

Supplementary materials

Table S1. The pKa values of molecular dynamics clustering conformation of each representative conformation.

State	E68	D234	retinal
<i>Gt</i> ACR1- <i>trans</i> (E68p-D234dp)	10.35	5.93	11.23
	10.06	6.07	12.34
	7.95	4.91	10.43
<i>Gt</i> ACR1- <i>cis</i> (E68p-D234dp)	9.11	4.38	11.54
	8.58	3.95	11.37
	9.32	2.58	10.99
L ₁ '-like (E68p-D234dp)	9.01	6.76	13.01
	8.96	6.21	12.41
	10.01	7.06	11.03
L ₁ -like (E68dp-D234p)	6.23	7.02	11.72
	2.38	7.56	10.87
	5.28	6.78	11.63
L ₂ -like (E68dp-D234dp)	6.52	5.14	10.09
	7.17	3.22	11.68
	2.7	4.66	9.64

Table S2 Atom type definition, charges and connectivity for retinal.

Atom name	Atom type	charge
C1	CG301	0.00
C2	CG321	-0.18
H21	HGA2	0.09
H22	HGA2	0.09
C3	CG321	-0.18
H31	HGA2	0.09
H32	HGA2	0.09
C4	CG321	-0.18
H41	HGA2	0.09
H42	HGA2	0.09
C5	CG2DC2	0.00
C6	CG2DC2	0.00
C7	CG2DC1	-0.15
H71	HGA4	0.15
C8	CG2DC1	-0.15
H81	HGA4	0.15
C9	CG2DC2	0.00
C10	CG2DC2	-0.15
H101	HGA4	0.15
C11	CG2DC1	-0.15
H111	HGA4	0.15
C12	CG2DC1	-0.15
H121	HGA4	0.15
C13	CG2DC2	0.00
C14	CG2DC2	-0.15
H141	HGA4	0.15
C15	CG321	0.05
H151	HGA2	0.09
H152	HGA2	0.09
OR	OG311	-0.65
HR	HGP1	0.42
C16	CG331	-0.27
H161	HGA3	0.09
H162	HGA3	0.09
H163	HGA3	0.09
C17	CG331	-0.27
H171	HGA3	0.09
H172	HGA3	0.09
H173	HGA3	0.09
C18	CG331	-0.27
H181	HGA3	0.09

H182	HGA3	0.09
H183	HGA3	0.09
C19	CG331	-0.27
H191	HGA3	0.09
H192	HGA3	0.09
H193	HGA3	0.09
C20	CG331	-0.27
H201	HGA3	0.09
H202	HGA3	0.09
H203	HGA3	0.09

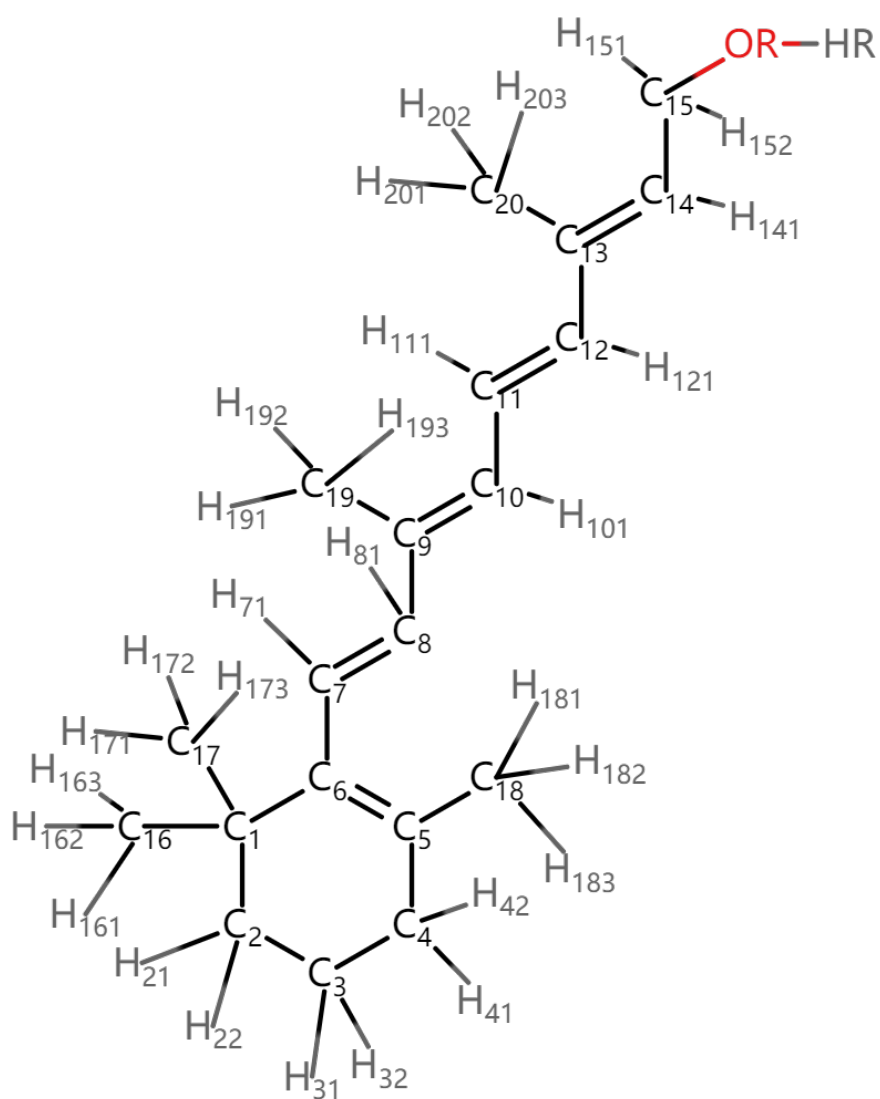


Table S3 Related bond parameters used in the force field for describing the C12-C13=C14-C15 groups in the protein. Units are presented in the brackets.

Atom type #1	Atom type #2	B ₀ [Å]	K _b [kJ·mol ⁻¹ ·Å ⁻²]
CG2DC1	CG2DC1	440.00	1.3400
CG2DC1	CG2DC2	300.00	1.4500
CG2DC1	HGA4	360.50	1.1000
CG2DC2	CG2DC2	440.00	1.3400
CG2DC2	CG331	383.00	1.5040
CG2DC2	CG321	365.00	1.5020
CG2DC2	HGA4	360.50	1.1000
CG321	HGA2	309.00	1.1110
CG321	OG311	428.00	1.4200
CG331	HGA3	322.00	1.1110

Table S4 Related angle parameters used in the force field for describing the C12-C13=C14-C15 groups in the protein. Units are presented in the brackets.

Atom type #1	Atom type #2	Atom type #3	θ ₀ [degree]	K _θ [kJ·mol ⁻¹ ·rad ⁻²]
CG2DC1	CG2DC1	HGA4	42.00	119.00
CG2DC1	CG2DC2	CG331	48.00	113.00
CG2DC2	CG2DC2	CG331	48.00	123.50
CG2DC2	CG331	HGA3	42.00	111.50
CG2DC2	CG2DC1	HGA4	42.00	118.00
CG2DC2	CG2DC2	CG321	48.00	123.50
HGA2	CG321	HGA2	35.50	109.00
HGA3	CG331	HGA3	35.50	108.40
OG311	CG321	HGA2	45.90	108.89

Table S5 Related dihedral parameters used in the force field for describing the C12-C13=C14-C15 groups in the protein. Units are presented in the brackets. n indicates multiplicity.

Atom type #1	Atom type #2	Atom type #3	Atom type #4	ψ ₀ [degree]	K _ψ [kJ·mol ⁻¹]	n
CG2DC1	CG2DC2	CG2DC2	CG321	180.00	0.5600	1
CG2DC1	CG2DC2	CG2DC2	CG321	180.00	7.00	2
CG2DC1	CG2DC2	CG331	HGA3	180.00	0.3000	3
CG2DC2	CG2DC2	CG321	HGA2	0.00	0.0300	3
CG2DC2	CG2DC2	CG321	OG311	180.00	1.9000	1
CG2DC2	CG2DC2	CG321	OG311	180.00	0.4000	2
CG2DC2	CG2DC2	CG321	OG311	180.00	0.6000	3
CG2DC2	CG321	OG311	HGP1	0.00	1.3000	1
CG2DC2	CG321	OG311	HGP1	0.00	0.7000	2
CG2DC2	CG321	OG311	HGP1	0.00	0.1400	3
HGA2	CG321	OG311	HGP1	0.00	0.1800	3
CG2DC2	CG2DC2	CG331	HGA3	180.00	0.3000	3

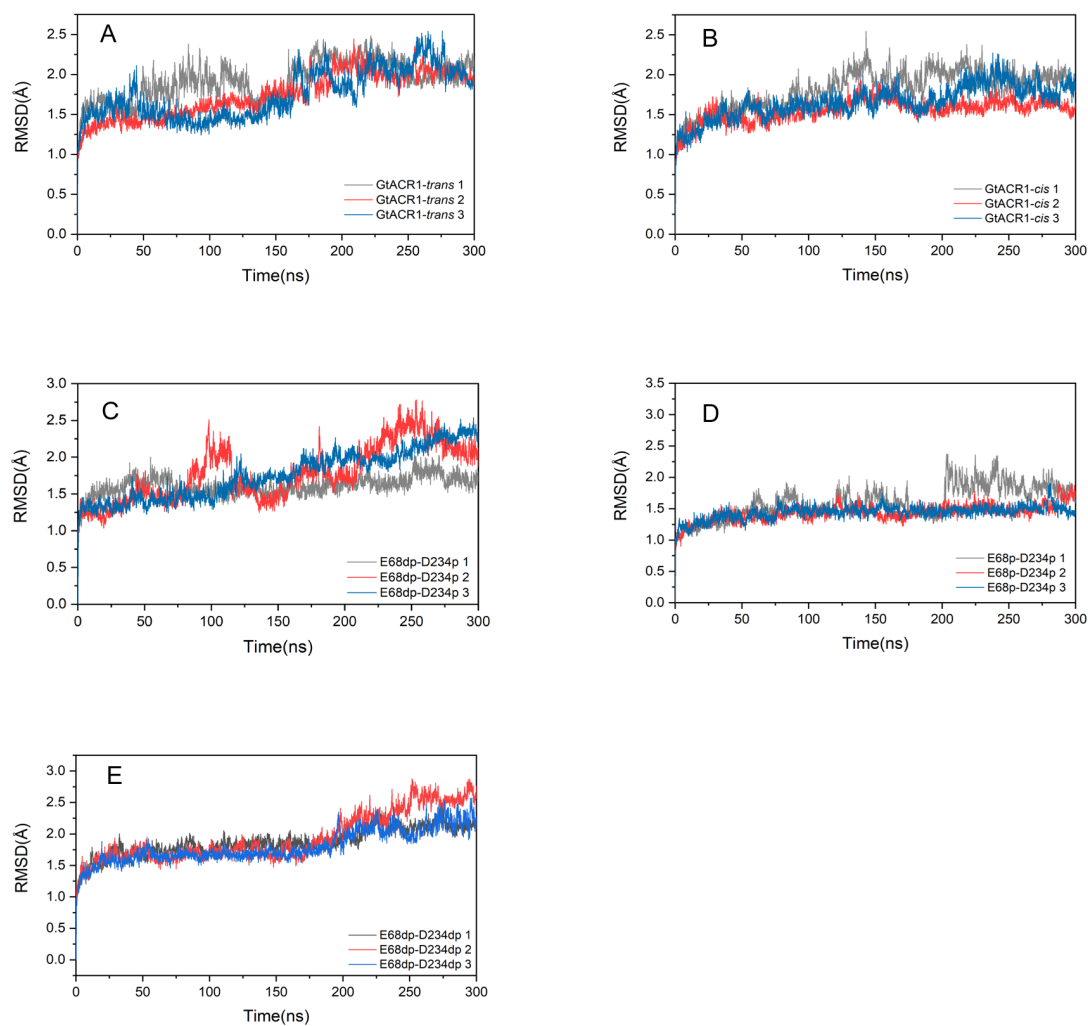


Figure S1. The time evolution of root mean square deviation (RMSD) of non-hydrogen atomic positions of (A) *Gt*ACR1-*trans*, (B) *Gt*ACR1-*cis*, (C) E68dp-D234dp, (D) E68p-D234dp and (E) E68dp-D234dp. Each state was performance three independent MD simulations.