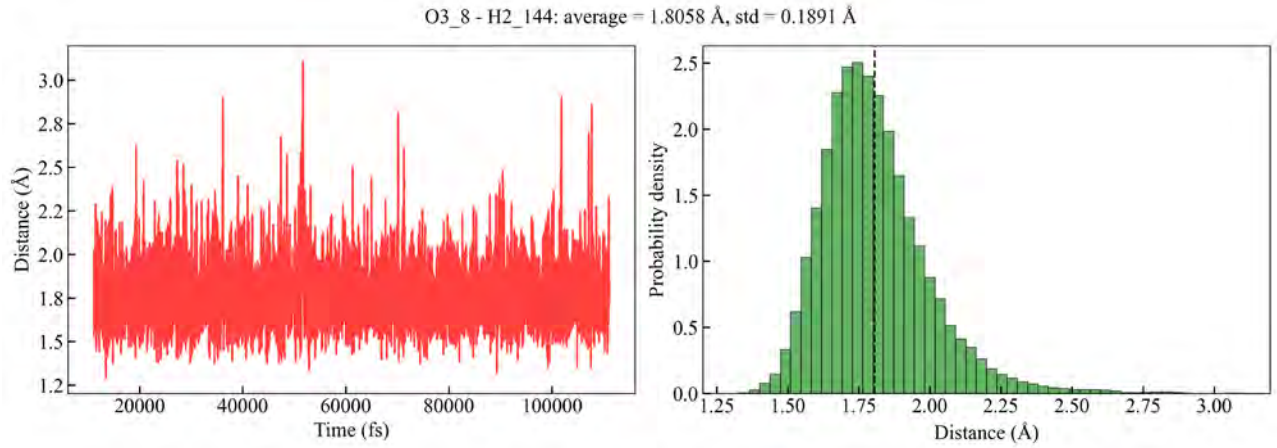
O3_748 - H2_884

Average distance = 1.8058 Å; standard deviation = 0.1804 Å; number of points = 100046



O3_8 - H2_144

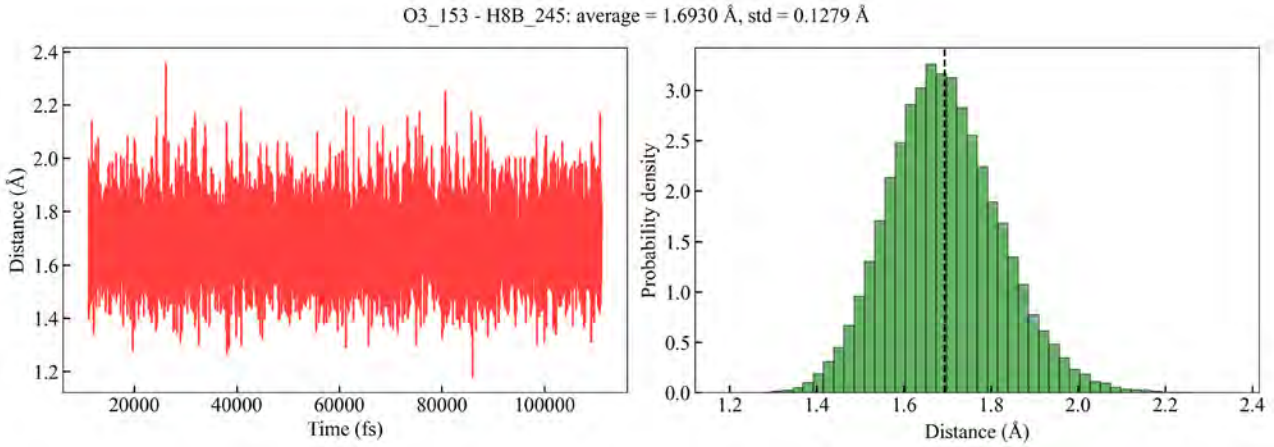
Average distance = 1.8058 Å; standard deviation = 0.1891 Å; number of points = 100046



O3 - H8B

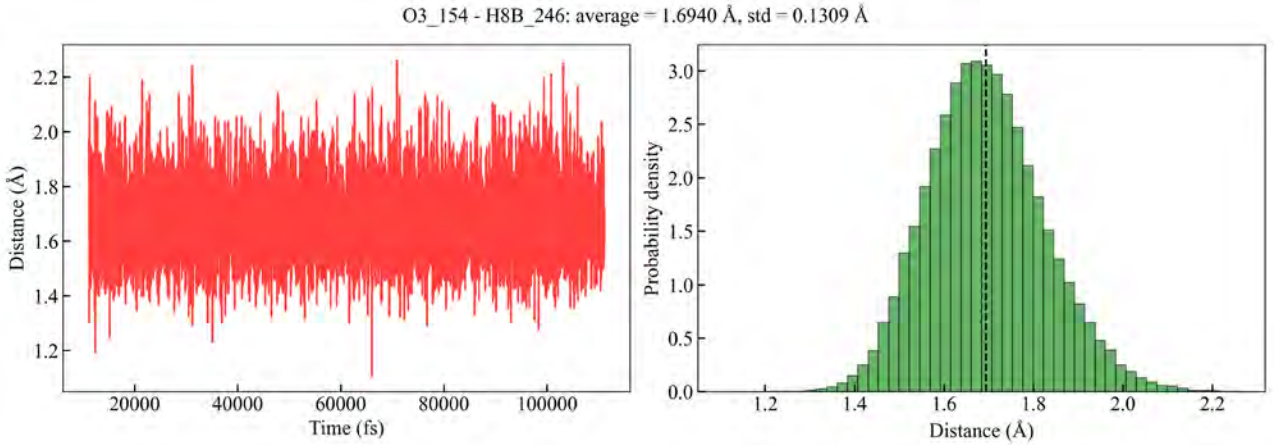
O3_153 - H8B_245

Average distance = 1.6930 Å; standard deviation = 0.1279 Å; number of points = 100046



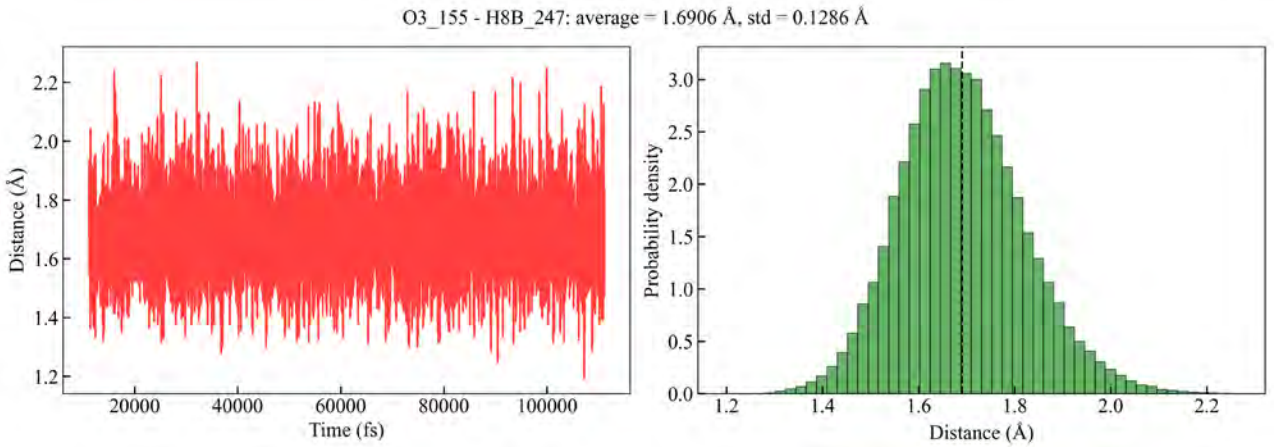
O3_154 - H8B_246

Average distance = 1.6940 Å; standard deviation = 0.1309 Å; number of points = 100046



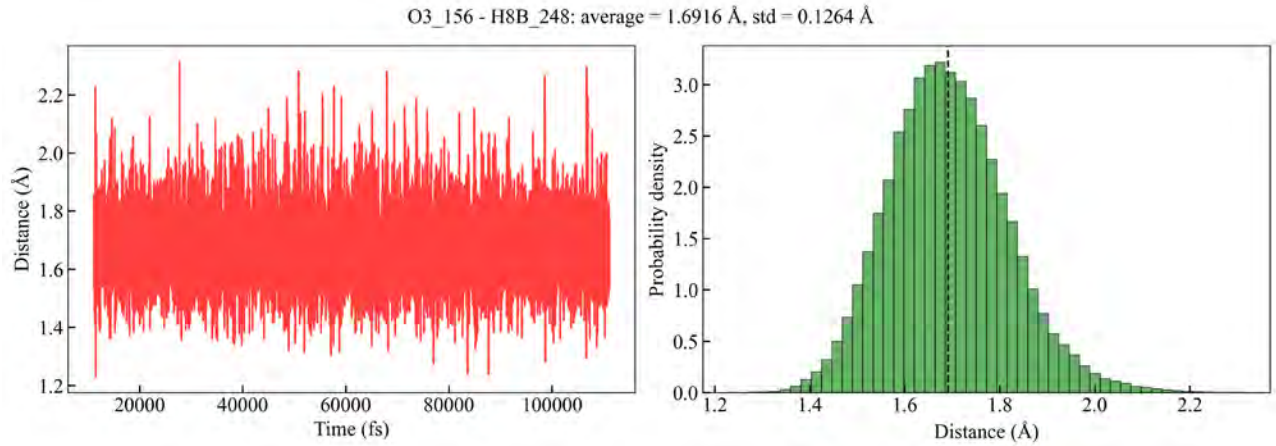
O3_155 - H8B_247

Average distance = 1.6906 Å; standard deviation = 0.1286 Å; number of points = 100046



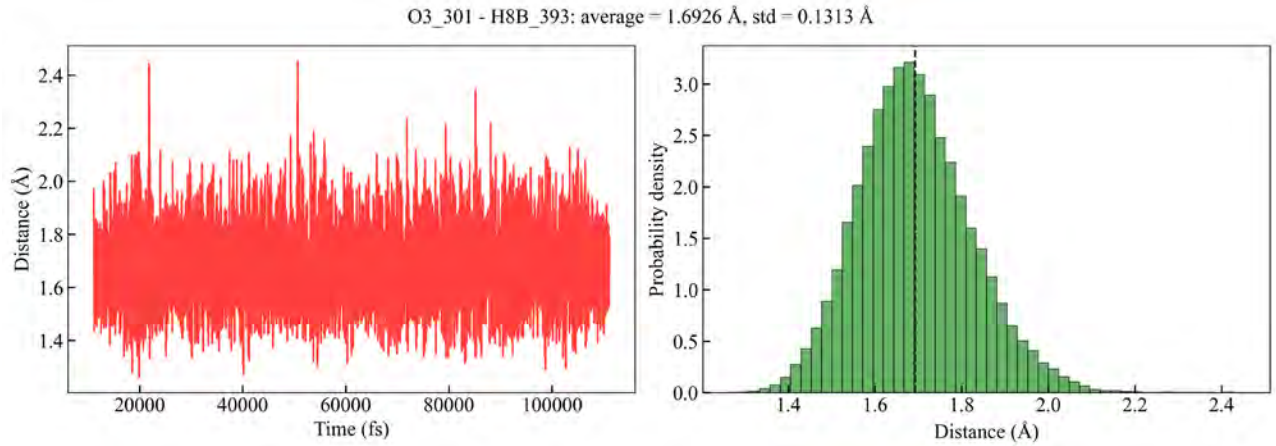
O3_156 - H8B_248

Average distance = 1.6916 Å; standard deviation = 0.1264 Å; number of points = 100046



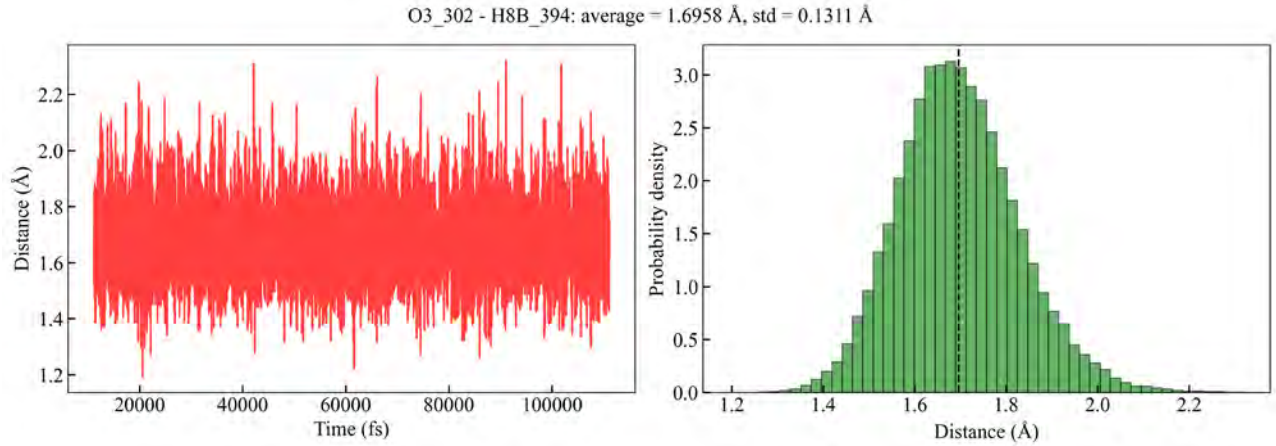
O3_301 - H8B_393

Average distance = 1.6926 Å; standard deviation = 0.1313 Å; number of points = 100046



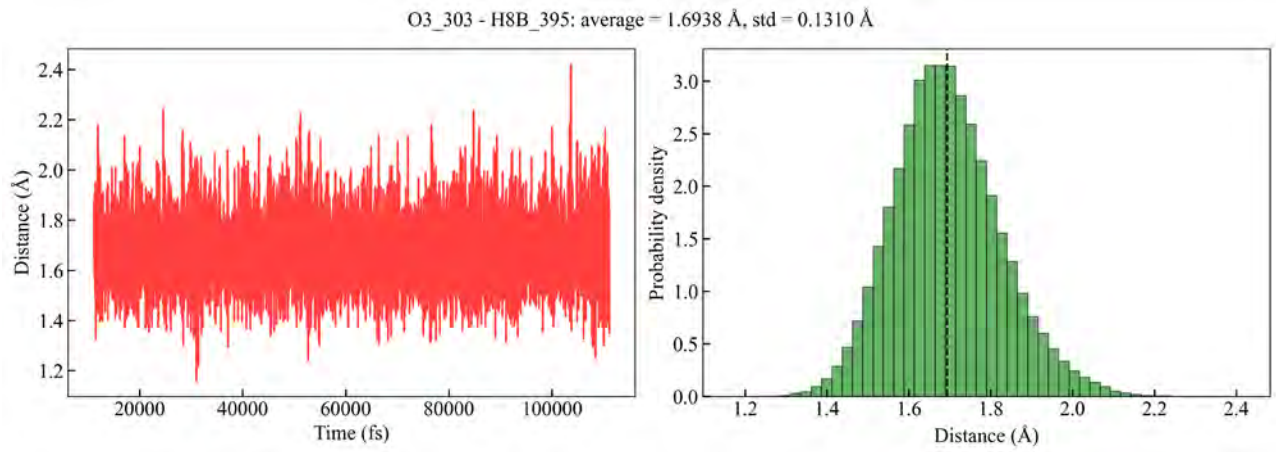
O3_302 - H8B_394

Average distance = 1.6958 Å; standard deviation = 0.1311 Å; number of points = 100046



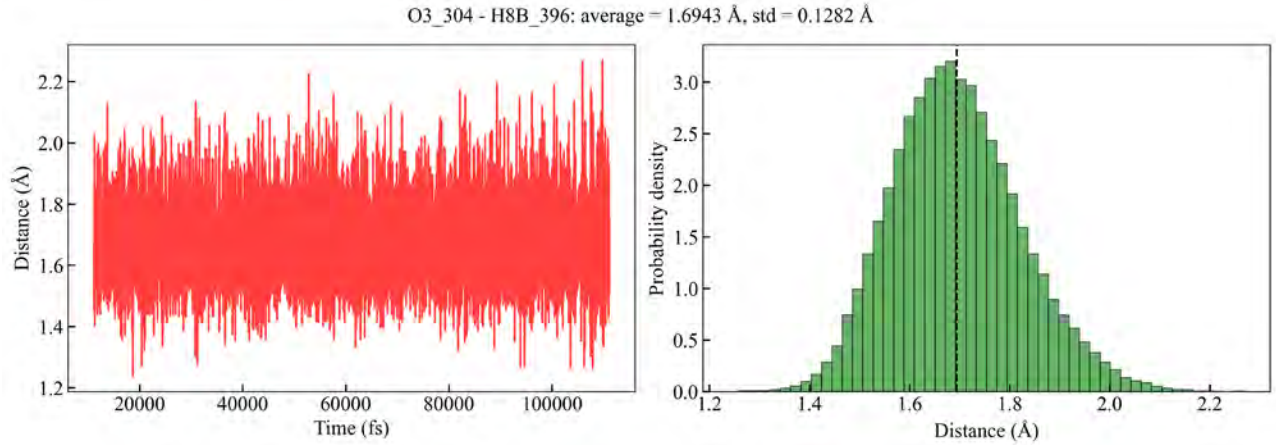
O3_303 - H8B_395

Average distance = 1.6938 Å; standard deviation = 0.1310 Å; number of points = 100046



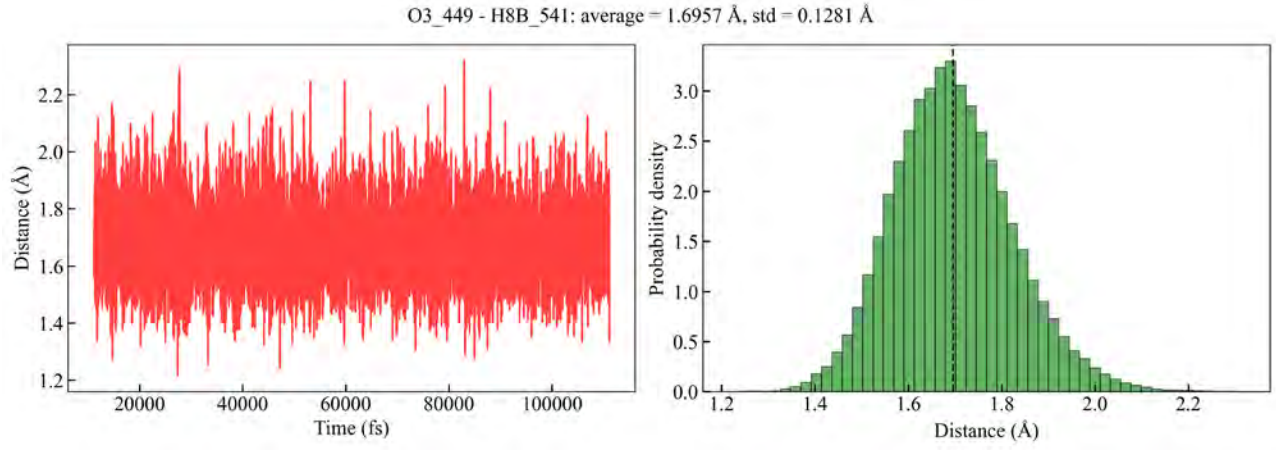
O3_304 - H8B_396

Average distance = 1.6943 Å; standard deviation = 0.1282 Å; number of points = 100046



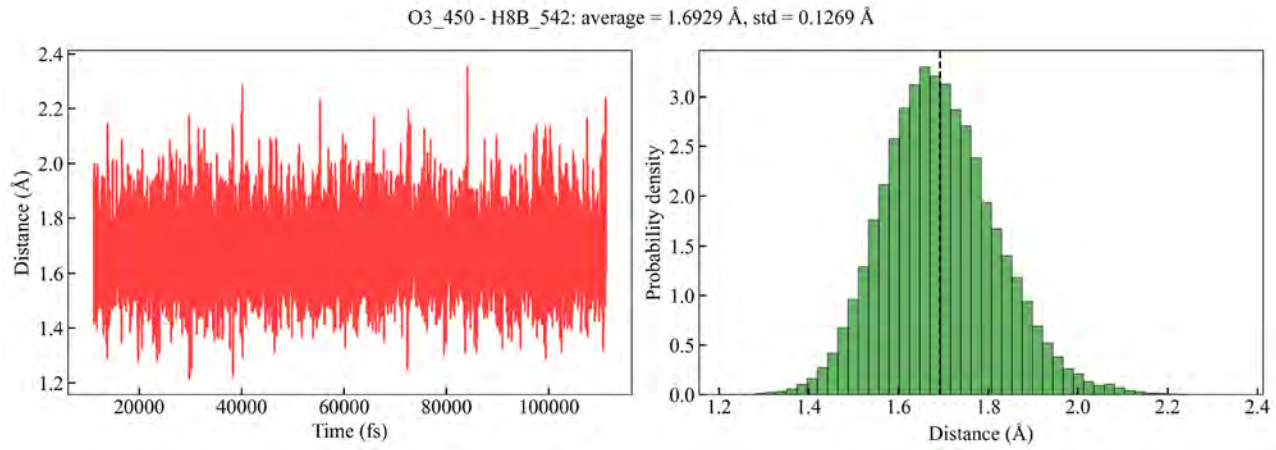
O3_449 - H8B_541

Average distance = 1.6957 Å; standard deviation = 0.1281 Å; number of points = 100046



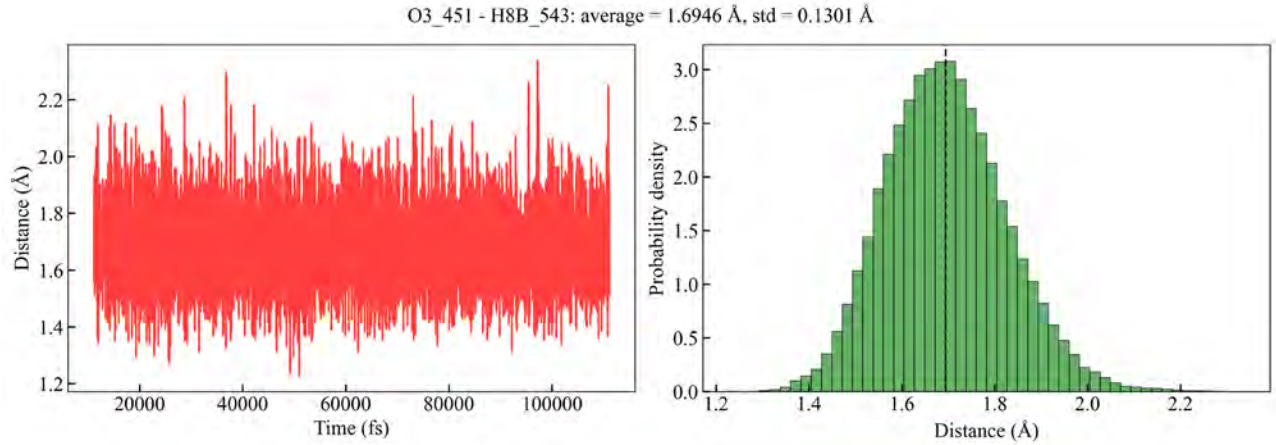
O3_450 - H8B_542

Average distance = 1.6929 Å; standard deviation = 0.1269 Å; number of points = 100046



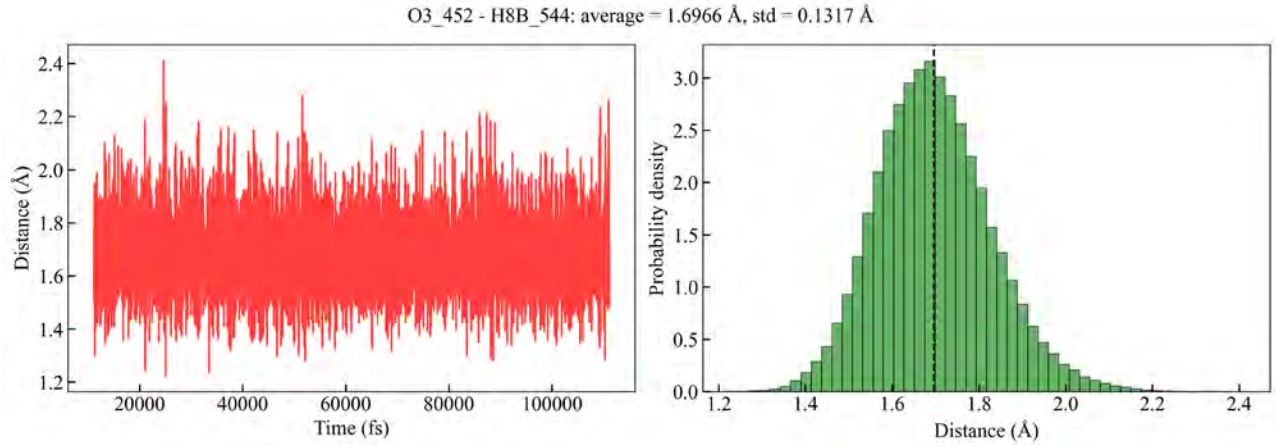
O3_451 - H8B_543

Average distance = 1.6946 Å; standard deviation = 0.1301 Å; number of points = 100046



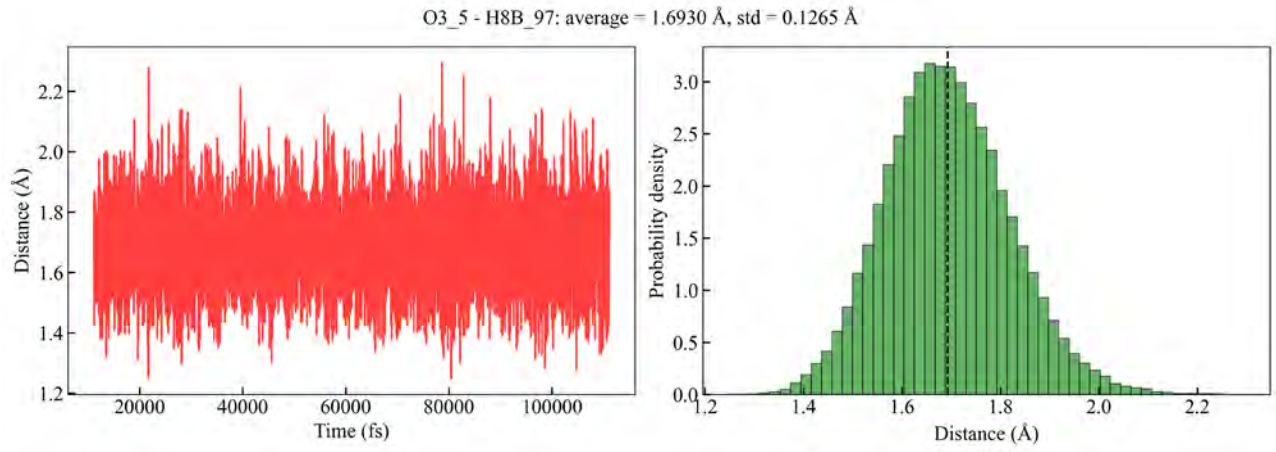
O3_452 - H8B_544

Average distance = 1.6966 Å; standard deviation = 0.1317 Å; number of points = 100046



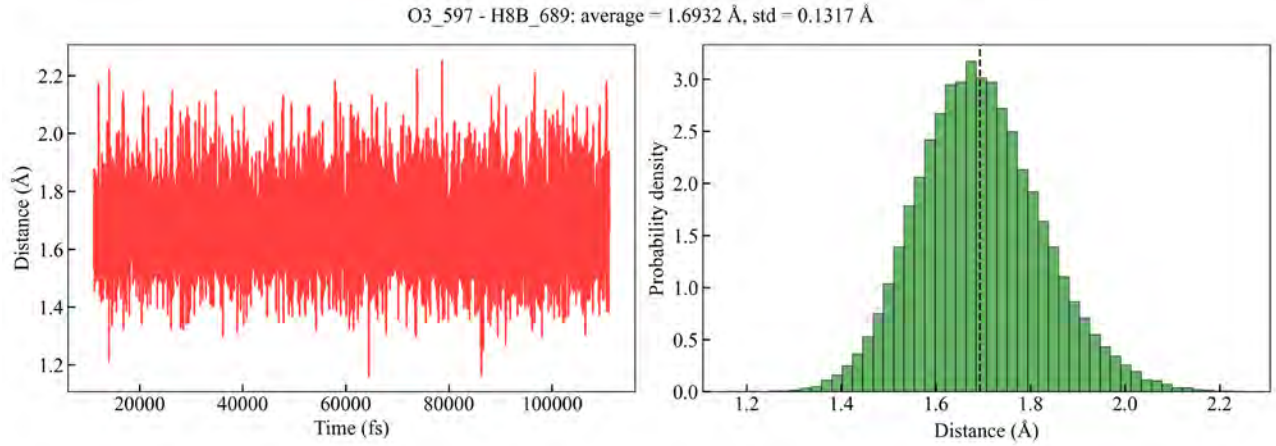
O3_5 - H8B_97

Average distance = 1.6930 Å; standard deviation = 0.1265 Å; number of points = 100046



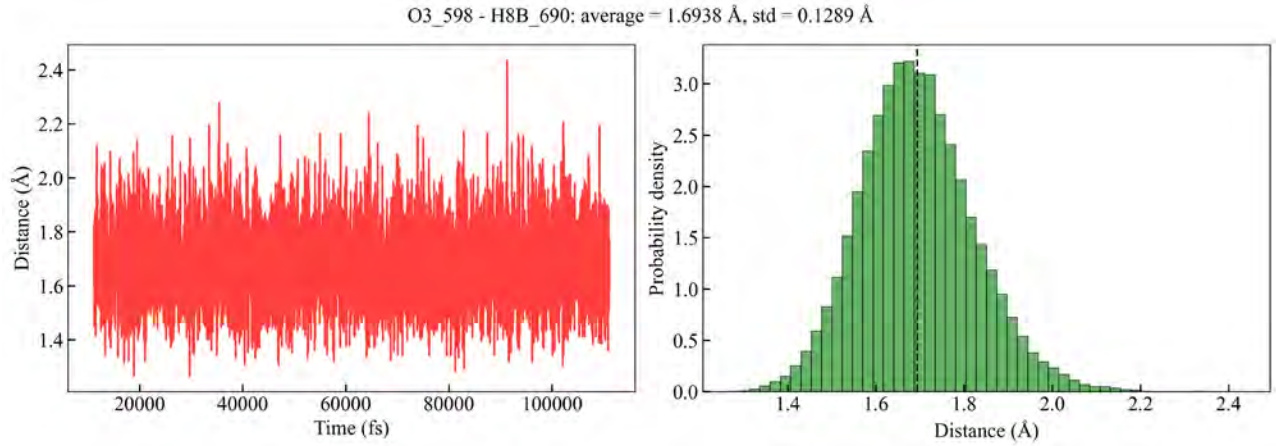
O3_597 - H8B_689

Average distance = 1.6932 Å; standard deviation = 0.1317 Å; number of points = 100046



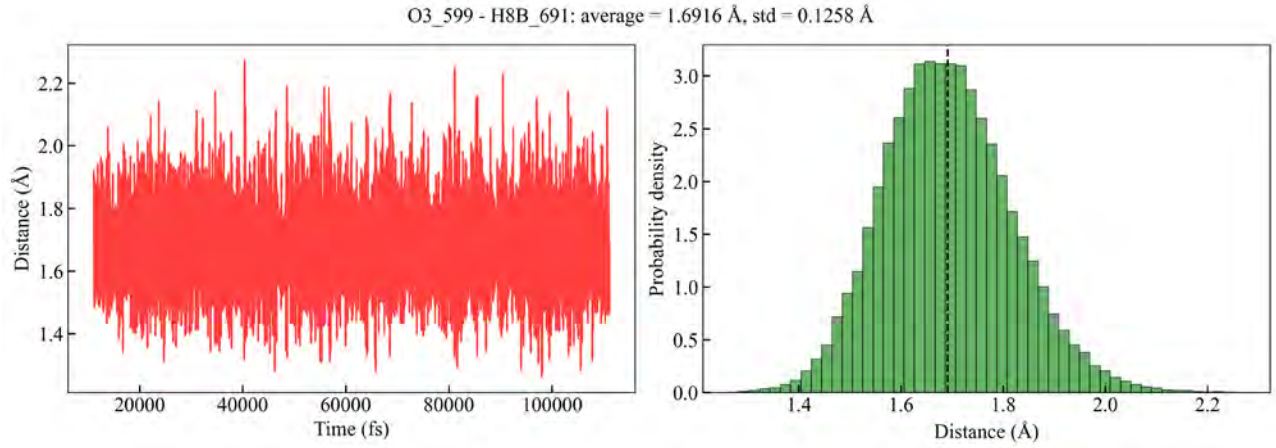
O3_598 - H8B_690

Average distance = 1.6938 Å; standard deviation = 0.1289 Å; number of points = 100046



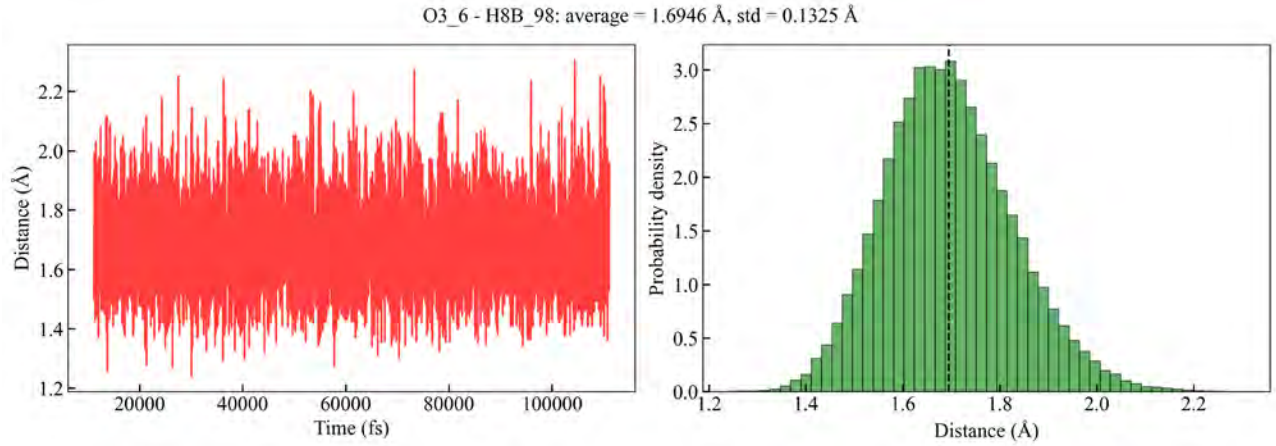
O3_599 - H8B_691

Average distance = 1.6916 Å; standard deviation = 0.1258 Å; number of points = 100046



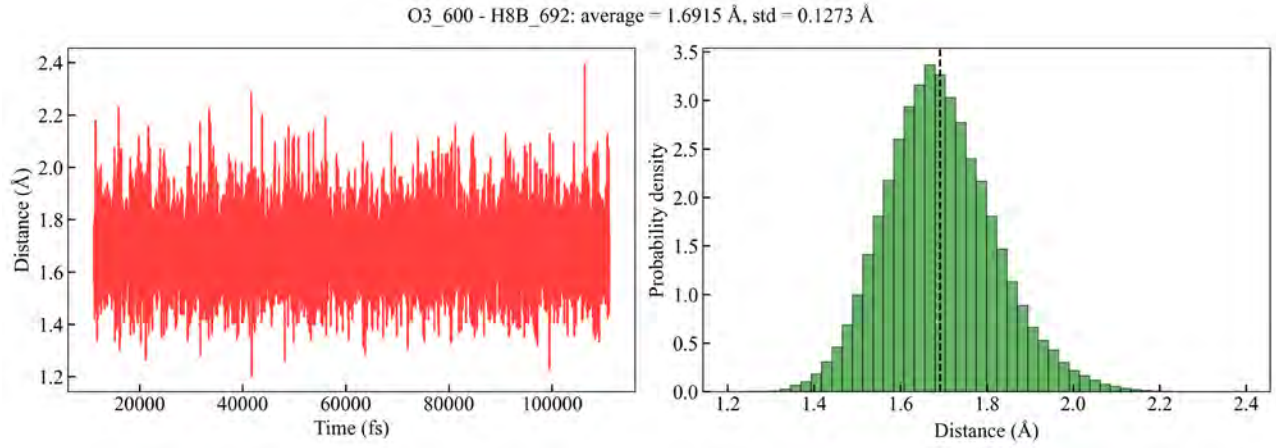
O3_6 - H8B_98

Average distance = 1.6946 Å; standard deviation = 0.1325 Å; number of points = 100046



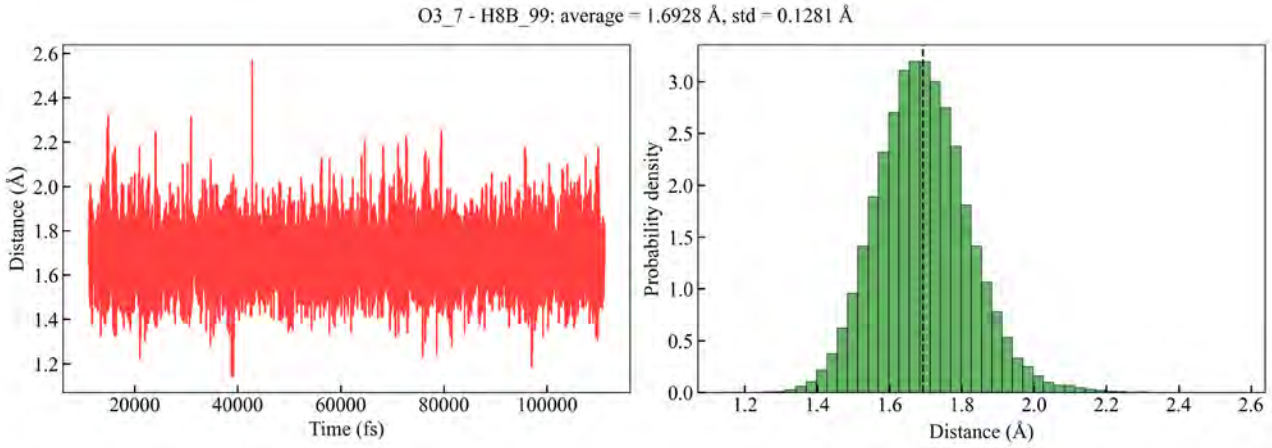
O3_600 - H8B_692

Average distance = 1.6915 Å; standard deviation = 0.1273 Å; number of points = 100046



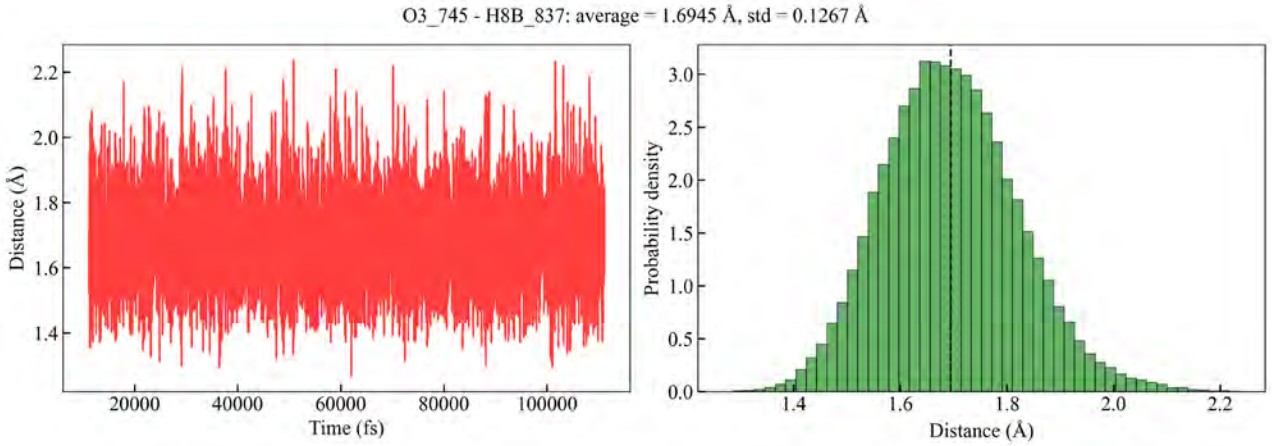
O3_7 - H8B_99

Average distance = 1.6928 Å; standard deviation = 0.1281 Å; number of points = 100046



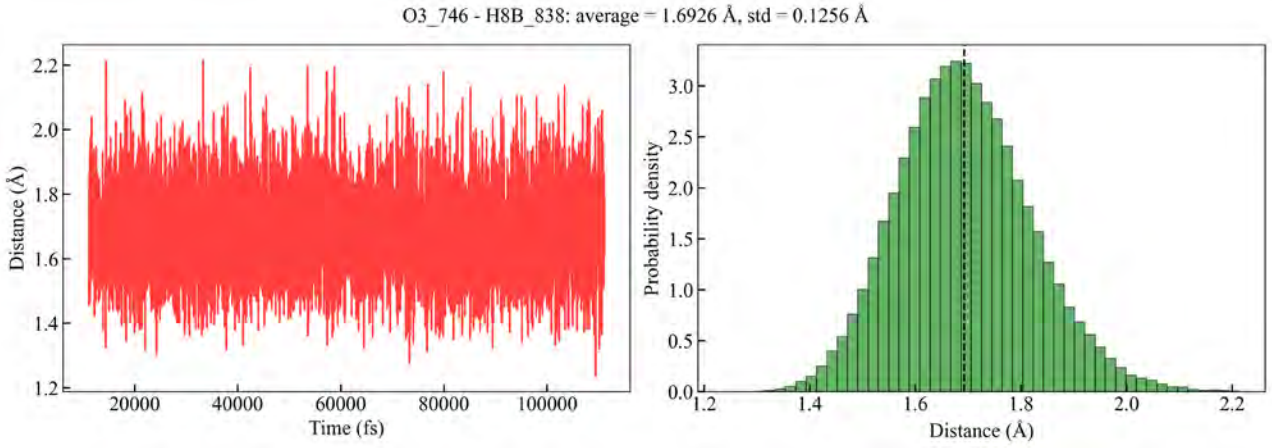
O3_745 - H8B_837

Average distance = 1.6945 Å; standard deviation = 0.1267 Å; number of points = 100046



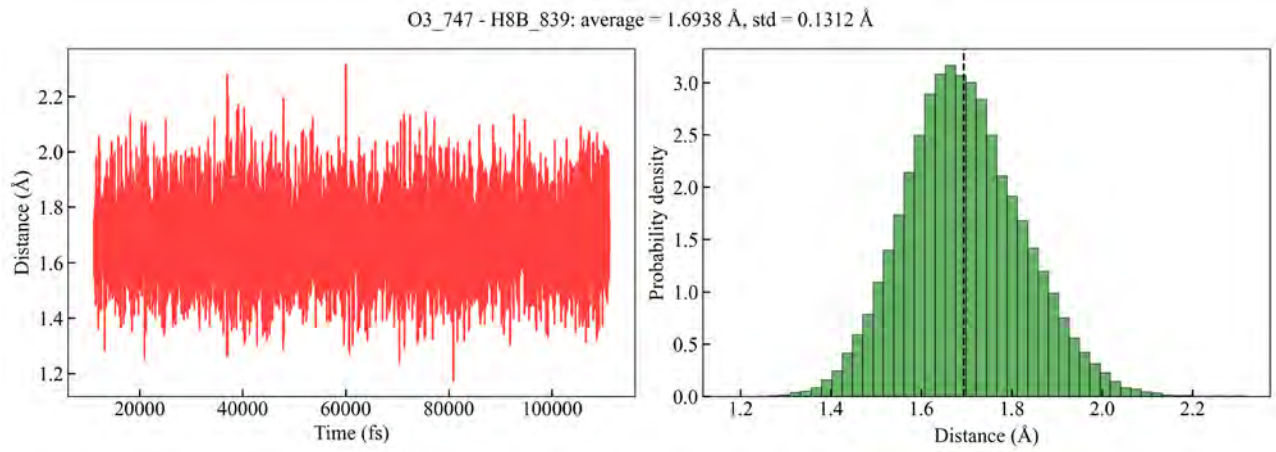
O3_746 - H8B_838

Average distance = 1.6926 Å; standard deviation = 0.1256 Å; number of points = 100046



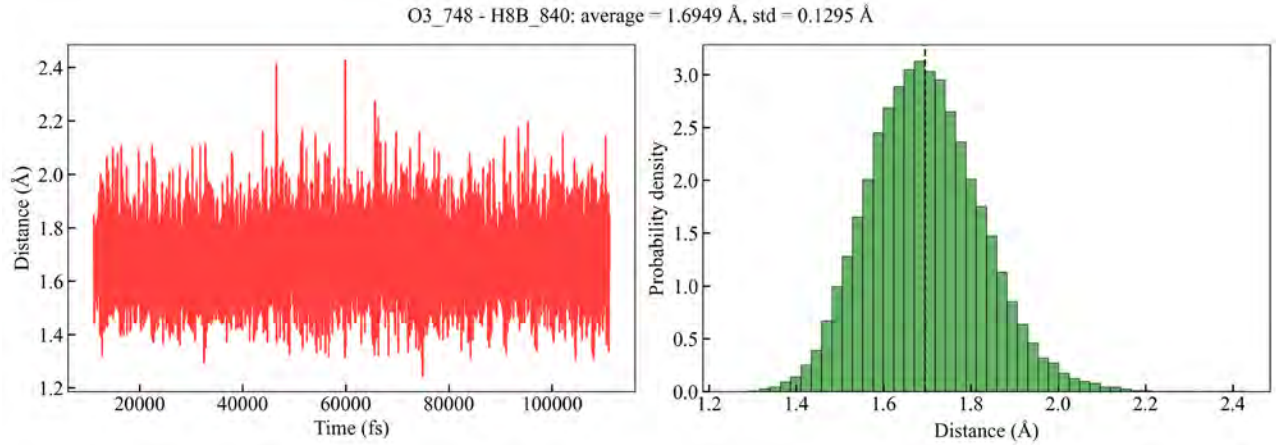
O3_747 - H8B_839

Average distance = 1.6938 Å; standard deviation = 0.1312 Å; number of points = 100046



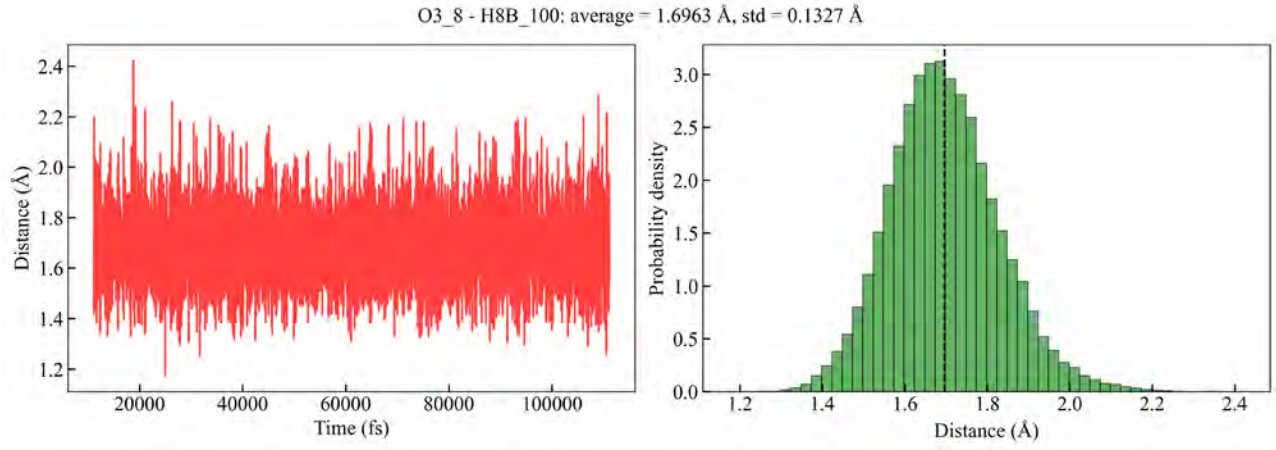
O3_748 - H8B_840

Average distance = 1.6949 Å; standard deviation = 0.1295 Å; number of points = 100046



O3_8 - H8B_100

Average distance = 1.6963 Å; standard deviation = 0.1327 Å; number of points = 100046



3.2.6. P3 at 453 K - Bond Distance Analysis at the surface

Table S23. Individual time-averaged hydrogen-involving atomic distances for all equivalent proton environments in the P3 surface AIMD trajectory at 453 K.

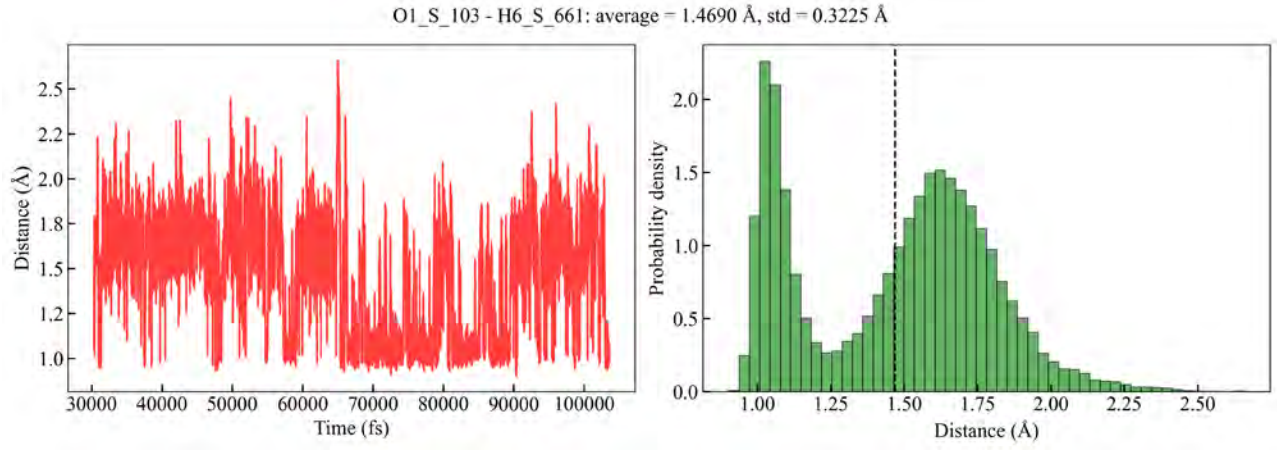
Bond type	Average distance (Å)	Standard dev. σ (Å)	Number of points
O1_S_103 - H6_S_661	1.4690	0.3225	73284
O1_S_104 - H6_S_662	1.4695	0.3152	73284
O1_S_13 - H6_S_769	1.5863	0.2555	73284
O1_S_14 - H6_S_770	1.5571	0.2749	73284
O1_S_48 - H6_S_882	1.4865	0.3021	73284
O1_S_77 - H6_S_557	1.5321	0.2875	73284
O1_S_78 - H6_S_558	1.5381	0.2878	73284
O2_S_1 - H3_S_583	1.8386	0.2380	73284
O2_S_2 - H3_S_584	1.8798	0.2286	73284
O2_S_35 - H3_S_479	1.7872	0.2340	73284
O2_S_35 - H3_S_881	3.5114	0.2769	73284
O2_S_36 - H3_S_480	1.8104	0.2680	73284
O2_S_66 - H3_S_804	1.8082	0.2713	73284
O2_S_91 - H3_S_691	1.8152	0.2516	73284
O2_S_92 - H3_S_692	1.7690	0.3102	73284
O3_S_41 - H8B_S_839	1.6864	0.1901	73284
O3_S_42 - H8B_S_840	1.6844	0.1869	73284
O3_S_71 - H8B_S_515	1.6801	0.1769	73284
O3_S_72 - H8B_S_516	1.6856	0.1826	73284
O3_S_8 - H8B_S_728	1.7068	0.1844	73284
O3_S_97 - H8B_S_589	3.3909	0.1924	73284
O3_S_98 - H8B_S_620	1.7141	0.1826	73284

Bond Distance Plots

O1 - H6

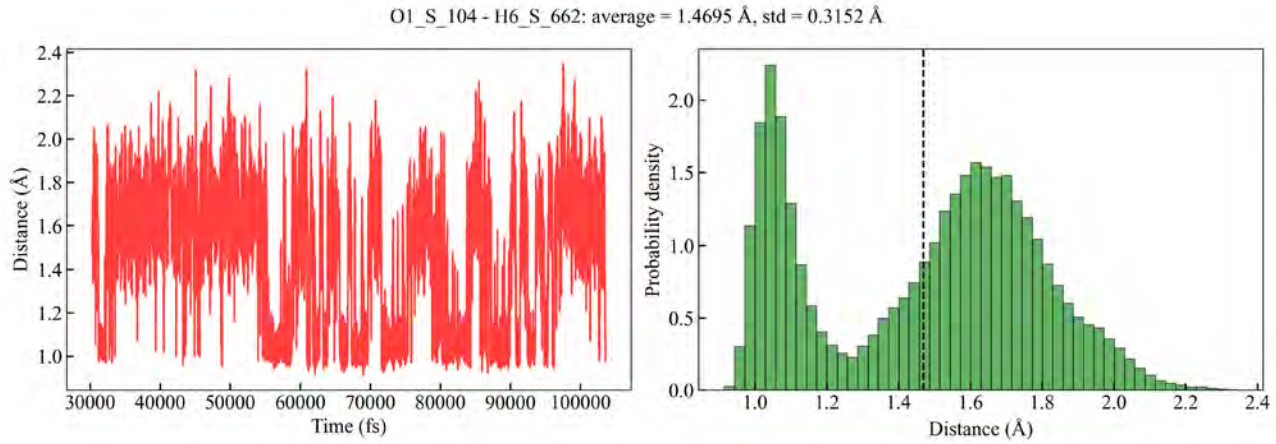
O1_S_103 - H6_S_661

Average distance = 1.4690 Å; standard deviation = 0.3225 Å; number of points = 73284



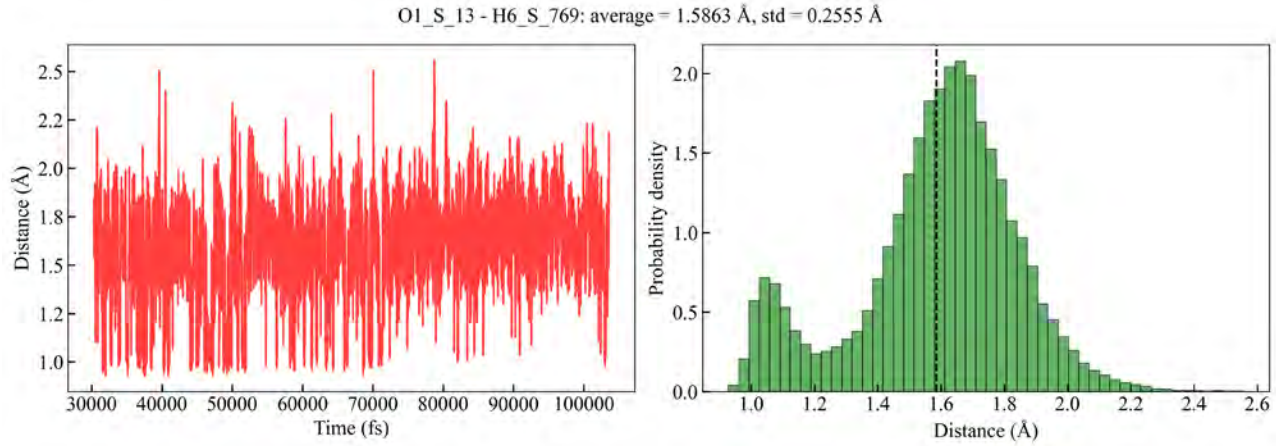
O1_S_104 - H6_S_662

Average distance = 1.4695 Å; standard deviation = 0.3152 Å; number of points = 73284



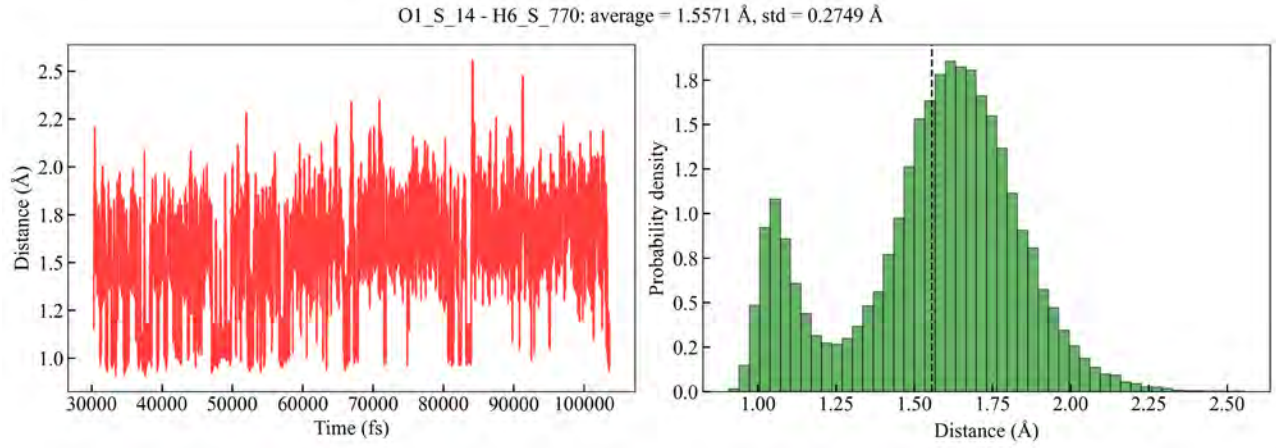
O1_S_13 - H6_S_769

Average distance = 1.5863 Å; standard deviation = 0.2555 Å; number of points = 73284



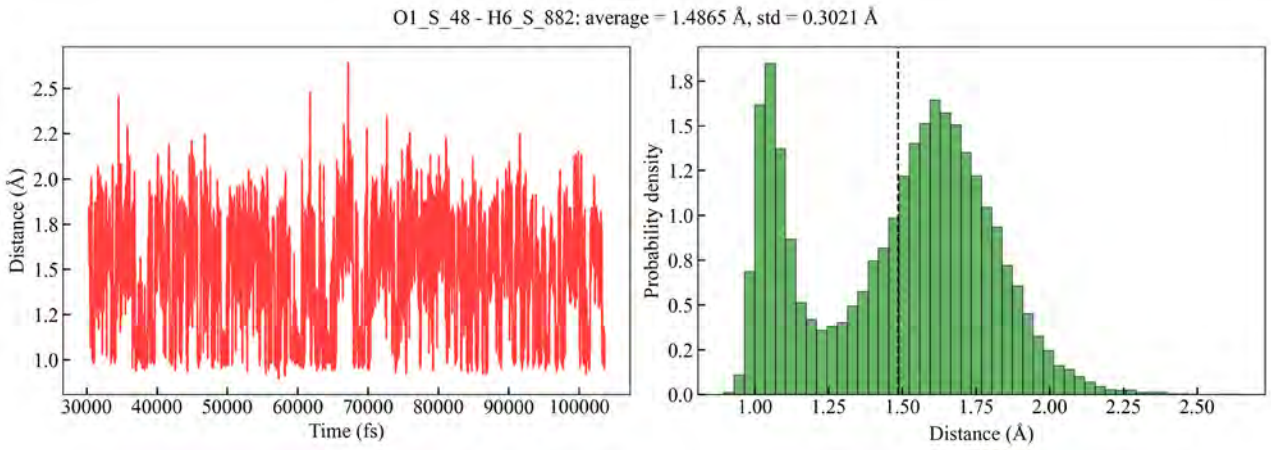
O1_S_14 - H6_S_770

Average distance = 1.5571 Å; standard deviation = 0.2749 Å; number of points = 73284



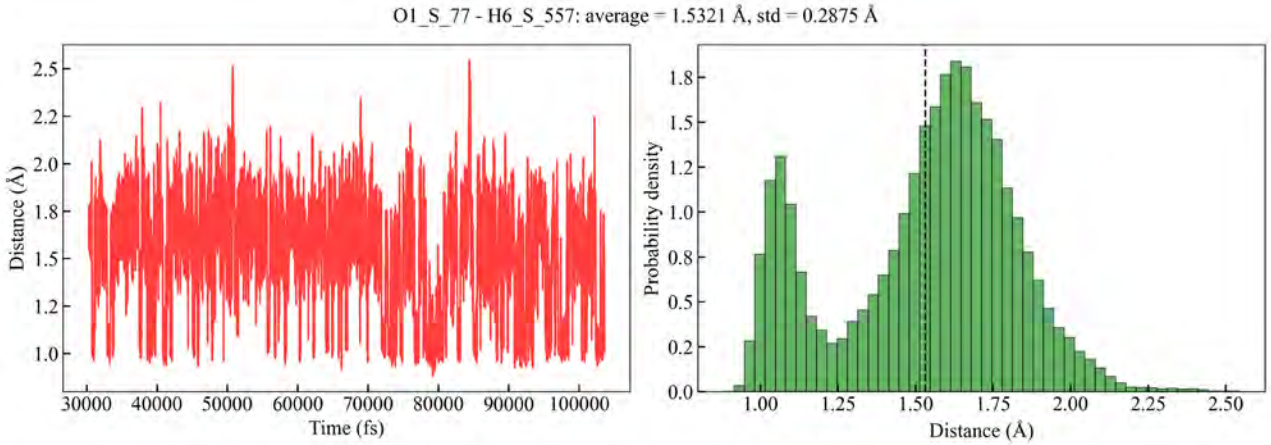
O1_S_48 - H6_S_882

Average distance = 1.4865 Å; standard deviation = 0.3021 Å; number of points = 73284



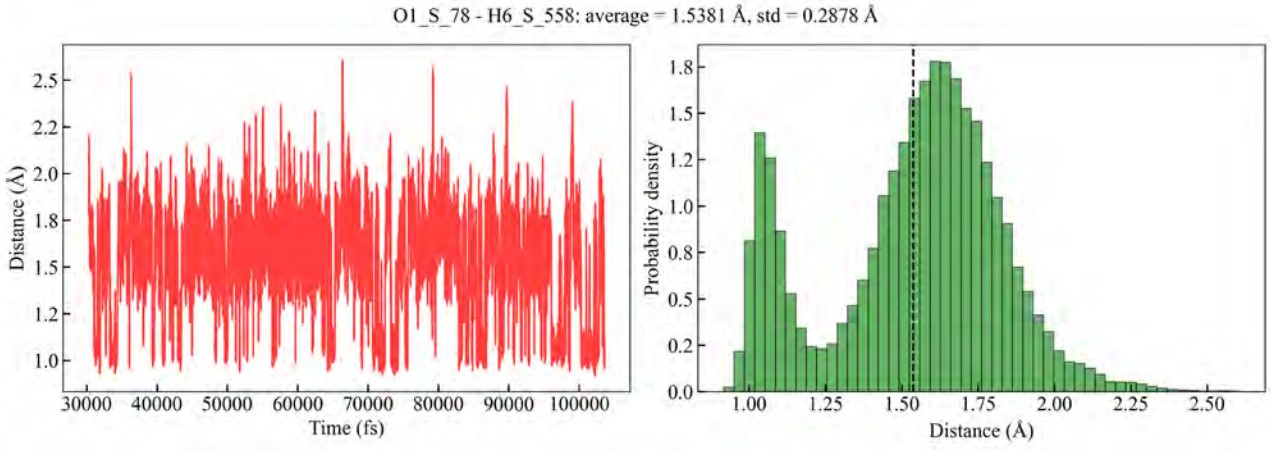
O1_S_77 - H6_S_557

Average distance = 1.5321 Å; standard deviation = 0.2875 Å; number of points = 73284



O1_S_78 - H6_S_558

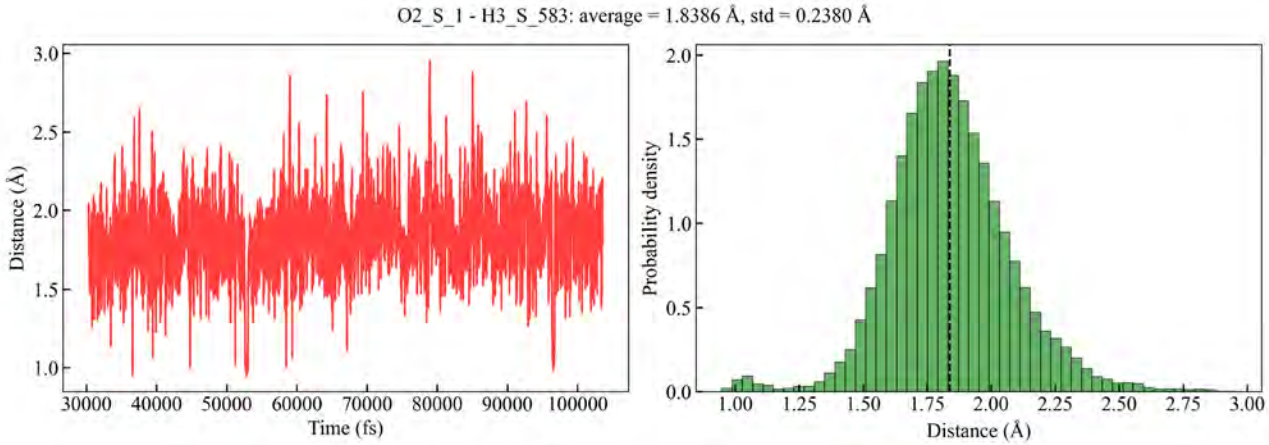
Average distance = 1.5381 Å; standard deviation = 0.2878 Å; number of points = 73284



O2 - H3

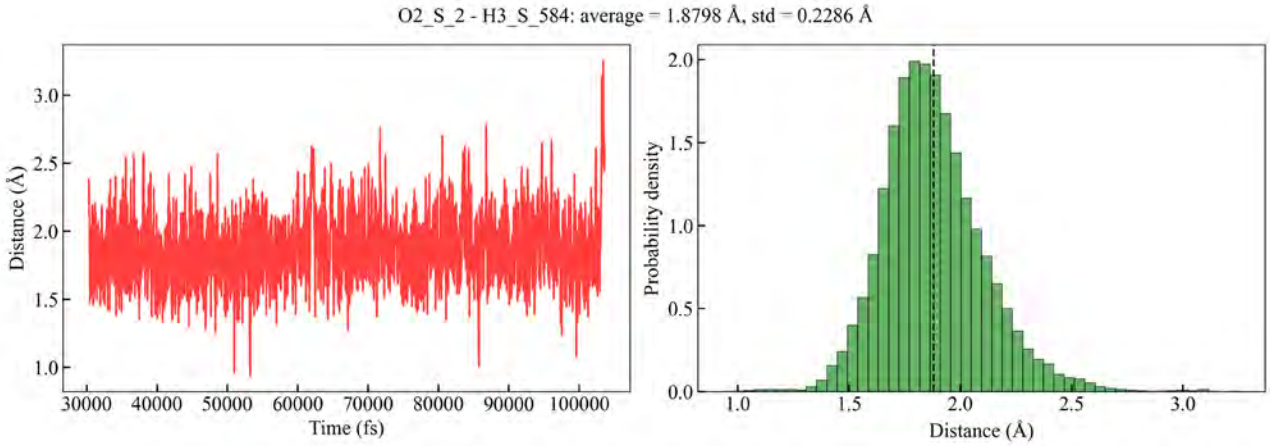
O2_S_1 - H3_S_583

Average distance = 1.8386 Å; standard deviation = 0.2380 Å; number of points = 73284



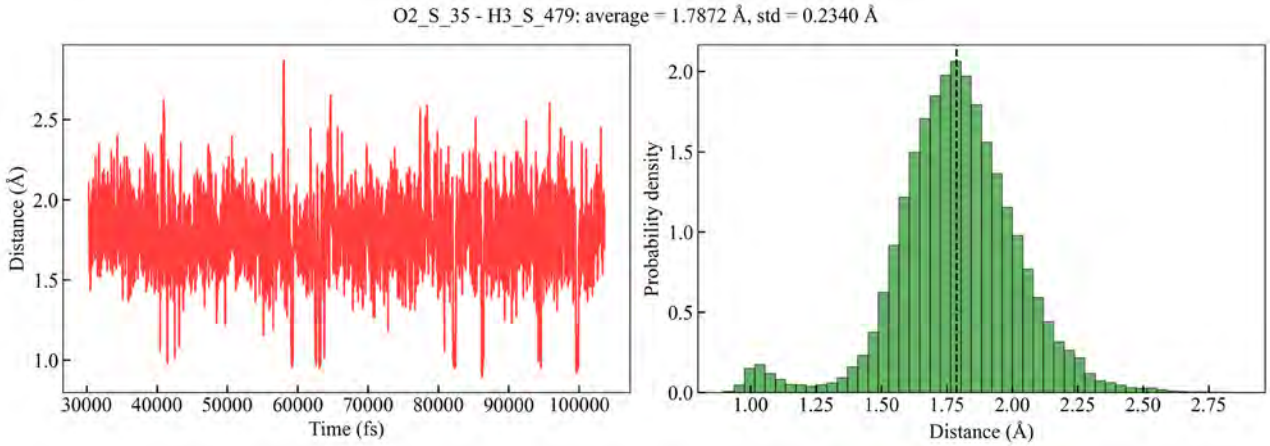
O2_S_2 - H3_S_584

Average distance = 1.8798 Å; standard deviation = 0.2286 Å; number of points = 73284



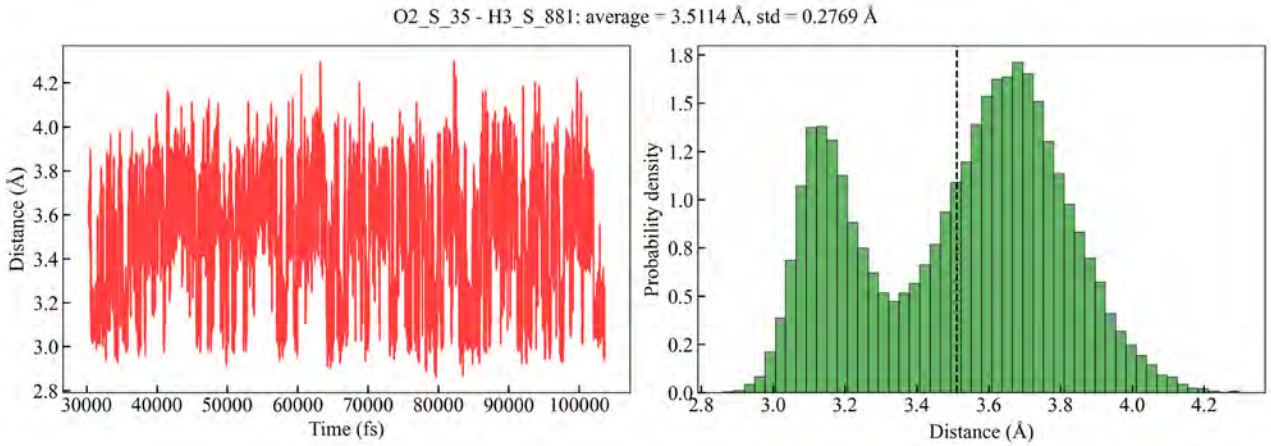
O2_S_35 - H3_S_479

Average distance = 1.7872 Å; standard deviation = 0.2340 Å; number of points = 73284



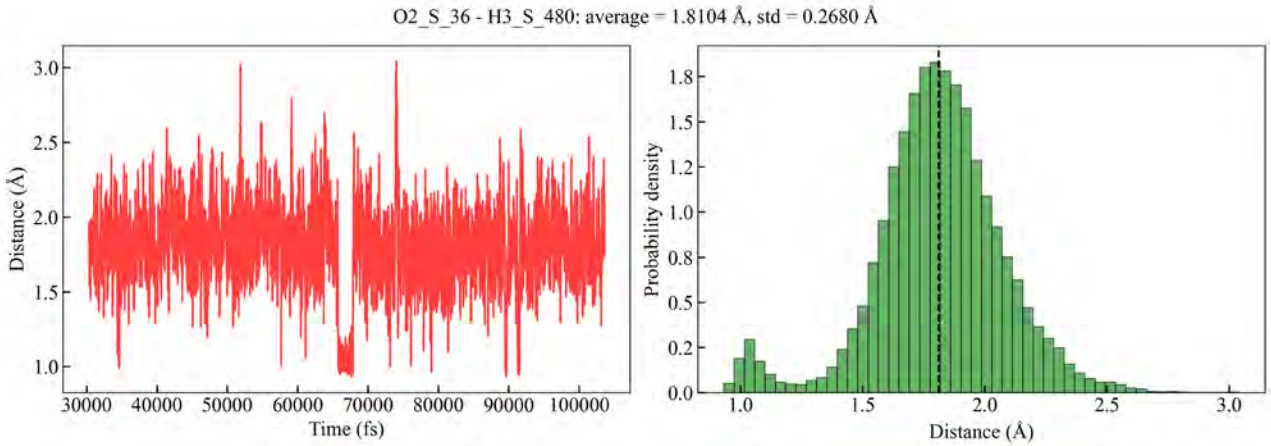
O2_S_35 - H3_S_881

Average distance = 3.5114 Å; standard deviation = 0.2769 Å; number of points = 73284



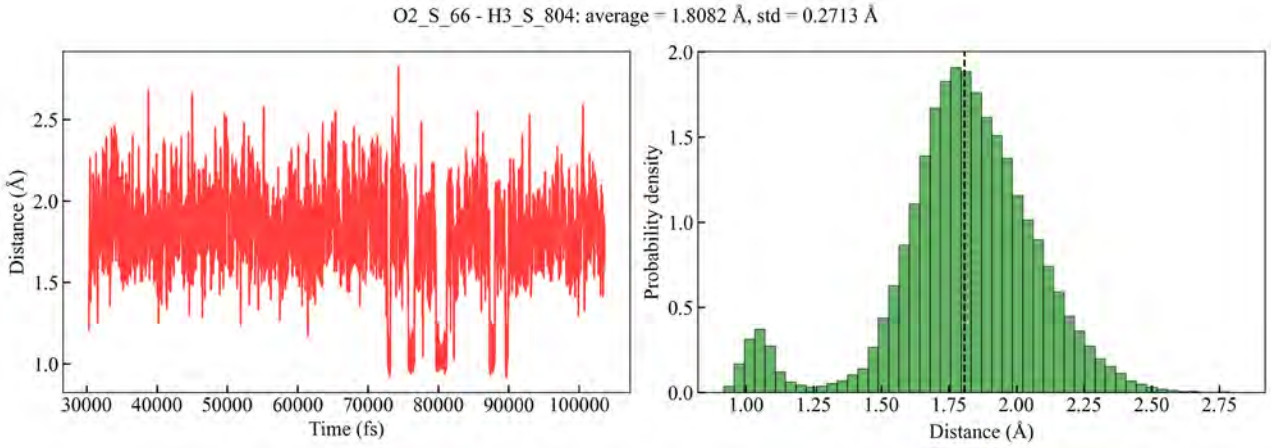
O2_S_36 - H3_S_480

Average distance = 1.8104 Å; standard deviation = 0.2680 Å; number of points = 73284



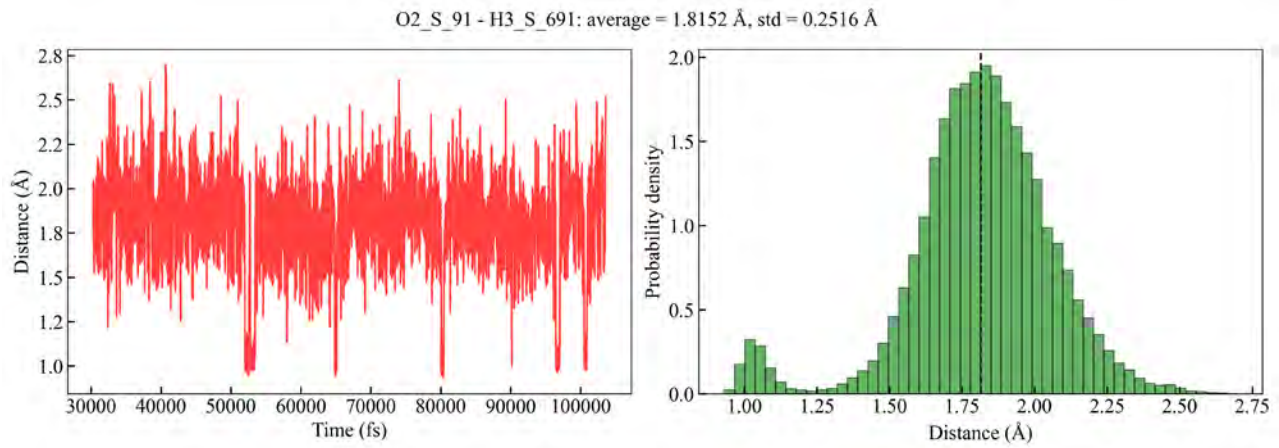
O2_S_66 - H3_S_804

Average distance = 1.8082 Å; standard deviation = 0.2713 Å; number of points = 73284



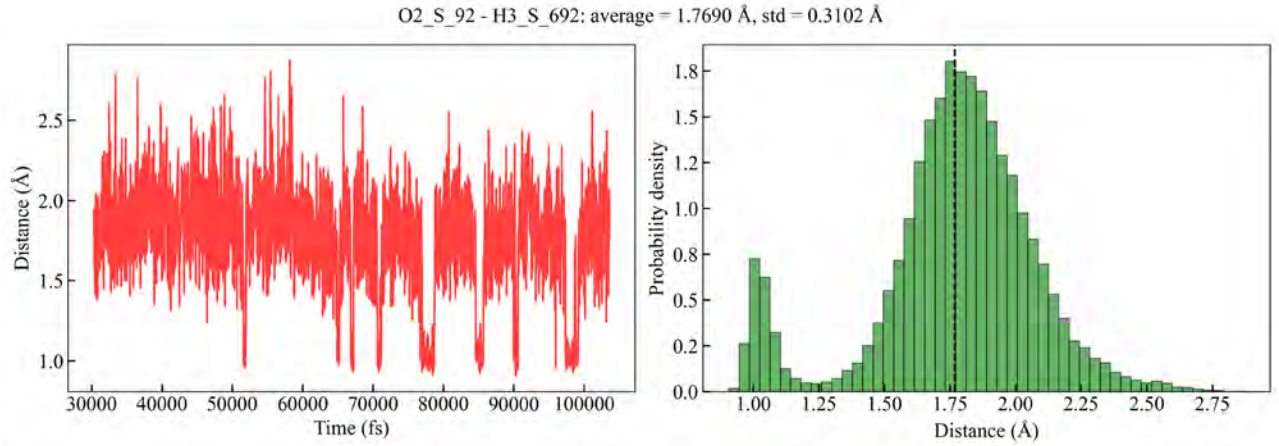
O2_S_91 - H3_S_691

Average distance = 1.8152 Å; standard deviation = 0.2516 Å; number of points = 73284



O2_S_92 - H3_S_692

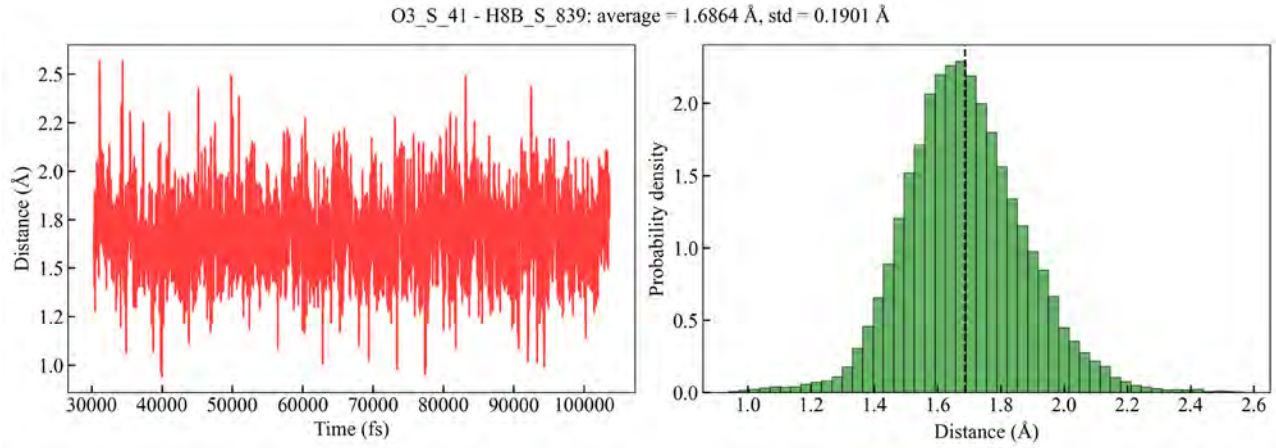
Average distance = 1.7690 Å; standard deviation = 0.3102 Å; number of points = 73284



O3 - H8B

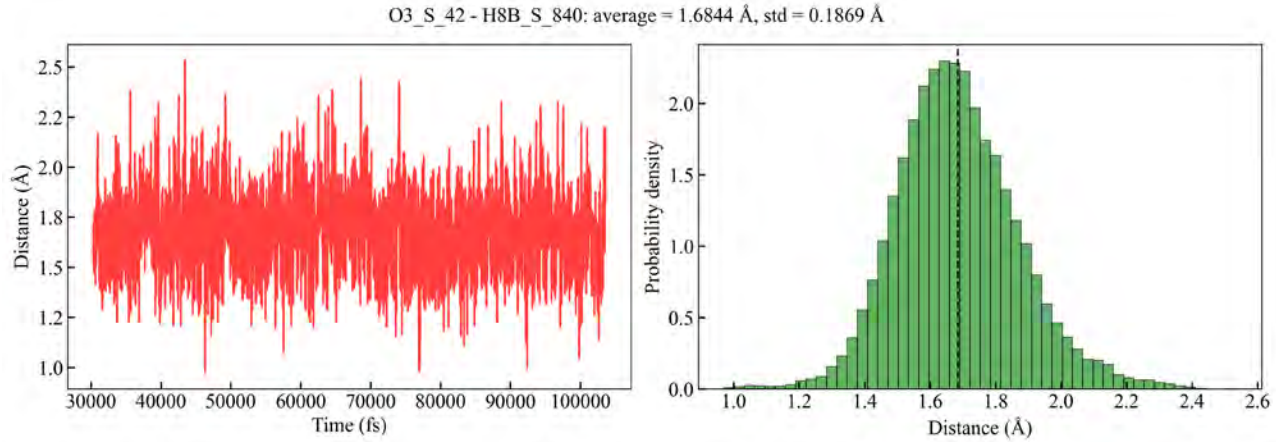
O3_S_41 - H8B_S_839

Average distance = 1.6864 Å; standard deviation = 0.1901 Å; number of points = 73284



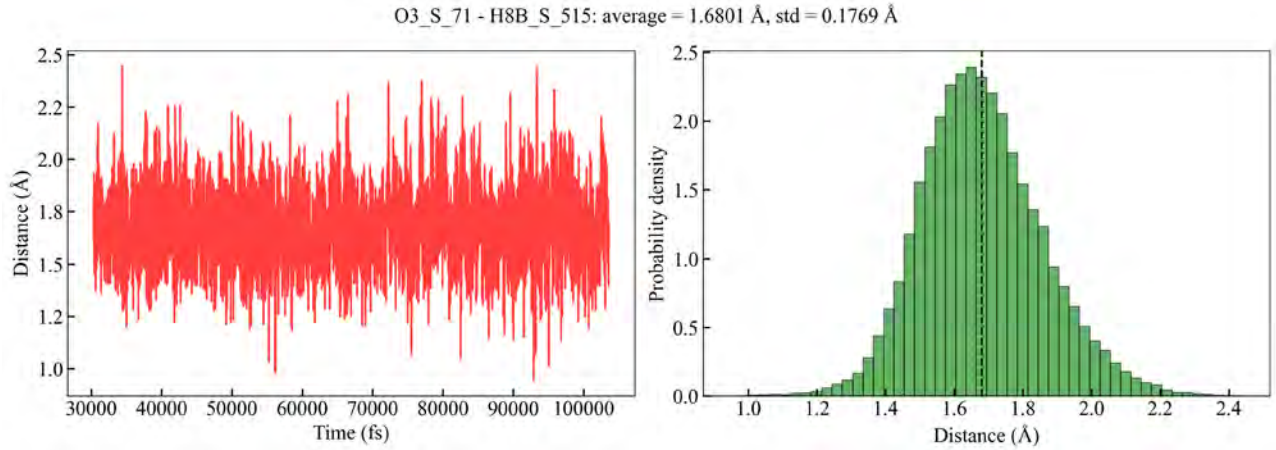
O3_S_42 - H8B_S_840

Average distance = 1.6844 Å; standard deviation = 0.1869 Å; number of points = 73284



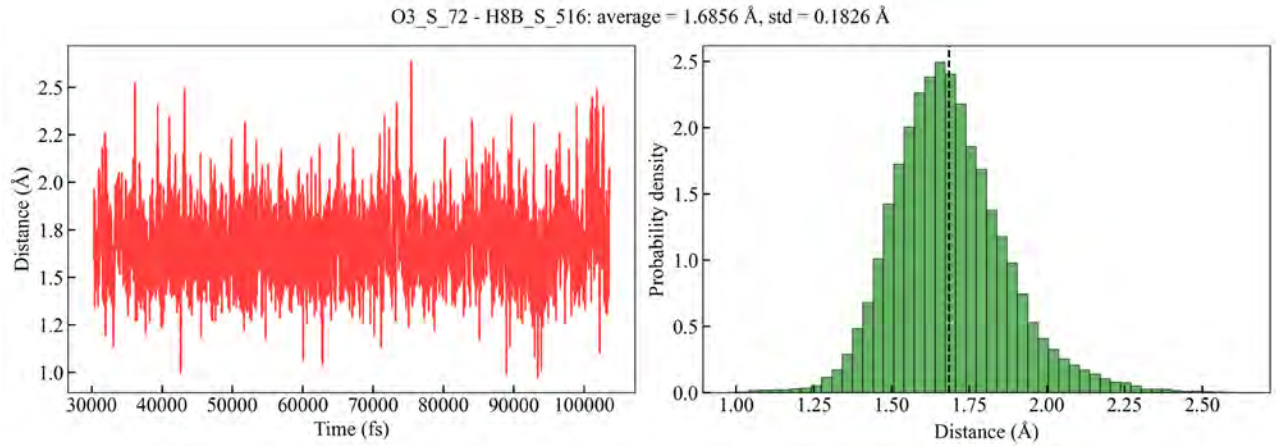
O3_S_71 - H8B_S_515

Average distance = 1.6801 Å; standard deviation = 0.1769 Å; number of points = 73284



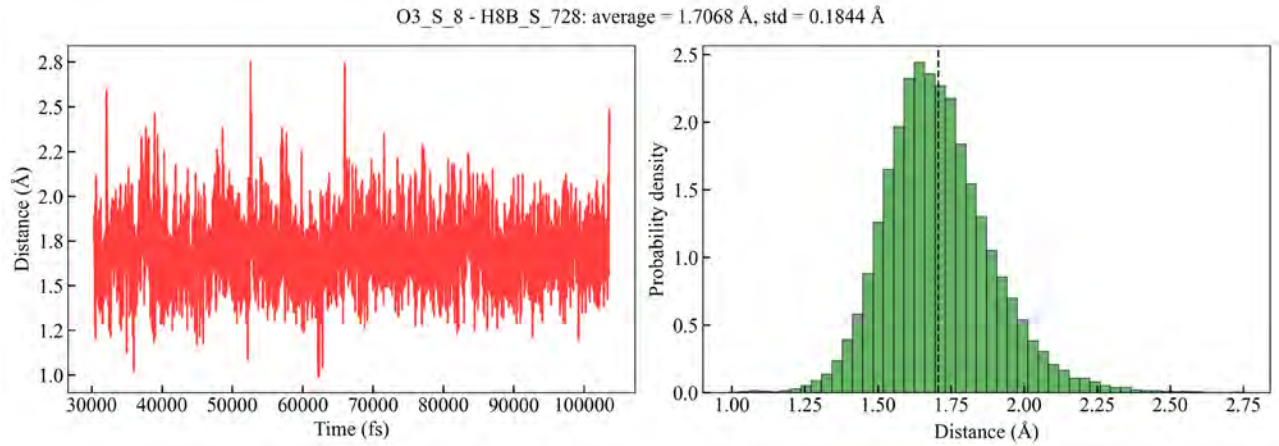
O3_S_72 - H8B_S_516

Average distance = 1.6856 Å; standard deviation = 0.1826 Å; number of points = 73284



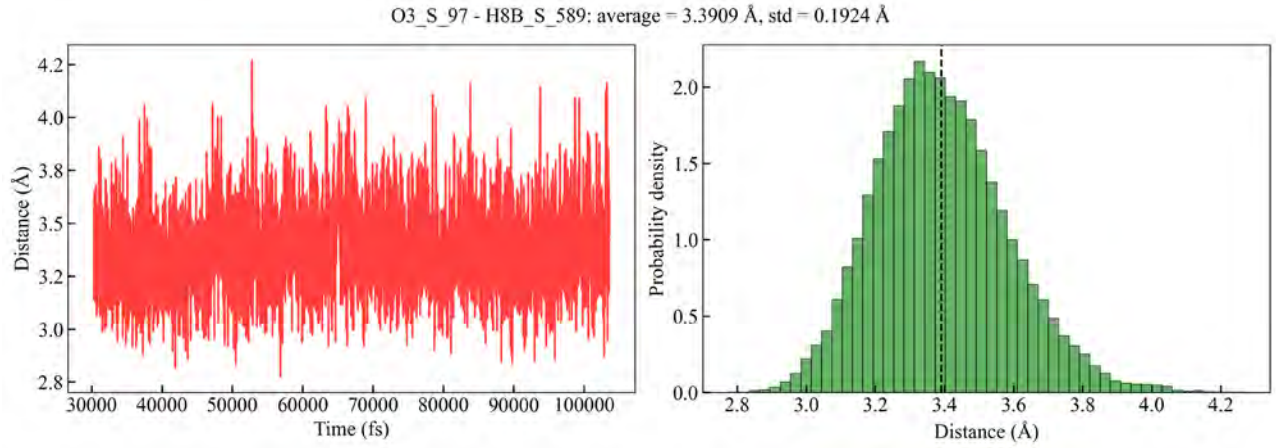
O3_S_8 - H8B_S_728

Average distance = 1.7068 Å; standard deviation = 0.1844 Å; number of points = 73284



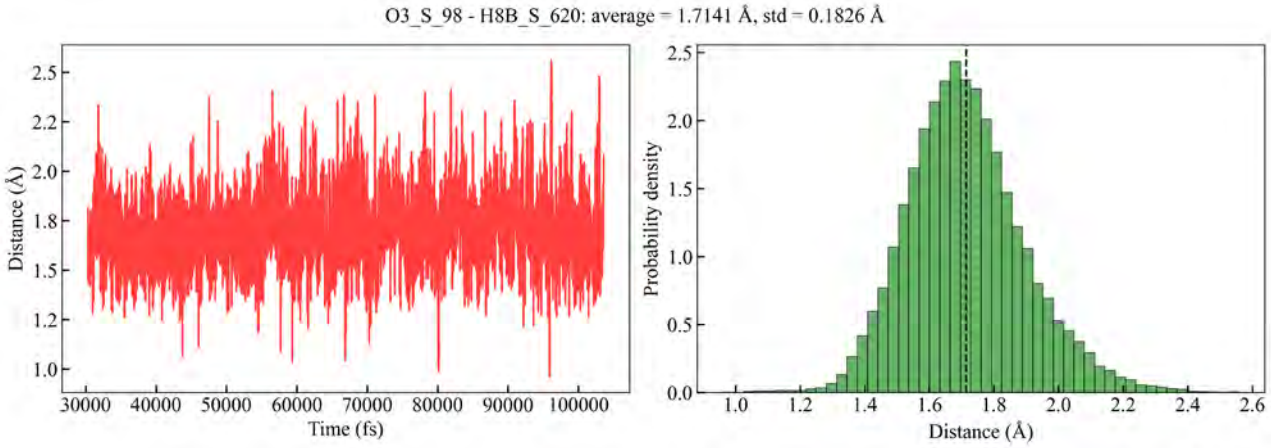
O3_S_97 - H8B_S_589

Average distance = 3.3909 Å; standard deviation = 0.1924 Å; number of points = 73284



O3_S_98 - H8B_S_620

Average distance = 1.7141 Å; standard deviation = 0.1826 Å; number of points = 73284


O3_S_98 - H8B_S_620: average = 1.7141 Å, std = 0.1826 Å
Distance (Å)
Time (fs)
Probability density
Distance (Å)