Supporting Information

Nano-bio interaction between human immunoglobulin G and nontoxic, near-infrared emitting water-borne silicon quantum dot micelles

Shanmugavel Chinnathambi^{1,2}*, Naoto Shirahata^{3,4, 5,}*, Mahima Kumar¹,

Subramani Karthikeyan⁶, Katsuhiko Abe¹, Vaijayanthi Thangavel¹ and Ganesh N. Pandian^{1*}

¹Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Institute for Advanced Study, Kyoto University, Kyoto 606-8501, Japan

²International Center for Young Scientists, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

³Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo 060-0814, Japan

⁴International Center for Materials Nanoarchitectonics (WPI-MANA), NIMS, Namiki, Tsukuba 305-0044, Japan

⁵Department of Physics, Chuo University, 1-13-27 Kasuga, Bunkyo, Tokyo 112-8551, Japan

⁶Centre for Healthcare Advancement, Innovation and Research, Vellore Institute of Technology, Chennai, 600 127, India

C.A. E-mail: CHINNATHAMBI.Shanmugavel.8s@kyoto-u.ac.jp: SHIRAHATA.Naoto@ nims.go.jp; NAMASIVAYAM.ganeshpandian.5z@kyoto-u.ac.jp

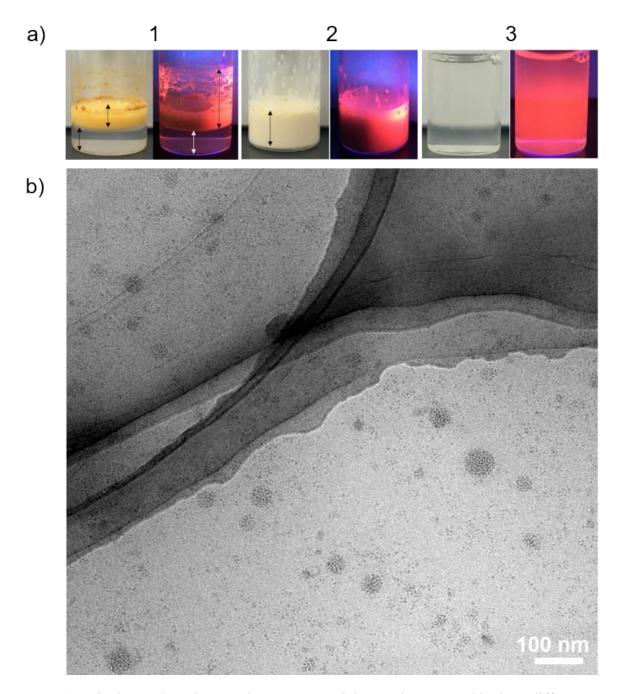


Figure S1. a). It is shown that SiQD-De/F127 nanoparticles can be prepared in three different ways. For each step, three sets of photos are shot using room lighting and UV light. Eight mL of Milli-Q water and 24 microliters of SiQD-De toluene were added to the glass bottle. Arrows on a left-pair image represent the amounts of toluene and water. b). An image of a SiQD-De/F127 nanoparticle TEM image. A Pluronic F127 molecule surrounds the constructed SiQDs-De cores, which range in diameter from 30 to 80 nm and are contrasted in the image.

The left-pair image was captured following toluene evaporation in the fume hood. A layer of SiQD-De (a yellow-colored band) has been left on top of the water, as is evident in the image on the left. SiQD-De is still present in small amounts inside the bottle's wall. The yellow-colored band in the right image of the pair's red-fluorescence confirms that it is made up of SiQD-De.

The middle-pair was obtained by shaking the glass bottle shown in the left-pair. The left image shows that the Si-De/F127 water solution is a milky color. The SiQD-De/F127 is well dispersed in the milky-colored solution, as seen in the right image.

The middle pair was diluted with Milli-Q water to produce the **right pair**. The left image shows a clear, colorless water solution. The successful encapsulation of SiQD-De with the Pluronic F127 molecule can be seen in the right image, which demonstrates that SiQD-De/F127 nanoparticles are highly dispersed in water.

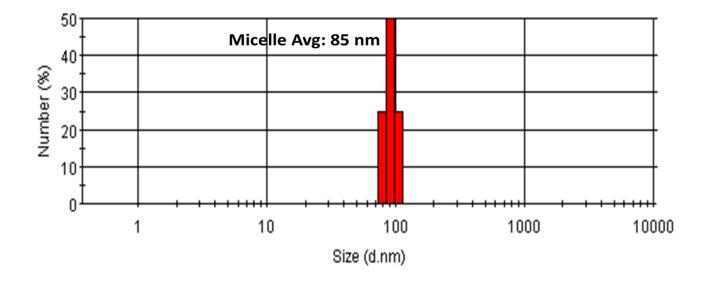


Figure S2. UV-visible absorption spectra, PL excitation (PLE) spectra, and PL spectra of two SiQD-De/F127 samples with different QD sizes.

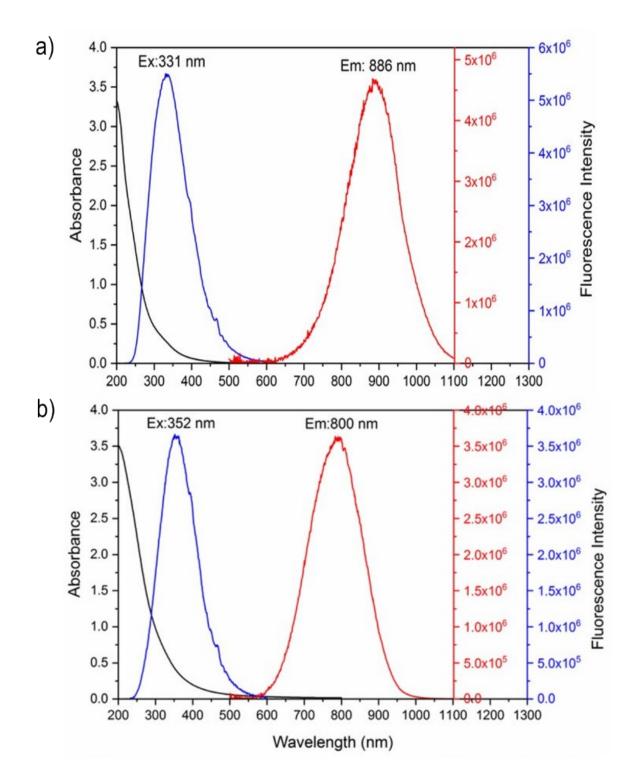


Figure S3. UV-visible absorption spectra, PL excitation (PLE) spectra, and PL spectra of two SiQD-De/F127 samples with different QD sizes. The diameters estimated from Scherrer broadening analysis are 4.8 nm, 4.0 nm. Both PLE spectra centered at 331, 352 nm, and their corresponding PL spectra centered at 886 and 800 nm spectrum are demonstrated for four SiQDs/F127 samples.

Table S1. The induced fit docking simulation produced 10 distinct binding poses. The gliding energy and docking score were used to determine the best positions.

100	A	В	С	D		E		F			G	H I	J	K	(M N	
1 5	tars	Title	Entry ID	Entry Nam	Date Added		Dat	e Modified		PDB	TITLE PDB	ID PDB C	LASS PDB	DEPO PDB f	orma PDB	R PDB	Rfree PDB R	RESOL PD
2		F127	1	F127.1		1/23/2023	10:57	1,	/23/2023 1	10:57 THE	СОМР 6КА	7 IMMU	JNE § 21-Ju	n-19	3.3	0.257	0.333	3 X-
		F127	2	F127.1	:	1/23/2023	10:57	1,	/23/2023 1	10:57 THE	сомр 6ка	7 IMMU	JNE S 21-Ju	n-19	3.3	0.257	0.333	3 X-I
4		F127	3	F127.1	:	1/23/2023	10:57	1,	/23/2023 1	10:57 THE	СОМР 6КА	7 IMMU	JNE S 21-Ju	n-19	3.3	0.257	0.333	3 X-
;		F127	4	F127.1		1/23/2023	10:57	1,	/23/2023 1	10:57 THE	СОМР 6КА	7 IMMU	JNE S 21-Ju	n-19	3.3	0.257	0.333	3 X-
5		F127	5	F127.1	:	1/23/2023	10:57	1,	/23/2023 1	10:57 THE	СОМР 6КА	7 IMMU	JNE § 21-Ju	n-19	3.3	0.257	0.333	3 X-
7		F127	6	F127.1		1/23/2023	10:57	1	/23/2023 1	10:57 THE	СОМР 6КА	7 IMMU	JNE § 21-Ju	n-19	3.3	0.257	0.333	3 X-
3		F127	7	F127.1		1/23/2023				10:57 THE			JNE § 21-Ju	n-19	3.3	0.257	0.333	3 X-
9		F127		F127.1		1/23/2023				10:57 THE			JNE S 21-Ju				0.333	3 X-
0		F127		F127.1		1/23/2023				10:57 THE			JNE S 21-Ju				0.333	3 X-
1		F127		F127.1		1/23/2023				10:57 THE			JNE S 21-Ju				0.333	3 X-
2			10			1, 20, 2020	10107	-,	20/2020		contra ora i				010			U A
	0	Р	Q	R	S	т	U	V	W	Х	Y	Z	AA	AB	AC	AD	AE	AF
F							-	entry id ba			-	d treated me						
-	-RAY DIFF				C:\Users\9		1		TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26174.		
	-RAY DIFF				C:\Users\9		2		TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26167.		
	-RAY DIFF				C:\Users\9		3		TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26167.		
							4		TRUE					TRUE				
	-RAY DIFF				C:\Users\9 C:\Users\9		4		TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		D -26154. D -26157.		
1	-RAY DIFF								TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26157. 0 -26162.		
					C:\Users\9		6											
	-RAY DIFF				C:\Users\9		7		TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26168.		
	-RAY DIFF				C:\Users\9		8		TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26152.		
0 >	-RAY DIFF				C:\Users\9		9		TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26160.		
		03	ABCD	1 000000	C·\llcorc\Q	InducedFit	10	4	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE		0 -26161.	4 4206.51	-4270
	-RAY DIFF AG	AH	AI	AJ	AK	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX
ı F	AG rime Solv	AH Prime Lipo	Al Prime Ener	AJ Prime Hbo	AK Prime Pack	AL Prime Self(r	AM ran protas	AN Potential El	AO RMS Deriv	AP Max Deriv	AQ Stretch Er	AR Bend Eneri	AS LJ-14 Eneri	AT El-14 Enerį	AU Van der W	AV Electrosta	AW t Dihedral Er	AX ran imp
2 1 F 2	AG rime Solv -4521.26	AH Prime Lipo -4745.06	Al Prime Ener -36428.5	AJ Prime Hbo -304.493	AK Prime Pack -24.449	AL Prime Self(1 -600.213	AM ran protas TRUE	AN Potential E 7.906	AO RMS Deriv 0	AP Max Deriv 0	AQ Stretch Er 0.175	AR Bend Eneri 6 0.996	AS LJ-14 Ener 1.981	AT El-14 Enerį 38.747	AU Van der W -1.188	AV Electrosta -33.798	AW t Dihedral Eı 0.992	AX ran imp TRUE
2 I F 2 3	AG rime Solv -4521.26 -4530.07	AH Prime Lipo -4745.06 -4743.68	Al Prime Ener -36428.5 -36438.6	AJ Prime Hbo -304.493 -303.735	AK Prime Pack -24.449 -24.449	AL Prime Self(1 -600.213 -600.222	AM ran protas TRUE TRUE	AN Potential E 7.906 7.906	AO RMS Deriv 0 0	AP Max Deriv 0 0	AQ Stretch Er 0.175 0.175	AR Bend Ener 0.996 0.996	AS LJ-14 Ener 1.981 1.981	AT El-14 Ener≨ 38.747 38.747	AU Van der W -1.188 -1.188	AV Electrosta -33.798 -33.798	AW t Dihedral Er 0.992 0.992	AX ran imp TRUE TRUE
2 F	AG rime Solv -4521.26 -4530.07 -4532.33	AH Prime Lipo -4745.06 -4743.68 -4748.42	Al Prime Ener -36428.5 -36438.6 -36432.8	AJ Prime Hbo -304.493 -303.735 -303.029	AK Prime Pack -24.449 -24.449 -24.449	AL Prime Self(r -600.213 -600.222 -600.337	AM ran protas TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906	AO RMS Deriv 0 0 0	AP Max Deriv 0 0 0	AQ Stretch Er 0.175 0.175	AR Bend Eneri 0.996 0.996 0.996	AS LJ-14 Eneri 1.981 1.981 1.981	AT El-14 Eners 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188	AV Electrosta -33.798 -33.798	AW t Dihedral Ei 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE
P F 2 3 4 5	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45	Al Prime Ener -36428.5 -36438.6 -36432.8 -36432.8	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939	AK Prime Pack -24.449 -24.449 -24.449 -24.449	AL Prime Self(r -600.213 -600.222 -600.337 -600.146	AM ran protas: TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906	AO RMS Deriv 0 0 0 0	AP Max Deriv 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996	AS LJ-14 Ener ₁ 1.981 1.981 1.981 1.981	AT El-14 Ener 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.798 -33.798 -33.798	AW t Dihedral Ei 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE
2 1 F 2 33 4 5 5 5	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4748	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36429.8	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(r -600.213 -600.222 -600.337 -600.146 -600.265	AM ran protas: TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv. 0 0 0 0 0	AP Max Deriv 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996	AS LJ-14 Ener 1.981 1.981 1.981 1.981 1.981	AT El-14 Ener 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188	AV 2 Electrosta -33.798 -33.798 -33.798 -33.798 -33.798	AW t Dihedral Er 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE
P F F F F	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4748 -4745.54	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36429.8 -36427.4	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.129	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(r -600.213 -600.222 -600.337 -600.146 -600.265 -600.358	AM ran protas: TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv. 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS LJ-14 Ener 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Ener 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798	AW t Dihedral Ei 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE
1 F 2 3 3 4 5 5 7 3	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4525.2	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4746.54 -4745.54 -4746.76	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36429.8 -36429.4 -36429.5	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.129 -304.662	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(r -600.213 -600.222 -600.337 -600.146 -600.265 -600.358 -600.293	AM ran protas: TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Enerr 5 0.996 5 0.996 5 0.996 5 0.996 5 0.996 5 0.996	AS LJ-14 Ener 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Ener 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV 2 Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798	AW t Dihedral Et 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE
1 F 2 3 3 4 5 5 77 3 39 9	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4534.44	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4748 -4745.54 -4745.54 -4746.76 -4743.32	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36429.8 -36429.5 -36429.5 -36420	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.129 -304.662 -302.873	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(-600.213 -600.222 -600.337 -600.146 -600.265 -600.358 -600.293 -600.378	AM ran protass TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ \$tretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS UJ-14 Ener ₁ 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Ener ₁ 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798	AW tDihedral Et 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE
F 2 3 4 5 5 7 7 3 9 0	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4524.14	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4748 -4745.54 -4745.54 -4746.76 -4743.32 -4740.87	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36430.3 -36429.8 -36427.4 -36429.5 -36420 -36417.1	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.129 -304.662 -302.873 -303.618	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(1 -600.213 -600.222 -600.337 -600.146 -600.265 -600.358 -600.293 -600.378 -600.323	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential El 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS LJ-14 Ener, 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Enerç 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799	AW t Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
I F 2 3 3 - 5 - 7 - 33 - 9 0 11	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4524.14	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4748 -4745.54 -4745.54 -4746.76 -4743.32	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36429.8 -36429.5 -36429.5 -36420	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.129 -304.662 -302.873	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(-600.213 -600.222 -600.337 -600.146 -600.265 -600.358 -600.293 -600.378	AM ran protass TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS UJ-14 Ener ₁ 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Ener ₁ 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799	AW t Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
F 5 6 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4524.14	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4748 -4745.54 -4745.54 -4746.76 -4743.32 -4740.87	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36430.3 -36429.8 -36427.4 -36429.5 -36420 -36417.1	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.129 -304.662 -302.873 -303.618	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(1 -600.213 -600.222 -600.337 -600.146 -600.265 -600.358 -600.293 -600.378 -600.323	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential El 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS LJ-14 Ener, 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Enerç 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799	AW t Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
F 5 6 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4524.14	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4748 -4745.54 -4745.54 -4746.76 -4743.32 -4740.87	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36430.3 -36429.8 -36427.4 -36429.5 -36420 -36417.1	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.129 -304.662 -302.873 -303.618	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(1 -600.213 -600.222 -600.337 -600.146 -600.265 -600.358 -600.293 -600.378 -600.323	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential El 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS LJ-14 Ener, 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Enerç 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799 -33.799	AW t Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
F 5 6 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	AG rime Solv 4521.26 4530.07 4532.33 -4532.38 -4527.38 -4525.2 4519.84 4534.44 4526.11 -4522.95	AH Prime Lipo -4743.68 -4743.68 -4748.42 -4746.45 -4745.54 -4745.54 -4746.76 -4743.32 -4740.87 -4742.84	Al Prime Ener -36428.5 -36432.8 -36430.3 -36429.8 -36427.4 -36429.5 -36420 -36417.1 -36420 BA	AJ Prime Hbo -304.493 -303.735 -303.029 -303.029 -303.499 -304.622 -304.622 -302.873 -303.618 -304.326	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(-600.213 -600.222 -600.337 -600.46 -600.265 -600.358 -600.358 -600.378 -600.378 -600.323 -600.292	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS U-14 Ener, 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 BM	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798	AW Dihedral Ei 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE
P F F F F F F F F F F F F F F F F F F F	AG rime Solv 4521.26 4530.07 4532.33 -4532.38 -4527.38 -4525.2 4519.84 4534.44 4526.11 -4522.95	AH Prime Lipo -4743.68 -4743.68 -4748.42 -4746.45 -4745.54 -4745.54 -4746.76 -4743.32 -4740.87 -4742.84	Al Prime Ener -36428.5 -36432.8 -36430.3 -36429.8 -36427.4 -36429.5 -36420 -36417.1 -36420 BA	AJ Prime Hbo -304.493 -303.735 -303.029 -303.029 -303.499 -304.622 -304.622 -302.873 -303.618 -304.326	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449	AL Prime Self(-600.213 -600.222 -600.337 -600.46 -600.265 -600.358 -600.358 -600.378 -600.378 -600.323 -600.292	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ (Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Ener ₁ 5 0.996 5 0.996 5 0.996 5 0.996 5 0.996 5 0.996 5 0.996 5 0.996 5 0.996	AS U-14 Ener, 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 BM	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798	AW Dihedral Ei 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
F 	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4534.44 -4534.44 -4534.44 -4524.95 AY rid versio	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4745.54 -4745.54 -4746.76 -4743.82 -4740.87 -4742.84 AZ gridbox xcc	Al Prime Ener -36428.5 -36438.6 -36430.3 -36420.8 -36427.4 -36427.4 -36427.4 -36427.4 -36427.4 -36427.4 -36420 -36420 -36417.1 -36420	A) Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -304.662 -304.662 -302.873 -303.618 -304.326 BB gridbox zcq	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 gridbox xrag	AL Prime Self(-600.213 -600.222 -600.337 -600.146 -600.265 -600.358 -600.358 -600.323 -600.323 -600.292	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 8.900 7.900	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ (Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Ener ₁ 6 0.996 6 0.996 6 0.996 6 0.996 6 0.996 6 0.996 6 0.996 6 0.996 6 0.996 9 0	AS U-14 Ener, 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Enerr 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 BN lide ligancg	AW Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE BP de gsco 1.513
	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4524.45 -4524.95 -4522.95	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4746.45 -4746.76 -4743.32 -4740.87 -4742.84 AZ gridbox xcr 15.417	Al Prime Ener -36428.5 -36438.6 -36432.8 -36430.3 -36429.5 -36429.5 -36420 -36417.1 -364200 BA gridbox ycc 29.159	A) Prime Hbo -304.493 -303.735 -303.299 -303.499 -303.129 -304.662 -302.873 -304.326 solution -304.326 BB gridbox zc(42.816	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 gridbox xrcg 21.766	AL Prime Self(-600.213 -600.222 -600.327 -600.358 -600.293 -600.323 -600.292 -600.292	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 8 8 9 9 9 9 9 9 10	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175	AR Bend Enery 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996	AS U-14 Ener; 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Ener(38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.1888 -1.1888 -1.1888 -1.1888 -1.1888 -1.1888 -1.1888 -1.	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 BN lide ligang 0.306	AW Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE BP de gsco 1.513 2.071
	AG rime Solv 4521.26 4530.07 4523.38 4525.2 4519.84 4526.11 4522.95 AY rid versio 66013 66013	AH Prime Lipo -4745.06 -4743.68 -4748.45 -4746.76 -4748.32 -4746.76 -4743.32 -4740.87 -4742.84 gridbox xcr 15.417 15.389	Al Prime Ener -36428.5 -36438.6 -36430.3 -36429.8 -36429.5 -36429.5 -36420. -36417.1 -364200 BA gridbox ycr 29.159 30.127	AJ Prime Hbo -304.493 -303.735 -303.299 -303.129 -304.662 -302.873 -303.618 -304.326 BB gridbox zcq 42.816 40.406	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 gridbox xrag gridbox xrag 21.766 21.311	AL Prime Self(-600.213 -600.222 -600.372 -600.146 -600.293 -600.293 -600.378 -600.292 BD g21.766 21.311	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 8 F rridbox lig gr 10	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175	AR Bend Energ 0.996	AS LJ-14 Ener, 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981 1.981	AT El-14 Energ 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 del ligan(g 0.138 0.188	AV (Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 BN BN BN BN BN BN BN BN BN BN BN BN BN	AW Dihedral Er 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4519.84 -4526.11 -4522.95 AY rid versio 66013 66013	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4748.42 -4745.54 -4745.54 -4745.54 -4743.32 -4740.87 -4742.84 AZ gridbox xci 15.417 15.389 16.448	Al Prime Ener -36428.5 -36432.8 -36432.8 -36432.8 -36429.8 -36427.4 -36429.5 -36420 -36417.1 -36420 BA gridbox ycr 29.159 30.127 28.055	AJ Prime Hbo -304.493 -303.735 -303.029 -303.029 -303.499 -304.622 -302.873 -304.622 -304.622 -304.326 BB gridbox zc(42.816 40.406 44.112	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 BC gridbox xrs g 21.766 21.311 21.818	AL Prime Self(-600.213 -600.213 -600.337 -600.337 -600.358 -600.358 -600.358 -600.323 -600.323 -600.292 BD pridbox yrr g 21.766 21.311 21.818	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 8 8 9 9 9 9 9 10 10 10	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 TRUE TRUE TRUE TRUE	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 1.996 1.996 1.996	AS U-14 Ener, 1.981	AT El-14 Energ 38.747 37.747 3	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 0.138 0.138 0.138 0.171	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 BN lide ligang 0.306 0.419 0.381	AW Dihedral Ei 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
P P P P P P P P P P P P P P	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4534.44 -4526.11 -4522.95 AY rid versio 66013 66013 66013 66013	AH Prime Lipo -4743.68 -4743.84 -4748.42 -4746.45 -47484746.76 -4743.32 -4740.87 -4743.32 -4740.87 -4742.84 AZ gridbox xcc 15.417 15.389 16.448 15.06 16.395	Al Prime Ener -36428.5 -36436.8 -36430.3 -36420.8 -36427.4 -36420.5 -36420 -364210 -364210 -36420 BA gridbox yct 29.159 30.127 28.055 28.828 28.778	A) Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -304.662 -304.662 -302.873 -303.618 -304.326 BB gridbox zc(g 42.816 40.406 44.112 43.04	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.149 -21.766 21.766 21.311 21.818 22.049 21.561	AL Prime Self(-600.213 -600.222 -600.337 -600.46 -600.358 -600.358 -600.323 -600.323 -600.292 BD rridbox yr; g 21.766 21.311 21.818 21.818 21.849 21.561	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 0.00 1.00 100 100 100 100	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ (Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 TRUE TRUE TRUE TRUE TRUE TRUE	AR Bend Enerj 0.996 0.997	AS U-14 Ener, 1.981 1.1 1.1 1.1 1.1 1.1 1.1 1.1 1	AT 88.747 38	AU Van der W -1.1888 -1.1888 -1.1888 -1.1888 -1.1888 -1.1888 -1.1888 -1.	AV Electrosta -33.798	AW Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.955 0.61 0.558	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
P F 2 3 4 5 5 7 7 3 9 0 1 2 3 9 0 1 2 3 9 0 1 2 3 9 0 1 2 3 9 0 0 1 2 3 9 0 0 1 1 2 3 9 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1	AG rime Solv -4521.26 -4530.33 -4536.86 -4527.38 -4525.2 -4519.84 -4524.45 -4524.45 -4522.95 AY rid versio 66013 66013 66013 66013 66013	AH Prime Lipo -4745.06 -4743.68 -4748.2 -4746.45 -4746.76 -4743.32 -4740.87 -4742.84 gridbox xcc 15.417 15.389 16.488 15.06 16.395 16.857	Al Prime Ener -36428.5 -36432.8 -36430.3 -36429.8 -36429.5 -36420 -36417.1 -364200 -36417.1 -364200 BA gridbox ycc 29.159 30.127 28.055 28.828 28.878 29.056	A) Prime Hbo -304.493 -303.735 -303.299 -303.499 -303.129 -304.662 -302.873 -303.618 -304.326 gridbox zcc 42.816 40.406 44.104 43.04 41.041 42.037	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.419 -24.429 -24.551 -21.766 -21.311 -21.551 -21.551 -21.561	AL Prime Self(-600.213 -600.222 -600.323 -600.358 -600.293 -600.323 -600.323 -600.292 -800.292 -800.292 -800.292 -1.311 21.818 22.049 21.561 21.863	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 0.00 0.00 10 10 10	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ (Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AR Bend Energ 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 0.996 1.0996 1.0996 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.00000 1.00000 1.00000 1.00000 1.00000 1.00000000	AS U-14 Ener; 1.981 1.98	AT El-14 Energ 38.747 38.74	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 0.138 0.138 0.138 0.188 0.171 0.165	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 BN lide ligancg 0.306 0.419 0.381 0.388 0.388 0.434	AW Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.955 0.61 0.554 0.553 0.631	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
I F 2 I 3 I 4 I 5 I 7 I 8 I 2 I 8 I 1 I 2 I 8 I 1 I 2 I 1 I 2 I 3 I 1 I 2 I 3 I	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4526.11 -4522.95 AY rid versio 66013 66013 66013 66013 66013 66013	AH Prime Lipo -4745.06 -4743.08 -4748.42 -4746.45 -4745.76 -4748.32 -4740.87 -4743.32 -4740.87 -4742.84 AZ gridbox xct 15.417 15.389 16.448 15.06 16.395 16.455 16.357	Al Prime Ener -36428.5 -36432.8 -36432.8 -36429.8 -36429.8 -36429.4 -36429.4 -36429.4 -36420 -36417.1 -36420 BA gridbox ycc 29.159 30.127 28.055 28.828 28.778 29.056 28.884	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.499 -304.662 -302.873 -303.618 -304.326 BB gridbox zccc 42.816 40.406 44.112 43.04 41.041 42.037	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.349 -24.349 -21.766 21.766 21.761 21.818 22.049 21.561 21.863 21.863	AL Prime Self (1 -600.213 -600.233 -600.337 -600.337 -600.378 -600.378 -600.323 -600.292 BD pridbox yrr gr 21.766 21.761 21.818 22.049 21.863 22.583	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 0.00 0.00 10 10 10 10 10 10	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175	AR Bend Energi 0.996 0.997 0.996 0.99	AS U-14 Enery 1.981	AT EI-14 Energ 38.747 39.747 3	AU Van der W -1.1888 -1.1888 -1.1888 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.798	AW Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.955 0.631 0.554 0.631 0.553 0.631 0.574	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
I F 2 3 3 - 5 - 7 - 3 - 0 - 1 2 1 2 3 - 4 - 5 - 6 - 7 - 3 - -	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4519.84 -4526.11 -4522.95 AY rid versio 66013 66013 66013 66013 66013 66013	AH Prime Lipo -4745.06 -4743.68 -4748.42 -4748.42 -4745.54 -4745.54 -4745.54 -4742.84 AZ gridbox xci 15.477 15.387 16.395 16.357 15.577	Al Prime Ener -36428.5 -36432.8 -36432.8 -36432.8 -36429.8 -36427.4 -36429.5 -36420 -36417.1 -36420 BA gridbox ycr 29.159 30.127 28.055 28.828 28.778 29.056 28.884 28.806	AJ Prime Hbo -304.493 -303.735 -303.029 -303.029 -303.619 -304.622 -302.873 -304.622 -304.622 -304.326 BB gridbox 2ct 42.816 42.816 42.816 44.112 43.04 41.1041 42.037 41.205 42.999	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -21.51 21.818 22.049 21.561 21.863 22.563 21.561 21.863 22.583 22.096	AL Prime Self(-600.213 -600.223 -600.337 -600.265 -600.358 -600.358 -600.323 -600.323 -600.323 -600.292 BD ridbox yrr g 21.766 21.311 21.818 22.049 21.861 21.861 21.863 22.583 22.595	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 0.00 0.00 10 10 10 10 10 10 10	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175	AR Bend Energ 0.996 0.096 0.096 0.096 0.096 0.096 0.096 0.096 0.096 0.096 0.096 0.096 0.0000 0.00000 0.00000 0.0000 0.00000 0.00000 0.0000 0.00000000	AS U-14 Enery 1.981	AT El-14 Energ 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 38.747 1.879 1.879 1.879 1.879 2.145 2.525 2.204	AU Van der W -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 -1.188 0.138 0.138 0.138 0.171 0.16 0.171 0.195 0.23 0.22	AV Electrosta -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 -33.798 0.349 0.301 0.356 0.381 0.356 0.381 0.356 0.381 0.356	AW Dihedral Ei 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.512 0.553 0.651 0.553 0.631 0.743	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
1 F 2 3 3 4 5 5 6 7 3 9 0 1 2 2	AG rime Solv -4521.26 -4530.07 -4532.33 -4536.86 -4527.38 -4525.2 -4519.84 -4526.11 -4522.95 AY rid versio 66013 66013 66013 66013 66013 66013	AH Prime Lipo -4745.06 -4743.08 -4748.42 -4746.45 -4748.42 -4745.76 -4748.32 -4740.87 -4742.84 AZ gridbox xci 15.417 15.389 16.448 15.06 16.395 16.455 15.317	Al Prime Ener -36428.5 -36432.8 -36432.8 -36429.8 -36429.8 -36429.4 -36429.4 -36429.4 -36420 -36417.1 -36420 BA gridbox ycc 29.159 30.127 28.055 28.828 28.778 29.056 28.884	AJ Prime Hbo -304.493 -303.735 -303.029 -302.939 -303.499 -303.499 -304.662 -302.873 -303.618 -304.326 BB gridbox zccc 42.816 40.406 44.112 43.04 41.041 42.037	AK Prime Pack -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.449 -24.349 -24.349 -21.766 21.766 21.761 21.818 22.049 21.561 21.863 21.863	AL Prime Self (1 -600.213 -600.233 -600.337 -600.337 -600.378 -600.378 -600.323 -600.292 BD pridbox yrr gr 21.766 21.761 21.818 22.049 21.863 22.583	AM ran protas TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AN Potential E 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 7.906 0.00 0.00 10 10 10 10 10 10	AO RMS Deriv. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AP Max Deriv 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	AQ Stretch Er 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 0.175 TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE	AR Bend Energi 0.996 0.997 0.996 0.99	AS U-14 Enery 1.981	AT EI-14 Energ 38.747 39.747 3	AU Van der W -1.1888 -1.1888 -1.1888 -1.188 -1.188 -1.188 -1.188 -1.188	AV Electrosta -33.798	AW Dihedral Er 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.992 0.955 0.631 0.554 0.631 0.553 0.631 0.574	AX ran imp TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE

BQ	BR	BS	BT	BU	BV	BW	BX	BY	BZ	CA	CB	CC	CD	CE	CF	CG	CH
glide lipo	glide hbon	glide meta	glide rewa	iglide evdw	glide ecoul	glide erotb	glide esite	glide emod	glide energ	glide einte	glide confr	glide poser	glide eff st	target tem	PDB CRYST	PDB CRYST	PDB CRYST
-0.699	-0.911	0	-2.25	-12.539	-12.713	7.907	C	-20.604	-25.252	4.02	181	278	0	298	59.926	107.42	171.35
-0.952	-0.29	0	-2.25	-14.226	-10.879	7.907	C	-18.808	-25.105	5.876	89	332	0	298	59.926	107.42	171.35
-1.33	-0.608	0	-2.25	-16.871	-6.608	7.907	C	-18.117	-23.479	5.309	68	310	0	298	59.926	107.42	171.35
-0.585	-0.585	0	-2.25	-8.438	-15.366	7.907	C	-19.064	-23.804	4.018	147	374	0	298	59.926	107.42	171.35
-0.806	-0.546	0	-2.25	-14.382	-11.371	7.907	C	-20.342	-25.753	4.897	51	283	0	298	59.926	107.42	171.35
-1.033	-0.575	0	-2.25	-15.091	-7.657	7.907	C	-18.817	-22.748	0.495	60	185	0	298	59.926	107.42	171.35
-0.858	0	0	-2.25	-15.895	-9.862	7.907	C	-18.203	-25.757	6.573	206	15	0	298	59.926	107.42	171.35
-1.045	-0.168	0	-2.25	-16.967	-9.27	7.907	C	-19.283	-26.237	6.971	109	145	0	298	59.926	107.42	171.35
-0.659	-0.553	0	-2.25	-13.967	-8.589	7.907	C	-16.691	-22.556	2.863	82	252	0	298	59.926	107.42	171.35
-0.332	-0.681	0	-2.25	-12.944	-8.912	7.907	0	-15.06	-21.856	4.697	105	171	0	298	59.926	107.42	171.35

CI	CJ	CK	CL	CM	CN
PDB CRYST	IFDScore				
90	90	90	8	P 21 21 21	-1819.91
90	90	90	8	P 21 21 21	-1819.86
90	90	90	8	P 21 21 21	-1819.76
90	90	90	8	P 21 21 21	-1819.76
90	90	90	8	P 21 21 21	-1819.61
90	90	90	8	P 21 21 21	-1819.23
90	90	90	8	P 21 21 21	-1818.95
90	90	90	8	P 21 21 21	-1818.8
90	90	90	8	P 21 21 21	-1818.4
90	90	90	8	P 21 21 21	-1818.34