Supplementary

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Table S1: Three types of hydrogen bonds between antibody and receptor

Type of interaction	Location	Antibody		Receptor		Dd-a*	No
		Residue	Atom	Residue	Atom		
(Main Chain-Main Chain)	HCDR3	ILE 101	N	THR 297	OXT	2.88	1
		TRP 103	N	THR 297	OXT	3.29	1
		GLY 105	O	Cys 287	N	1.63	1
		GLY 105	O	VAL 288	N	2.63	1
		GLU 106	O	CYS 296	N	3.12	1
		GLU 106	O	THR 297	N	1.95	1
(Main Chain-Side Chain)	HCDR2	SER 54	N	GLU 239	OE2	2.48	1
		GLY 55	O	HIS 205	NE2	3.46	1
		GLY 56	N	HIS 205	NE2	2.10	1
		GLY 56	O	HIS 205	ND1	1.02	1
		GLY 56	O	CYS 287	SG	2.18	1
		GLY 57	N	HIS 205	ND1	2.44	1
		GLY 57	N	HIS 205	NE2	1.27	1
		THR 58	N	MET 142	SD	3.39	1
		TYR 59	O	GLN 139	NE2	3.49	2
		TYR 59	OH	VAL 138	O	2.75	1
		TYR 59	N	GLN 139	OE1	3.48	1
		TYR 59	N	GLN 139	NE2	3.36	1
		TYR 59	OH	VAL 288	O	3.33	1
		TYR 60	N	GLN 139	NE2	1.97	1
		LYZ 65	NZ	ARG 140	O	2.49	1
	HCDR3	ASP 99	OD1	THR 297	O	2.67	2
		ASP 99	OD1	THR 297	OXT	3.03	2
		ASP 99	OD2	THR 297	O	3.46	2
		GLY 105	O	CYS 287	SG	2.59	1
		GLU 106	N	CYS 287	SG	1.94	1
		GLU 106	OE2	SER 295	O	1.71	2
		GLU 106	OE2	CYS 296	N	3.31	1
		GLU 106	O	CYS 296	SG	2.98	1
		GLU 106	N	CYS 296	SG	3.38	1
		PRO 107	O	CYS 296	SG	3.88	1
Side Chain-Side Chain	HCDR2	SER 52	OG	HIS 205	NE2	3.20	2
		SER 52	OG	GLU 239	OE1	2.66	1
		SER 54	OG	GLU 239	OE1	1.23	1
		SER 54	OG	GLU 239	OE2	1.28	1
		TYR 60	OH	LYS 121	NZ	2.77	1
	HCDR3	GLU 106	OE1	GLN 286	OE1	2.90	4
		GLU 106	OE1	CYS 287	SG	3.91	1
		GLU 106	OE2	CYS 287	SG	3.61	1
Total Hydrogen interactions							48

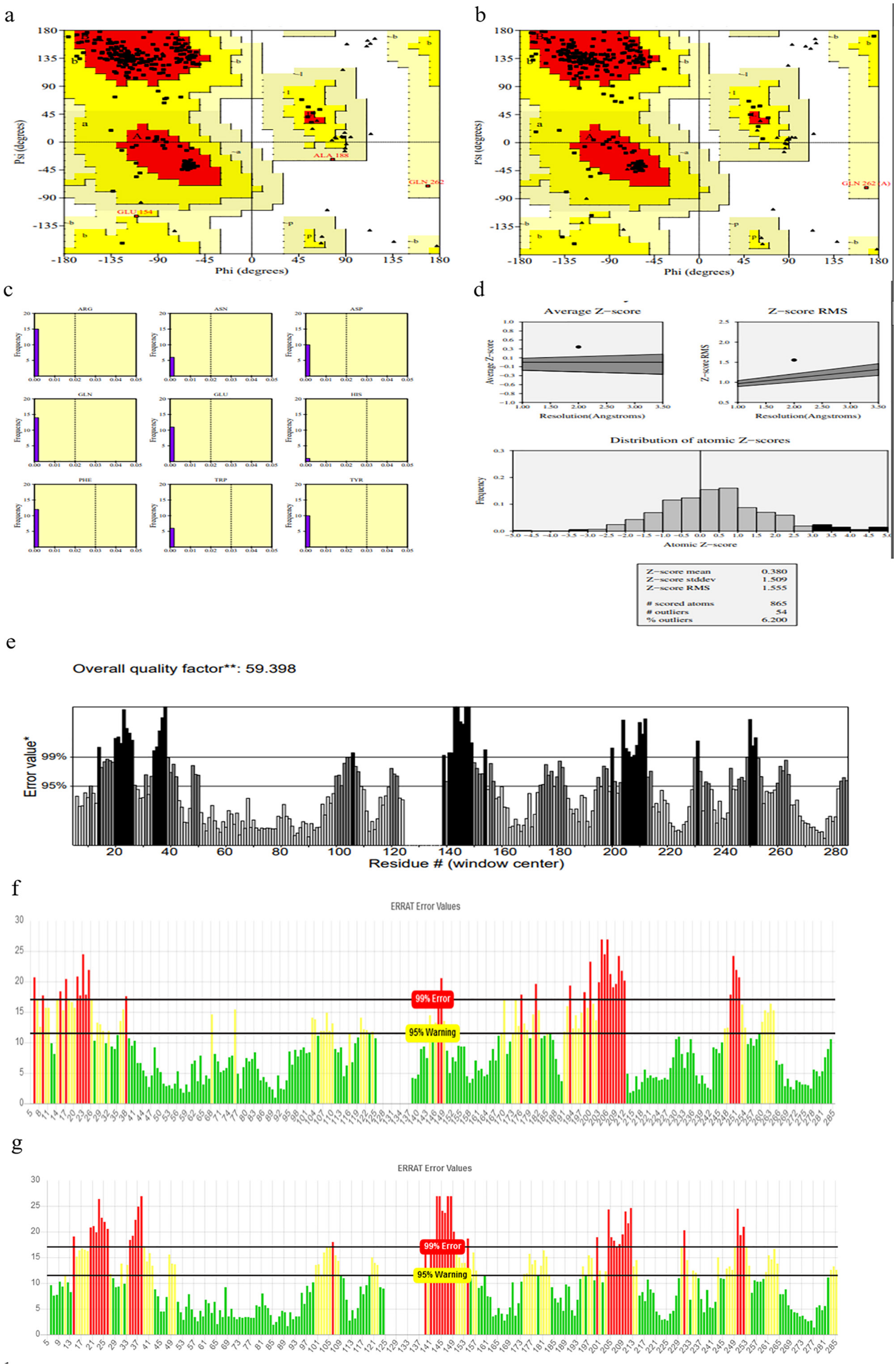
*Distance Between Donor and Acceptor, H: Heavy chain, L: Light chain, FR: Framework 2, CDR: complementary determining region.

Table S2: Hydrophobic and Ionic interactions between antibody and receptor

Type of interaction	Antibody		CD38 Receptor
	Location	Residue	Residue
Hydrophobic	HFR2	TRP 47	PRO 291
	HCDR2	TYR 59	VAL 138
		TYR 59	VAL 288
		TYR 59	PRO 291
	HCDR3	TRP 103	PHE 284
		TRP 103	ILE 278
		PHE 104	PHE 135
		PHE 104	TRP 241
		PHE 104	PHE 284
		PHE 104	VAL 288
		PRO 107	PRO 291
		PHE 109	PRO 291
Ionic	HCDR2	ASP 62	ARG 140
		LYS 65	ASP 141
	HCDR3	GLU 106	LYS 283

Table S3: Aromatic-Aromatic and Cation-Pi interactions between antibody and receptor

Type of interaction	Antibody		CD38 Receptor	Distance
	Location	Residue	Residue	
Aromatic-Aromatic	HCDR2	TYR 59	PHE 135	6.94
	HCDR3	PHE 104	PHE 135	5.90
		PHE 104	TRP 241	4.71
Cation-Pi	HCDR2	TYR 60	LYS 121	3.86


a
Psi (degrees)
Phi (degrees)
GLU 154
ALA 188
GLN 262
b
GLN 262 (A)
c
ARG
ASN
ASP
GLN
GLU
HIS
PHE
TRP
TYR
Frequency
d
Average Z−score
Z−score RMS
Resolution(Angstroms)
Distribution of atomic Z−scores
Atomic Z−score
Frequency
Z−score mean 0.380
Z−score stddev 1.509
Z−score RMS 1.555
scored atoms 865
outliers 54
% outliers 6.200
e
Overall quality factor**: 59.398
Error value*
99%
95%
Residue # (window center)
f
ERRAT Error Values
99% Error
95% Warning
g
ERRAT Error Values
99% Error
95% Warning

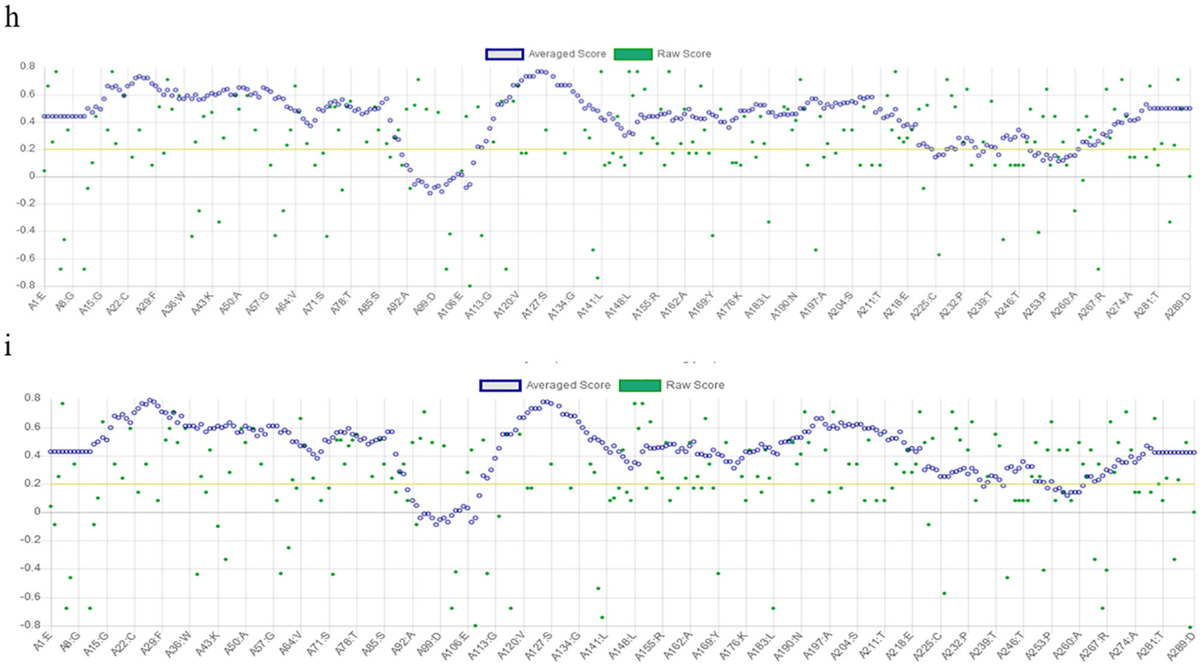


Figure S1: Ramachndran plot before refinement (a), Ramachndran plot after refinement (b), RMS distances from planarity (c), analysis of entire structure according to z score (d), ERRAT2 program analysis (e), ERRAT error value before refinement (f) ERRAT error value after refinement (g) verify3D analysis before refinement (h) verify3D analysis after refinement (i)

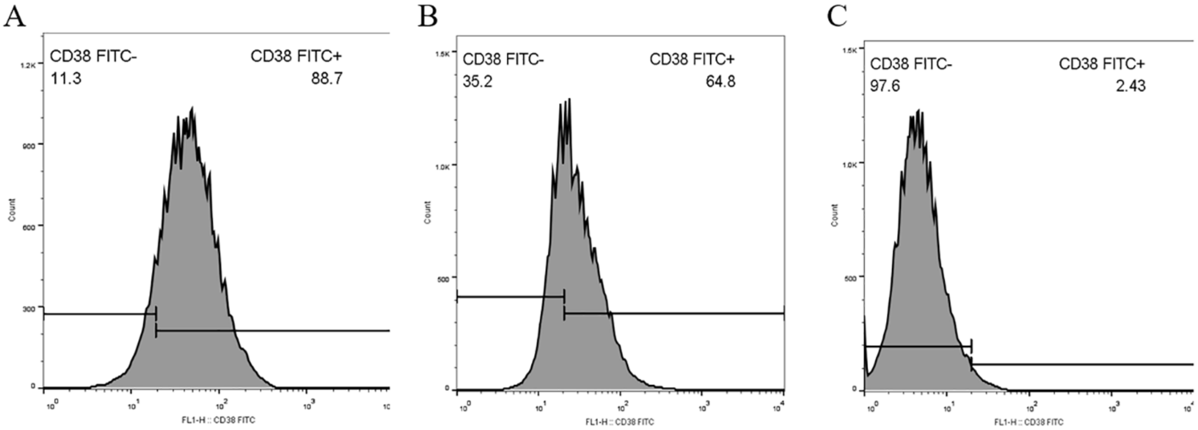


Figure S2: Daudi CD38 expression level (a) Jorkat CD38 expression level (b) K562 CD38 expression level (c)

Table S4: sequences data of insilico input; CD38, different parts of extracellular Scfv- hinge including linker and some manner of daratumumab based anti-CD38 scFv which changing their length and displacement, provided the initial information for *in silic*o analysis.

Protein	Sequences
Hinge 1	AKPTTTPAPRPPTPAPTIASQPLSLRPEACRPAAGGAVHTRGLDFACDIYI
Hinge 2	TTTPAPRPPTPAPTIASQPLSLRPEACRPAAGGAVHTRGLDFACD
Hinge 3	KPTTTPAPRPPTPAPTIASQPLSLRPEACRPAAGGAVHTRGLDFACD
linker	(G4S)1-7
Light Chain	EIVLTQSPATLSLSPGERATLSCRASQSVSSYLAWYQQKPGQAPRLLIYDASNRATGIPARFSGSGSGTDFTLTISSLEPEDFAVYYCQQRSNWPPTFGQGTKVEIK
Heavy chain	EVQLLESGGGLVQPGGSLRLSCAVSGFTFNSFAMSWVRQAPGKGLEWVSAISGSGGGTYYADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYFCAKDKILWFGEPVFDYWGQGTLVTV
scFv	EIVLTQSPATLSLSPGERATLSCRASQSVSSYLAWYQQKPGQAPRLLIYDASNRATGIPARFSGSGSGTDFTLTISSLEPEDFAVYYCQQRSNWPPTFGQGTKVEIK(G4S)1-7 EVQLLESGGGLVQPGGSLRLSCAVSGFTFNSFAMSWVRQAPGKGLEWVSAISGSGGGTYYADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYFCAKDKILWFGEPVFDYWGQGTLVTV
scFv	EVQLLESGGGLVQPGGSLRLSCAVSGFTFNSFAMSWVRQAPGKGLEWVSAISGSGGGTYYADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYFCAKDKILWFGEPVFDYWGQGTLVTV(G4S)1-7 EIVLTQSPATLSLSPGERATLSCRASQSVSSYLAWYQQKPGQAPRLLIYDASNRATGIPARFSGSGSGTDFTLTISSLEPEDFAVYYCQQRSNWPPTFGQGTKVEIK
Sequence 197 from Patent EP3334765	EVQLVESGGGLVQAGGSLRLSCAASGRTYAMGWYRQAPGKQRDLVATISGAGNTKYADSVKGRFTISRDNAKNTMYLQMNSLKPEDTAVYYCAAGKWFPAANEYWGQGTQVTVSS
Sequence 293 from Patent EP3334765	EVQLVESGGGLVQAGGSLRLSCIATGKVFSIYDMGWYRQAPGKQRELVAEITSSGTTHYDDFVSGRFTISRDNAKNTVYLQMNTLKAEDTAVYYCRANHVFGGSYWGQGTQVTVSS
Sequence 196 from Patent EP3334765	QVKLEESGGGLVQAGGSLRLSCVASGTIVSISTMGWYRQAPGKQRELVATITRRGRTNYTDSVKGRFTISRDNAKNTVYLQMNSLKPEDTAVYYCNAEVQLDIWASAYDYWGQGTQVTVASTRRMHTS
Sequence 195 from Patent EP3334765	DVQLVESGGGLVQAGDSLRLSCAASGRTFSSYAMAWFRQAPGKEREIVSSISTSGGITDYADSVKGRFTISKDSAKMNTVYLQMNSLEPEDTAVYYCAARTWYLRTSLQYDYWGQGTQVTVSSTRRMHTS
Sequence 194 from Patent EP3334765	AVQLVDSGGGLAQTGGSLRLSCAASQGIFTINAMGWYRQVPGKQRELVAEVSSGGRTDYADSVKGRFTISRDNAKNTVYLQMNSLKPEDTGVYYCRVSGWHVFVGDRIVWGQGTLVTVSSTRRMHTS
Sequence 193 from Patent EP3334765	EVQLVESGGGLVQAGGSLRLSCAASGLTFSSYIMGWFRQAPGEERELVAEISSGGMTSYADSVKGRFTISRDNAKKTGYLQMNSLKPEDTAVYYCAAPERGSIWYSRYEYKYWGQGTQVTVSSTRRMHTS
Sequence 192 from Patent EP3334765	QVQLVESGGGLVQAGDSLRLSCAASGRAYATMAWFRQAPGKEREFVAHLRVSGDTTYYTDSVKGRFTISRDNAKNTAYLQMNMLKPEDTAVYYCAAGPYGILAAARVSNPGNYDYWGQGTQVTVSSTRRMHTS
Mu375	DVQLQESGGGLVQAGGSLRLSCTGSGRTFRNYPMAWFRQAPGKEREFVAGITWVGASTLYADFAKGRFTISRDNAKNTVYLQMNSLKPEDTAVYSCAAGRGIVAGRIPAEYADWGQGTQVTVSSEPKTPKPQPAAAHHHHHHGAAEQKLISEEDLNGAA
Mu551	DVQLQESGGGLVQAGHSLRLSCVGSGSRFDNYAMGWFRQAPGKEREFVAAISWSSGTTRYLDTVKGRFTISRDNAKSTVYLQMNSLKPEDTAVYYCAARYQPRYYDSGDMDGYEYDNWGQGTQVTVSSEPKTPKPQPAAAHHHHHHGAAEQKLISEEDLNGAA
scFv (daratumomab)	EVQLLESGGGLVQPGGSLRLSCAVSGFTFNSFAMSWVRQAPGKGLEWVSAISGSGGGTYYADSVKGRFTISRDNSKNTLYLQMNSLRAEDTAVYFCAKDKILWFGEPVFDYWGQGTLVTVSSGGGGSGGGGSGGGGSEIVLTQSPATLSLSPGERATLSCRASQSVSSYLAWYQQKPGQAPRLLIYDASNRATGIPARFSGSGSGTDFTLTISSLEPEDFAVYYCQQRSNWPPTFGQGTKVEIK
CD38	MANCEFSPVSGDKPCCRLSRRAQLCLGVSILVLILVVVLAVVVPRWRQQWSGPGTTKRFPETVLARCVKYTEIHPEMRHVDCQSVWDAFKGAFISKHPCNITEEDYQPLMKLGTQTVPCNKILLWSRIKDLAHQFTQVQRDMFTLEDTLLGYLADDLTWCGEFNTSKINYQSCPDWRKDCSNNPVSVFWKTVSRRFAEAACDVVHVMLNGSRSKIFDKNSTFGSVEVHNLQPEKVQTLEAWVIHGGREDSRDLCQDPTIKELESIISKRNIQFSCKNIYRPDKFLQCVKNPEDSSCTSEI