Proteins: Structure, Function, and Bioinformatics

Supporting Information

RosettaCM for antibodies with very long HCDR3s and low template availability

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Content

Supporting Material

Table S1: Antibody Template Structures

PDB-ID	**Name**	**Resolution (Å)**
1aqk	Three-Dimensional Structure Of A Human Fab With High Affinity For Tetanus Toxoid	1.84
1b2w	Comparison Of The Three-Dimensional Structures Of A Humanized And A Chimeric Fab Of An Anti-Gamma-Interferon Antibody	2.9
1bj1	Vascular Endothelial Growth Factor In Complex With A Neutralizing Antibody	2.4
1bvk	Humanized Anti-Lysozyme Fv Complexed With Lysozyme	2.7
1ce1	1.9a Structure Of The Therapeutic Antibody Campath-1h Fab In Complex With A Synthetic Peptide Antigen	1.9
1cz8	Vascular Endothelial Growth Factor In Complex With An Affinity Matured Antibody	2.4
1dee	Structure Of S. Aureus Protein A Bound To A Human Igm Fab	2.7
1dfb	Structure Of A Human Monoclonal Antibody Fab Fragment Against Gp41 Of Human Immunodeficiency Virus Type I	2.7
1dn0	Structure Of The Fab Fragment From A Human Igm Cold Agglutinin	2.28
1dql	Crystal Structure Of An Unliganded (Native) Fv From A Human Igm Anti-Peptide Antibody	2.6
1fvd	X-Ray Structures Of The Antigen-Binding Domains From Three Variants Of Humanized Anti-P185-Her2 Antibody 4d5 And Comparison With Molecular Modeling	2.5
1fve	X-Ray Structures Of The Antigen-Binding Domains From Three Variants Of Humanized Anti-P185-Her2 Antibody 4d5 And Comparison With Molecular Modeling	2.7
1g9m	Hiv-1 Hxbc2 Gp120 Envelope Glycoprotein Complexed With Cd4 And Induced Neutralizing Antibody 17b	2.2
1gc1	Hiv-1 Gp120 Core Complexed With Cd4 And A Neutralizing Human Antibody	2.5
1hez	Antibody-Antigen Complex	2.7
1igm	Three Dimensional Structure Of An Fv From A Human Igm Immunoglobulin	2.3
1iqd	Human Factor VIII C2 Domain Complexed To Human Monoclonal BO2C11 Fab.	2
1jps	Crystal Structure Of Tissue Factor In Complex With Humanized Fab D3h44	1.85

1l7i	Crystal Structure Of The Anti-Erbb2 Fab2C4	1.8
1mhp	Crystal Structure Of A Chimeric Alpha1 Integrin I-Domain In Complex With The Fab Fragment Of A Humanized Neutralizing Antibody	2.8
1n0x	Crystal Structure Of A Broadly Neutralizing Anti-HIV-1 Antibody In Complex With A Peptide Mimotope	1.8
1nfd	An Alpha-Beta T Cell Receptor (Tcr) Heterodimer In Complex With An Anti-Tcr Fab Fragment Derived From A Mitogenic Antibody	2.8
1nl0	Crystal Structure Of Human Factor IX Gla Domain In Complex Of An Inhibitory Antibody, 10C12	2.2
1rhh	Crystal Structure Of The Broadly HIV-1 Neutralizing Fab X5 At 1.90 Angstrom Resolution	1.9
1rz7	Crystal Structure Of Human Anti-Hiv-1 Gp120-Reactive Antibody 48d	2
1s3k	Crystal Structure Of A Humanized Fab (Hu3s193) In Complex With The Lewis Y Tetrasaccharide	1.9
1tzh	Crystal Structure Of The Fab YADS1 Complexed With H-VEGF	2.6
1tzi	Crystal Structure Of The Fab YADS2 Complexed With H-VEGF	2.8
1u6a	Crystal Structure Of The Broadly Neutralizing Anti-HIV Fab F105	2.81
1vge	Tr1.9 Fab Fragment Of A Human Igg1 Kappa Autoantibody	2
1w72	Crystal Structure Of HLA-A1:MAGE-A1 In Complex With Fab-Hyb3	2.15
1wt5	The Crystal Structure Of A Humanized Antibody Fv 528	2.1
1za3	The Crystal Structure Of The Ysd1 Fab Bound To DR5	3.35
2a9m	Structural Analysis Of A Tight-Binding Fluorescein-Scfv; Apo Form	2.1
2a9n	A Mutation Designed To Alter Crystal Packing Permits Structural Analysis Of A Tight-Binding Fluorescein-Scfv Complex	3
2agj	Crystal Structure Of A Glycosylated Fab From An Igm Cryoglobulin With Properties Of A Natural Proteolytic Antibody	2.6
2aj3	Crystal Structure Of A Cross-Reactive HIV-1 Neutralizing CD4-Binding Site Antibody Fab M18	2.03
2b1h	Crystal Structure Analysis Of Anti-HIV-1 V3 Fab 2219 In Complex With UG29 Peptide	2
2b2x	VLA1 Rdeltah I-Domain Complexed With A Quadruple Mutant Of The AQC2 Fab	2.2

2cmr	Crystal Structure Of The HIV-1 Neutralizing Antibody D5 Fab Bound To The Gp41 Inner-Core Mimetic 5-Helix	2
2d7t	Crystal Structure Of Human Anti Polyhydroxybutyrate Antibody Fv	1.7
2eiz	Crystal Structure Of Humanized HYHEL-10 Fv Mutant(HW47Y)-Hen Lysozyme Complex	1.9
2eks	Crystal Structure Of Humanized Hyhel-10 FV-HEN Lysozyme Complex	2
2f5a	Crystal Structure Of Fab' From The Hiv-1 Neutralizing Antibody 2f5	2.05
2fb4	Dir Primaerstruktur Des Kristallisierbaren Monoklonalen Immunoglobulins Igg1 Kol. Ii. Aminosaeuresequenz Der L-Kette, Lambda-Typ, Subgruppe I (German)	1.9
2fjf	Structure Of The G6 Fab, A Phage Derived VEGF Binding Fab	2.65
2fjh	Structure Of The B20-4 Fab, A Phage Derived Fab Fragment, In Complex With VEGF	3.1
2fl5	Cofactor-Containing Antibodies: Crystal Structure Of The Original Yellow Antibody	3
2g75	Crystal Structure Of Anti-SARS M396 Antibody	2.28
2ghw	Crystal Structure Of SARS Spike Protein Receptor Binding Domain In Complex With A Neutralizing Antibody, 80R	2.3
2h9g	Crystal Structure Of Phage Derived Fab Bdf1 With Human Death Receptor 5 (DR5)	2.32
2hfg	Crystal Structure Of Hbr3 Bound To CB3s-Fab	2.61
2hwz	Fab Fragment Of Humanized Anti-Viral Antibody MEDI-493 (Synagis TM)	1.8
2j6e	Crystal Structure Of An Autoimmune Complex Between A Human Igm Rheumatoid Factor And Igg1 Fc Reveals A Novel Fc Epitope And Evidence For Affinity Maturation	3
2jb5	Fab Fragment In Complex With Small Molecule Hapten, Crystal Form-1	2.8
2ny1	HIV-1 Gp120 Envelope Glycoprotein (I109C, T257S, S334A, S375W, Q428C) Complexed With CD4 And Antibody 17b	1.99
2nyy	Crystal Structure Of Botulinum Neurotoxin Type A Complexed With Monoclonal Antibody CR1	2.61
2nz9	Crystal Structure Of Botulinum Neurotoxin Type A Complexed With Monoclonal Antibody AR2	3.79
2qqk	Neuropilin-2 A1a2b1b2 Domains In Complex With A Semaphorin-Blocking Fab	2.75
2qqn	Neuropilin-1 B1 Domain In Complex With A VEGF-Blocking Fab	2.2

2qr0	Structure Of VEGF Complexed To A Fab Containing TYR And SER In The Cdrs	3.5
2qsc	Crystal Structure Analysis Of Anti-HIV-1 V3-Fab F425-B4e8 In Complex With A V3-Peptide	2.8
2r0k	Protease Domain Of HGFA With Inhibitor Fab58	3.51
2r0l	Short Form HGFA With Inhibitory Fab75	2.2
2r56	Crystal Structure Of A Recombinant Ige Fab Fragment In Complex With Bovine Beta-Lactoglobulin Allergen	2.8
2r8s	High Resolution Structure Of A Specific Synthetic FAB Bound To P4-P6 RNA Ribozyme Domain	1.95
2uzi	Crystal Structure Of HRAS(G12V) - Anti-RAS Fv Complex	2
2v7n	Unusual Twinning In Crystals Of The Cits Binding Antibody Fab Fragment F3p4	1.92
2vxq	Crystal Structure Of The Major Grass Pollen Allergen Phl P 2 In Complex With Its Specific Ige-Fab	1.9
2vxv	Crystal Structure Of Human Igg ABT-325 Fab Fragment	1.49
2wuc	Crystal Structure Of HGFA In Complex With The Allosteric Non- Inhibitory Antibody Fab40.Deltatrp And Ac-KQLR-Chloromethylketone	2.7
2xra	Crystal Structure Of The HK20 Fab In Complex With A Gp41 Mimetic 5- Helix	2.3
2xtj	The Crystal Structure Of PCSK9 In Complex With 1D05 Fab	2.7
2xwt	Crystal Structure Of The Tsh Receptor In Complex With A Blocking Type Tshr Autoantibody	1.9
2xzc	Crystal Structure Of Phosphonate-Modified Recombinant A.17 Antibody FAB Fragment	1.36
2yc1	Crystal Structure Of The Human Derived Single Chain Antibody Fragment (Scfv) 9004G In Complex With Cn2 Toxin From The Scorpion Centruroides Noxius Hoffmann	1.9
2yk1	Structure Of Human Anti-Nicotine Fab Fragment In Complex With Nicotine	1.85
2yss	Crystal Structure Of Humanized HYHEL-10 FV Mutant(HQ39KW47Y)-HEN Lysozyme Complex	2.4
3aaz	Crystal Structure Of The Humanized Recombinant Fab Fragment Of A Murine; Antibody	2.2
3auv	Predicting Amino Acid Preferences In The Complementarity Determining Regions Of An Antibody-Antigen Recognition Interface	2.4

3b2u	Crystal Structure Of Isolated Domain III Of The Extracellular Region Of The Epidermal Growth Factor Receptor In Complex With The Fab Fragment Of IMC-11F8	2.58
3bdy	Dual Specific Bh1 Fab In Complex With VEGF	2.6
3bn9	Crystal Structure Of MT-SP1 In Complex With Fab Inhibitor E2	2.17
3c09	Crystal Structure The Fab Fragment Of Matuzumab (Fab72000) In Complex With Domain III Of The Extracellular Region Of EGFR	3.2
3dvg	Crystal Structure Of K63-Specific Fab Apu.3A8 Bound To K63-Linked Di-Ubiquitin	2.6
3dvn	Crystal Structure Of K63-Specific Fab Apu2.16 Bound To K63-Linked Di-Ubiquitin	2.7
3efd	The Crystal Structure Of The Cytoplasmic Domain Of Kcsa	2.6
3eo0	Structure Of The Transforming Growth Factor-Beta Neutralizing Antibody GC-1008	1.75
3eo9	Crystal Structure The Fab Fragment Of Efalizumab	1.8
3eot	Crystal Structure Of LAC031, An Engineered Anti-VLA1 Fab	1.9
3eyf	Crystal Structure Of Anti-Human Cytomegalovirus Antibody 8f9 Plus Gb Peptide	2.3
3fn0	Crystal Structure Of HIV-1 Neutralizing Human Fab Z13e1 In Complex With A 12-Residue Peptide Containing The Z13e1 Epitope On Gp41	1.8
3fzu	Igg1 Fab Characterized By H/D Exchange	2.5
3g04	Crystal Structure Of The TSH Receptor In Complex With A Thyroid-Stimulating Autoantibody	2.55
3g6a	Crystal Structure Of Anti-IL-13 Antibody CNTO607	2.1
3gbn	Crystal Structure Of Fab CR6261 In Complex With The 1918 H1N1 Influenza Virus Hemagglutinin	2.2
3ghe	Crystal Structure Of Anti-HIV-1 Fab 537-10D In Complex With V3 Peptide MN	2.4
3giz	Crystal Structure Of The Fab Fragment Of Anti-CD20 Antibody Ofatumumab	2.2
3gjf	Rational Development Of High-Affinity T-Cell Receptor-Like Antibodies	1.9
3gkw	Crystal Structure Of The Fab Fragment Of Nimotuzumab. An Anti-Epidermal Growth Factor Receptor Antibody	2.5
3go1	Crystal Structure Of Anti-HIV-1 Fab 268-D In Complex With V3 Peptide MN	1.89
3grw	FGFR3 In Complex With A Fab	2.1

3h42	Crystal Structure Of PCSK9 In Complex With Fab From LDLR Competitive Antibody	2.3
3hae	Rational Development Of High-Affinity T-Cell Receptor-Like Antibodies	2.9
3hc0	BHA10 Igg1 Wild-Type Fab - Antibody Directed At Human LTBR	1.9
3hc3	BHA10 Igg1 Fab Double Mutant Variant - Antibody Directed At Human LTBR	1.72
3hc4	BHA10 Igg1 Fab Quadruple Mutant Variant - Antibody Directed At Human LTBR	1.62
3hi6	Crystal Structure Of Intermediate Affinity I Domain Of Integrin LFA-1 With The Fab Fragment Of Its Antibody AL-57	2.3
3hmx	Crystal Structure Of Ustekinumab FAB/IL-12 Complex	3
3hr5	M1prime Peptide From Ige Bound By Humanized Antibody 47H4 Fab	2.4
3i9g	Crystal Structure Of The LT1009 (SONEPCIZUMAB) Antibody Fab Fragment In Complex With Sphingosine-1-Phosphate	1.9
3idg	Crystal Structure Of The HIV-1 Cross Neutralizing Monoclonal Antibody 2F5 In Complex With Gp41 Peptide ALDKWD	1.86
3idx	Crystal Structure Of HIV-Gp120 Core In Complex With CD4-Binding Site Antibody B13, Space Group C222	2.5
3inu	Crystal Structure Of An Unbound KZ52 Neutralizing Anti-Ebolavirus Antibody.	2.5
3juy	Crystal Structure Of A 3B3 Variant, A Broadly Neutralizing HIV-1 Scfv Antibody	2.5
3k2u	Crystal Structure Of HGFA In Complex With The Allosteric Inhibitory Antibody Fab40	2.35
3kdm	Crystal Structure Of Human Anti-Steroid Fab 5F2 In Complex With Testosterone	1.5
3kr3	Crystal Structure Of IGF-II Antibody Complex	2.2
3kym	Crystal Structure Of Li33 Igg2 Di-Fab	2.62
3l5x	Crystal Structure Of The Complex Between IL-13 And H2L6 FAB	1.9
3l95	Crystal Structure Of The Human Notch1 Negative Regulatory Region (NRR) Bound To The Fab Fragment Of An Antagonist Antibody	2.19
3lh2	Crystal Structure Of HIV Epitope-Scaffold 4E10_1VI7A_S0_002_N 4E10 Fv Complex	2.65
3lmj	Structure Of Human Anti HIV 21c Fab	2.2
3lzf	Crystal Structure Of Fab 2D1 In Complex With The 1918 Influenza Virus Hemagglutinin	2.8
3m8o	Human Iga1 Fab Fragment	1.55

3ma9	Crystal Structure Of Gp41 Derived Protein Complexed With Fab 8066	2.05
3mac	Crystal Structure Of GP41-Derived Protein Complexed With Fab 8062	2.5
3mlw	Crystal Structure Of Anti-HIV-1 V3 Fab 1006-15D In Complex With An MN V3 Peptide	2.7
3mly	Crystal Structure Of Anti-HIV-1 V3 Fab 3074 In Complex With A UR29 V3 Peptide	1.7
3mme	Structure And Functional Dissection Of PG16, An Antibody With Broad And Potent Neutralization Of HIV-1	3.97
3n85	Crystallographic Trimer Of HER2 Extracellular Regions In Complex With Tryptophan-Rich Antibody Fragment	3.2
3n9g	Crystal Structure Of The Fab Fragment Of The Human Neutralizing Anti-West Nile Virus Mab CR4354	1.43
3na9	Crystal Structure Of Fab15	1.7
3naa	Crystal Structure Of Fab15 Mut5	1.7
3nab	Crystal Structure Of Fab15 Mut6	2.32
3nac	Crystal Structure Of Fab15 Mut7	1.8
3ncj	Crystal Structure Of Fab15 Mut8	1.6
3nfs	Crystal Structure The Fab Fragment Of Therapeutic Antibody Daclizumab	2.6
3nh7	Crystal Structure Of The Neutralizing Fab Fragment Abd1556 Bound To The BMP Type I Receptor IA	2.7
3nps	Crystal Structure Of Membrane-Type Serine Protease 1 (MT-SP1) In Complex With The Fab Inhibitor S4	1.5
3oau	Antibody 2G12 Recognizes Di-Mannose Equivalently In Domain- And Non-Domain-Exchanged Forms, But Only Binds The HIV-1 Glycan Shield If Domain-Exchanged	1.9
3oaz	A Non-Self Sugar Mimic Of The HIV Glycan Shield Shows Enhanced Antigenicity	1.75
3p0y	Anti-EGFR/HER3 Fab DL11 In Complex With Domain III Of EGFR Extracellular Region	1.8
3p30	Crystal Structure Of The Cluster II Fab 1281 In Complex With HIV-1 Gp41 Ectodomain	3.3
3pgf	Crystal Structure Of Maltose Bound MBP With A Conformationally Specific Synthetic Antigen Binder (Sab)	2.1

3piq	Crystal Structure Of Human 2909 Fab, A Quaternary Structure-Specific Antibody Against HIV-1	3.33
3pnw	Crystal Structure Of The Tudor Domain Of Human TDRD3 In Complex With An Anti-TDRD3 FAB	2.05
3pp4	Epitope Characterization And Crystal Structure Of GA101 Provide Insights Into The Molecular Basis For The Type I / Type II Distinction Of Anti- CD20 Antibodies	1.6
3qcu	Crystal Structure Of The LT3015 Antibody Fab Fragment In Complex With Lysophosphatidic Acid (14:0)	1.98
3qeh	Crystal Structure Of Human N12-I15, An ADCC And Non-Neutralizing Anti-HIV-1 Env Antibody	2.59
3qhf	Crystal Structure Of Fab Del2d1, A Deletion Variant Of Anti-Influenza Antibody 2D1	1.65
3qot	Crystal Structure Of Human Germline Antibody 1-69/B3	1.9
3qrg	Crystal Structure Of Antirsvf Fab B21m	1.7
3qwo	Crystal Structure Of A Motavizumab Epitope-Scaffold Bound To Motavizumab Fab	1.9
3r1g	Structure Basis Of Allosteric Inhibition Of BACE1 By An Exosite-Binding Antibody	2.8
3s34	Structure Of The 1121B Fab Fragment	2.2
3sdy	Crystal Structure Of Broadly Neutralizing Antibody CR8020 Bound To The Influenza A H3 Hemagglutinin	2.85
3se9	Crystal Structure Of Broadly And Potently Neutralizing Antibody VRC-PG04 In Complex With HIV-1 Gp120	2
3skj	Structural And Functional Characterization Of An Agonistic Anti-Human Epha2 Monoclonal Antibody	2.5
3so3	Structures Of Fab-Protease Complexes Reveal A Highly Specific Non-Canonical Mechanism Of Inhibition.	2.1
3sob	The Structure Of The First YWTD Beta Propeller Domain Of LRP6 In Complex With A FAB	1.9
3sqo	PCSK9 J16 Fab Complex	2.7
3tcl	Crystal Structure Of HIV-1 Neutralizing Antibody CH04	1.91
3tnm	Crystal Structure Of A32 Fab, An ADCC Mediating Anti-HIV-1 Antibody	1.85
3u0t	Fab-Antibody Complex	2.5

3u30	Crystal Structure Of A Linear-Specific Ubiquitin Fab Bound To Linear Ubiquitin	2.43
3u4b	Ch04h/Ch02l Fab P4	2.89
3u6r	Three Dimensional Structure Of Broadly Neutralizing Anti - Hepatitis C Virus (HCV) Glycoprotein E2 Single Chain FV Fragment 1:7	2.67
3u7y	Structure Of NIH45-46 Fab In Complex With Gp120 Of 93TH057 HIV	2.45
3uc0	Crystal Structure Of Domain I Of The Envelope Glycoprotein Ectodomain From Dengue Virus Serotype 4 In Complex With The Fab Fragment Of The Chimpanzee Monoclonal Antibody 5H2	2.71
3uji	Crystal Structure Of Anti-HIV-1 V3 Fab 2558 In Complex With MN Peptide	1.6
3ujj	Crystal Structure Of Anti-HIV-1 V3 Fab 4025 In Complex With Con A Peptide	2
3uls	Crystal Structure Of Fab12	2.49
3ux9	Structural Insights Into A Human Anti-IFN Antibody Exerting Therapeutic Potential For Systemic Lupus Erythematosus	2.8
3w9e	Structure Of Human Monoclonal Antibody E317 Fab Complex With HSV-2 Gd	2.3
3wd5	Crystal Structure Of Tnfalpha In Complex With Adalimumab Fab Fragment	3.1
3x3f	TRAIL-R2 Extracellular Region Complexed To A Fab Fragment From Human Agonist Antibody KMTR2	2.1
3zl4	Antibody Structural Organization: Role Of Kappa - Lambda Chain Constant Domain Switch In Catalytic Functionality	1.95
3ztn	Structure Of Influenza A Neutralizing Antibody Selected From Cultures Of Single Human Plasma Cells In Complex With Human H1 Influenza Haemagglutinin.	3
4buh	Human Ige Against The Major Allergen Bet V 1 - Crystal Structure Of Clone M0418 Scfv	1.3
4cni	Crystal Structure Of The Fab Portion Of Olokizumab In Complex With IL- 6	2.2
4d9l	Fab Structure Of Anti-HIV-1 Gp120 V2 Mab 697	2.48
4d9q	Inhibiting Alternative Pathway Complement Activation By Targeting The Exosite On Factor D	2.28
4dgy	Structure Of The Hepatitis C Virus Envelope Glycoprotein E2 Antigenic Region 412-423 Bound To The Broadly Neutralizing Antibody HCV1, C2 Form	1.8
4dke	Crystal Structure Of Human Interleukin-34 Bound To Fab1.1	3
4dkf	Crystal Structure Of Human Interleukin-34 Bound To Fab2	2.61
4dn3	Crystal Structure Of Anti-Mcp-1 Antibody Cnto888	2.6

4edw	Nerve Growth Factor In Complex With Fab From Humanized Version Of Mouse Mab 911 (Tanezumab)	2.48
4eow	Crystal Structure Of A Disease-Associated Anti-Human GM-CSF Autoantibody MB007	1.97
4ers	A Molecular Basis For Negative Regulation Of The Glucagon Receptor	2.64
4evn	Crystal Structure Of Fab CR6261 (Somatic Heavy Chain With Germline-Reverted Light Chain)	2.85
4f57	Fab Structure Of A Neutralizing Antibody L1 From An Early Subtype A HIV-1 Infected Patient	1.7
4f58	Fab Structure Of A Neutralizing Antibody L3 From An Early Subtype A HIV-1 Infected Patient	2.49
4fqc	Crystal Structure Of PGT121 Fab Bound To A Complex-Type Sialylated N-Glycan	2.4
4fqi	Crystal Structure Of Fab CR9114 In Complex With A H5N1 Influenza Virus Hemagglutinin	1.71
4fql	Influenza B Ha Antibody (Fab) Cr8033	1.9
4fqq	Crystal Structure Of Germline Antibody PGT121-GL Fab	2.42
4fze	Crystal Structure Of N26_I1 Fab, An ADCC Mediating Anti-HIV-1 Antibody.	2
4g5z	Crystal Structure Of The Therapeutical Antibody Fragment Of Canakinumab In Its Unbound State	1.83
4g6f	Crystal Structure Of 10E8 Fab In Complex With An HIV-1 Gp41 Peptide	2.1
4g7v	Crystal Structure Of Voltage Sensing Domain Of Ci-VSP With Fragment Antibody (R217E, 2.5 A)	2.5
4g80	Crystal Structure Of Voltage Sensing Domain Of Ci-VSP With Fragment Antibody (WT, 3.8 A)	3.58
4gsd	H5.3 Fab Structure	2.25
4gxv	Crystal Structure Of Anti-Influenza Virus Antibody 1F1	1.45
4h8w	Crystal Structure Of Non-Neutralizing And ADCC-Potent Antibody N5-I5 In Complex With HIV-1 Clade A/E Gp120 And Scd4.	1.85
4hcr	Crystal Structure Of Human Madcam-1 D1D2 Complexed With Fab PF-547659	2.3
4hf5	Crystal Structure Of Fab 8F8 In Complex A H2N2 Influenza Virus Hemagglutinin	3
4hfu	Crystal Structure Of Fab 8M2 In Complex With A H2N2 Influenza Virus Hemagglutinin	3.11

4hfw	Anti Rotavirus Antibody	2.6
4hg4	Crystal Structure Of Fab 2G1 In Complex With A H2N2 Influenza Virus Hemagglutinin	3.2
4hha	Anti-Human Cytomegalovirus (HCMV) Fab KE5 With Epitope Peptide AD-2S1	1.6
4hie	Anti-Streptococcus Pneumoniae 23F Fab 023.102	1.9
4hk0	UCA Fab (Unbound) From CH65-CH67 Lineage	2.5
4hk3	I2 Fab (Unbound) From CH65-CH67 Lineage	3
4hpo	Crystal Structure Of RV144-Elicited Antibody CH58 In Complex With V2 Peptide	1.69
4hpy	Crystal Structure Of RV144-Elicited Antibody CH59 In Complex With V2 Peptide	1.5
4hs6	Hepatitus C Envelope Glycoprotein E2 Fragment 412-423 With Humanized And Affinity-Matured Antibody MRCT10.V362	1.53
4hs8	Hepatitus C Envelope Glycoprotein E2 Fragment 412-423 With Humanized And Affinity-Matured Antibody Hu5b3.V3	2.6
4hwe	Crystal Structure Of Ectodomain 3 Of The IL-13 Receptor Alpha1 In Complex With A Human Neutralizing Monoclonal Antibody Fragment	2.43
4i18	Crystal Structure Of Human Prolactin Receptor Complexed With Fab Fragment	3.24
4i77	Lebrikizumab Fab Bound To IL-13	1.9
4imk	Uncrossed Fab Binding To Human Angiopoietin 2	2.2
4iml	Crossfab Binding To Human Angiopoietin 2	2.93
4ioi	Meditope-Enabled Trastuzumab In Complex With CQFDLSTRRLKC	1.95
4irz	Crystal Structure Of A4b7 Headpiece Complexed With Fab Natalizumab	2.84
4j4p	The Complex Of Human Ige-Fc With Two Bound Fab Fragments	2.91
4j6r	Crystal Structure Of Broadly And Potently Neutralizing Antibody VRC23 In Complex With HIV-1 Gp120	1.64
4jam	Crystal Structure Of Broadly Neutralizing Anti-Hiv-1 Antibody Ch103	1.65
4jdv	Crystal Structure Of Germ-Line Precursor Of NIH45-46 Fab	1.65
4jfx	Structure Of Phosphotyrosine (Ptyr) Scaffold Bound To Ptyr Peptide	1.95
4jfz	Structure Of Phosphoserine (Psab) Scaffold Bound To Pser Peptide	1.75
4jg1	Structure Of Phosphoserine/Threonine (Pstab) Scaffold Bound To Pthr Peptide	1.55
4jha	Crystal Structure Of RSV-Neutralizing Human Antibody D25	1.6

4jkp	Restricting HIV-1 Pathways For Escape Using Rationally-Designed Anti-HIV-1 Antibodies	2.82
4jlr	Crystal Structure Of A Designed Respiratory Syncytial Virus Immunogen In Complex With Motavizumab	2.71
4jn2	An Antidote For Dabigatran	1.71
4jpi	Crystal Structure Of A Putative VRC01 Germline Precursor Fab	2.1
4jpk	Crystal Structure Of The Germline-Targeting HIV-1 Gp120 Engineered Outer Domain Eod-GT6 In Complex With A Putative VRC01 Germline Precursor Fab	2.4
4jqi	Structure Of Active Beta-Arrestin1 Bound To A G Protein-Coupled Receptor Phosphopeptide	2.6
4jy5	Crystal Structure Of Human Fab PGT122, A Broadly Reactive And Potent HIV-1 Neutralizing Antibody	1.75
4jzj	Crystal Structure Of Receptor-Fab Complex	2.8
4jzn	Three Dimensional Structure Of Broadly Neutralizing Human Anti - Hepatitis C Virus (HCV) Glycoprotein E2 Fab Fragment HC84-1	2.05
4jzo	Three Dimensional Structure Of Broadly Neutralizing Human Anti - Hepatitis C Virus (HCV) Glycoprotein E2 Fab Fragment HC84-27	2.22
4k3j	Crystal Structure Of Onartuzumab Fab In Complex With MET And HGF-Beta	2.8
4k94	Crystal Structure Of KIT D4D5 Fragment In Complex With Anti-Kit Antibody Fab19	2.4
4k9e	Crystal Structure Of KIT D4D5 Fragment In Complex With Anti-Kit Antibodies Fab79D	2.7
4kmt	Crystal Structure Of Human Germline Antibody 5-51/O12	2.1
4kq3	Crystal Structure Of Anti-IL-17A Antibody CNTO3186	1.92
4ky1	Humanized HP1/2 Fab	2.97
4leo	Crystal Structure Of Anti-HER3 Fab RG7116 In Complex With The Extracellular Domains Of Human Her3 (ERBB3)	2.64
4lex	Unliganded Crystal Structure Of Mab7	2.02
4lf3	Inhibitory Mechanism Of An Allosteric Antibody Targeting The Glucagon Receptor	2.73
4liq	Structure Of The Extracellular Domain Of Human CSF-1 Receptor In Complex With The Fab Fragment Of RG7155	2.6
4lkc	An Antibody Against The C-Terminal Domain Of PCSK9 Lowers LDL Cholesterol Levels In Vivo	2.2

4lkx	Humanized Antibody 4B12 Fab Complexed With A Cemx Segment	1.92
4llu	Structure Of Pertuzumab Fab With Light Chain Clambda At 2.16A	2.16
4lly	Crystal Structure Of Pertuzumab Clambda Fab With Variable And Constant Domain Redesigns (VRD2 And CRD2) At 1.6A	1.6
4lmq	Development And Preclinical Characterization Of A Humanized Antibody Targeting CXCL12	2.77
4lss	Crystal Structure Of Broadly And Potently Neutralizing Antibody VRC01 In Complex With HIV-1 Clade A Strain KER_2018_11 Gp120	2.59
4lst	Crystal Structure Of Broadly And Potently Neutralizing Antibody VRC01 In Complex With HIV-1 Clade C Strain ZM176.66 Gp120	2.55
4lsu	Crystal Structure Of Broadly And Potently Neutralizing Antibody VRC-PG20 In Complex With HIV-1 Clade A/E 93TH057 Gp120	2.3
4m1d	Crystal Structure Of Anti-HIV-1 Fab 447-52D In Complex With V3 Cyclic Peptide MN	1.8
4m5y	Crystal Structure Of Broadly Neutralizing Fab 5J8	1.55
4m62	Ontogeny Of Recognition Specificity And Functionality For The Anti-HIV Neutralizing Antibody 4E10	1.8
4m6n	Crystal Structure Of Anti-IL-23 Antibody CNTO1959 At Ph 6.5	2
4m6o	Crystal Structure Of Anti-NGF Antibody CNTO7309	2.8
4mwf	Structure Of Hepatitis C Virus Envelope Glycoprotein E2 Core Bound To Broadly Neutralizing Antibody AR3C	2.64
4mxv	Structure Of Lymphotoxin Alpha Bound To Anti-Lta Fab	3.2
4n0y	Structure Of The Hepatitis C Envelope Glycoprotein E1 Antigenic Region 314-324 Bound To The Cross-Neutralizing Antibody IGH526	1.75
4n9g	Crystal Structure Of A Computationally Designed RSV-Presenting Epitope Scaffold And Its Elicited Antibody 17HD9	2.5
4nik	Structure Of Human Gankyrin In Complex To The Single Chain Antibody F5	2.5
4nki	Crystal Structure Of A Fab	2.41
4nm4	Crystal Structure Of Broadly Neutralizing Antibody CR8043	2.65
4nnp	Crystal Structure Of Apo Manganese ABC Transporter Mntc From Staphylococcus Aureus Bound To An Antagonistic Fab Fragment	2.69
4np4	Clostridium Difficile Toxin B CROP Domain In Complex With FAB Domains Of Neutralizing Antibody Bezlotoxumab	2.89

4npy	Crystal Structure Of Germline Fab PGT121, A Putative Precursor Of The Broadly Reactive And Potent HIV-1 Neutralizing Antibody	1.8
4nrx	Crystal Structure Of HIV-1 Neutralizing Antibody M66 In Complex With Gp41 MPER Peptide	2.21
4nrz	Crystal Structure Of HIV-1 Neutralizing Antibody M66.6	2.42
4nug	Crystal Structure Of HIV-1 Broadly Neutralizing Antibody PGT151	1.86
4nwt	Crystal Structure Of The Anti-Human NGF Fab APE1531	1.75
4nyl	Crystal Structure Of Adalimumab FAB Fragment	2.8
4nzu	Crystal Structure Of The Primary Monoclonal Antibody 13PL Fab' From A Multiple Myeloma Patient	1.2
4o5l	Crystal Structure Of Broadly Neutralizing Antibody F045-092	1.5
4oaw	Fab Structure Of Anti-HIV Gp120 V2 Mab 2158	2.8
4od2	Crystal Structure Of The Fab Fragment Of An Anti-DR5 Antibody Bound To DR5	3.2
4odx	4E10 Germline Encoded Precursor No.7 In Complex With Epitope Scaffold T117	3.1
4ogy	Crystal Structure Of Fab DX-2930 In Complex With Human Plasma Kallikrein At 2.1 Angstrom Resolution	2.1
4ojf	Humanised 3D6 Fab Complexed To Amyloid Beta 1-8	2
4olu	Crystal Structure Of Antibody VRC07 In Complex With Clade A/E 93TH057 HIV-1 Gp120 Core	2.2
4olv	Crystal Structure Of Antibody VRC07-G54F In Complex With Clade A/E 93TH057 HIV-1 Gp120 Core	2.5
4olw	Crystal Structure Of Antibody VRC07-G54H In Complex With Clade A/E 93TH057 HIV-1 Gp120 Core	2.71
4olx	Crystal Structure Of Antibody VRC07-G54L In Complex With Clade A/E 93TH057 HIV-1 Gp120 Core	2.2
4olz	Crystal Structure Of Antibody VRC07-G54W In Complex With Clade A/E 93TH057 HIV-1 Gp120 Core	2.1
4om0	Crystal Structure Of Antibody VRC07-G54Y In Complex With Clade A/E 93TH057 HIV-1 Gp120 Core	2.29
4om1	Crystal Structure Of Antibody VRC07-I30Q, G54W, S58N In Complex With Clade A/E 93TH057 HIV-1 Gp120 Core	2.13
4oqt	LINGO-1/Li81 Fab Complex	3.23

4ot1	Structural Basis For The Recognition Of Human Cytomegalovirus Glycoprotein B By The Neutralizing Human Antibody SM5-1	2.11
4p59	HER3 Extracellular Domain In Complex With Fab Fragment Of MOR09825	3.4
4ps4	Crystal Structure Of The Complex Between IL-13 And M1295 FAB	2.8
4ptu	Crystal Structure Of Anti-23F Strep Fab C05 With Rhamnose	1.51
4py7	Crystal Structure Of Fab 3.1	2.7
4q2z	Fab Fragment Of HIV Vaccine-Elicited CD4bs-Directed Antibody, GE356, From A Non-Human Primate	1.93
4qci	PDGF-B Blocking Antibody Bound To PDGF-BB	2.3
4qf1	Crystal Structure Of Unliganded CH59UA, The Inferred Unmutated Ancestor Of The RV144 Anti-HIV Antibody Lineage Producing CH59	2.4
4qhl	I3.2 (Unbound) From CH103 Lineage	3.15
4qhm	I3.1 (Unbound) From CH103 Lineage	3.23
4qhu	Crystal Structure Of IL-17A/Fab6785 Complex	2.2
4qxg	Antigen Binding Fragment Of An Anti IFNAR1 Antibody	2.3
4r7d	Fab Hu 15c1	2.75
4r8w	Crystal Structure Of H7 Hemagglutinin From A/Anhui/1/2013 In Complex With A Neutralizing Antibody CT149	2.8
4r96	Structure Of A Llama Glama Fab 48A2 Against Human Cmet	3.31
4rav	Crystal Structure Of Scfvc4 In Complex With The First 17 AA Of Huntingtin	2.5
4ris	Structural Analysis Of The Unmutated Ancestor Of The HIV-1 Envelope V2 Region Antibody CH58 Isolated From An RV144 HIV-1 Vaccine Efficacy Trial Vaccinee And Associated With Decreased Transmission Risk	2.3
4rrp	Crystal Structure Of The Fab Complexed With Antigen Asf1p, Northeast Structural Genomics Consortium (NESG) Target Pdr16	2.79
4rx4	Crystal Structure Of VH1-46 Germline-Derived CD4-Binding Site-Directed Antibody 8ANC134 In Complex With HIV-1 Clade A Q842.D12 Gp120	3.45
4s1r	Crystal Structure Of A VRC01-Lineage Antibody, 45-VRC01.H08.F-117225, In Complex With Clade A/E HIV-1 Gp120 Core	3.21
4s1s	Crystal Structure Of A VRC01-Lineage Antibody, 45-VRC01.H5.F-185917, In Complex With Clade A/E HIV-1 Gp120 Core	3.39
4tsa	Structure Of A Lysozyme Fab Complex	2.27
4tsb	Structure Of A Lysozyme Antibody Complex	1.95

4tsc	Structure Of A Lysozyme Antibody Complex	1.92
4ttd	Structure Of A Lysozyme Antibody Complex	2.15
4u6v	Mechanisms Of Neutralization Of A Human Anti-Alpha Toxin Antibody	2.56
4ud3	Structure Of A Redesigned Cross-Reactive Antibody To Dengue Virus With Increased In Vivo Potency	2.49
4ut7	Crystal Structure Of The Scfv Fragment Of The Broadly Neutralizing Human Antibody Ede2 A11	1.7
4ut9	Crystal Structure Of Dengue 2 Virus Envelope Glycoprotein Dimer In Complex With The Scfv Fragment Of The Broadly Neutralizing Human Antibody EDE1 C10	3.2
4uta	Crystal Structure Of Dengue 2 Virus Envelope Glycoprotein In Complex With The Fab Fragment Of The Broadly Neutralizing Human Antibody EDE1 C8	3
4uu9	Crystal Structure Of The Human C5a In Complex With MEDI7814 A Neutralising Antibody	2.12
4uv4	Crystal Structure Of Anti-FPR Fpro0165 Fab Fragment	3.08
4uv7	The Complex Structure Of Extracellular Domain Of EGFR And GC1118A	2.1
4v1d	Ternary Complex Among Two Human Derived Single Chain Antibody Fragments And Cn2 Toxin From Scorpion Centruroides Noxius.	3.1
4wuk	Crystal Structure Of Apo CH65 Fab	1.7
4wuu	Structure Of ESK1 In Complex With HLA-A*0201/WT1	3.05
4x4x	Retrofitting Antibodies With Stabilizing Mutations. Herceptin Scfv Mutant.	2.25
4x4y	Retrofitting Antibodies With Stabilizing Mutations. Herceptin Scfv Mutant K30D/S52D.	2.49
4x7s	Structure Of Omalizumab Fab Fragment Crystal Form 1	1.9
4xak	Crystal Structure Of Potent Neutralizing Antibody M336 In Complex With MERS Co-V RBD	2.45
4xc1	Crystal Structure Of Human 4E10 Fab In Complex With Its Peptide Epitope On HIV-1 GP41: Crystals Cryoprotected With Sn-Glycerol 3-Phosphate	1.63
4xgz	Crystal Structure Of Human Paxillin LD2 Motif In Complex With Fab Fragment	2.5
4xml	Crystal Structure Of Fab Of HIV-1 Gp120 V3-Specific Human Monoclonal Antibody 2424	2.68
4xnq	Antibody Hemagglutinin Complexes	2
4xtr	Structure Of Get3 Bound To The Transmembrane Domain Of Pep12	2.05

4xvj	Structure Of The Hepatitis C Virus Envelope Glycoprotein E2 Antigenic 2 Region 412-423 Bound To The Broadly Neutralizing Antibody Hc33.1	2
4xvt	Crystal Structure Of HIV-1 93TH057 Coree Gp120 With Antibody 45-VRC01.H01+07.O-863513/45-VRC01.L01+07.O-110653 (VRC07_1995)	1.69
4xx1	Low Resolution Structure Of LCAT In Complex With Fab1	3.6
4xxd	Crystal Structure Of Mid-Region Amyloid Beta Capture By Solanezumab	2.41
4y5v	Diabody 305 Complex With Epor	2.6
4y5x	Diabody 305 Complex With Epor	3.15
4ydi	Crystal Structure Of Broad And Potently Neutralizing VRC01-Class Antibody Z258-VRC27.01, Isolated From Human Donor Z258, In Complex With HIV-1 Gp120 From Clade A Strain Q23.17	3.45
4ydk	Crystal Structure Of Broadly And Potently Neutralizing Antibody C38-VRC16.01 In Complex With HIV-1 Clade AE Strain 93TH057 Gp120	2.05
4ydl	Crystal Structure Of Broadly And Potently Neutralizing Antibody C38-VRC18.02 In Complex With HIV-1 Clade AE Strain 93TH057gp120	1.8
4ygv	Reversal Agent For Dabigatran	1.76
4yhl	Reversal Agent For Dabigatran	2.09
4yho	Reversal Agent For Dabigatran	1.82
4yhy	Crystal Structure Of 309M3-B In Complex With Trimethylated Lys	1.9
4yhz	Crystal Structure Of 304M3-B Fab In Complex With H3k4me3 Peptide	2.3
4yjz	Human Antibody H2526 In Complex With Influenza Hemagglutinin H1 Solomon Islands/03/2006	2.72
4yk4	Human Antibody 641 I-9 In Complex With Influenza Hemagglutinin H1 Solomon Islands/03/2006	2.8
4ypg	Structural Insights Into The Neutralization Properties Of A Human Anti-Interferon Monoclonal Antibody	3
4ywg	Crystal Structure Of 830A In Complex With V1V2	3
4z0x	Structure Of Hepatitis C Virus Envelope Glycoprotein E2 Antigenic Region 434-446 Bound To The Broadly Neutralizing Antibody HC26AM	2
4z5r	Rontalizumab Fab Bound To Interferon-A2	3
4zd3	Structure Of A Transglutaminase 2-Specific Autoantibody Fab Fragment	2.4
4zfg	Dual-Specificity Fab 5A12 In Complex With Angiopoietin 2	2.27
4zs6	Receptor Binding Domain And Fab Complex	3.17

4zyk	Crystal Structure Of Quaternary-Specific RSV-Neutralizing Human Antibody AM14	2
5aam	Structure Of A Redesigned Cross-Reactive Antibody To Dengue Virus With Increased In Vivo Potency	2.49
5alb	Ticagrelor Antidote Candidate MEDI2452 In Complex With Ticagrelor	2.16
5anm	Crystal Structure Of Ige Fc In Complex With A Neutralizing Antibody	2.85
5awn	Crystal Structure Of Human Anti-HIV-1 Broadly Neutralizing Antibody 3BC176 Fab	1.89
5b71	Crystal Structure Of Complement C5 In Complex With SKY59	2.11
5bjz	Crystal Structure Of Maltose Binding Protein In Complex With An Allosteric Synthetic Antibody	1.95
5bk1	Crystal Structure Of Maltose Binding Protein In Complex With An Endosteric Synthetic Antibody	2.15
5bk2	Crystal Structure Of Maltose Binding Protein In Complex With A Peristeric Synthetic Antibody	2.6
5bk3	Crystal Structure Of The Neutralizing Anti-Circumsporozoite Protein 580 Antibody	2.8
5bk5	Crystal Structure Of The Anti-Circumsporozoite Protein 663 Germline Antibody	3
5bo1	Crystal Structure Of A Human Jag1 Fragment In Complex With An Anti-Jag1 Fab	2.56
5bv7	Crystal Structure Of Human LCAT (L4F, N5D) In Complex With Fab Of An Agonistic Antibody	2.45
5bvj	The Molecular Mode Of Action And Species Specificity Of Canakinumab, A Human Monoclonal Antibody Neutralizing IL-1beta	2
5bzd	Crystal Structure Of PCDN-27A, An Antibody From The PCDN Family Of HIV-1 Antibodies	2.7
5bzw	Crystal Structure Of PCDN-27B, An Antibody From The PCDN Family Of HIV-1 Antibodies	2.9
5c2b	Anti-CXCL13 Parental Scfv - 3B4	1.4
5c6w	Anti-CXCL13 Scfv - E10	1.54
5c8j	A Yidc-Like Protein In The Archaeal Plasma Membrane	3.5
5cck	Crystal Structure Of Human Anti-HIV-1 Broadly Neutralizing Antibody 3BC315 Fab	1.95
5cd3	Structure Of Immature VRC01-Class Antibody DRVIA7	2.9

5cex	Crystal Structure Of Fab 32H+109L, A Putative Precursor Of The PGT121 Family Of Potent HIV-1 Antibodies	2.11
5cgy	Fab Fragment Of Chikungunya Virus Neutralizing Human Monoclonal Antibody 4J21	2.07
5chn	Fab Fragments Of Chikungunya Virus Neutralizing Human Monoclonal Antibody 5M16	2.05
5cil	Crystal Structure Of Non-Neutralizing Version Of 4E10 (WDWD) With Epitope Bound	1.81
5cin	Crystal Structure Of Non-Neutralizing Version Of 4E10 (Deltaloop) With Epitope Bound	1.7
5cus	Crystal Structure Of Serbb3-Fab3379 Complex	3.2
5czv	Crystal Structure Of Notch3 NRR In Complex With 20350 Fab	3.19
5czx	Crystal Structure Of Notch3 NRR In Complex With 20358 Fab	2.1
5d1z	Isdb NEAT1 Bound By Clone D4-10	3.17
5d6c	Structure Of 4497 Fab Bound To Synthetic Wall Teichoic Acid Fragment	1.72
5d72	Crystal Structure Of MOR04252, A Neutralizing Anti-Human GM-CSF Antibody Fab Fragment In Complex With Human GM-CSF	2.6
5d7s	Crystal Structure Of MOR04357, A Neutralizing Anti-Human GM-CSF Antibody Fab Fragment	1.88
5d9q	Crystal Structure Of The BG505 SOSIP Gp140 HIV-1 Env Trimer In Complex With The Broadly Neutralizing Fab PGT122 And Scfv NIH45-46	4.4
5dd0	Crystal Structures In An Anti-HIV Antibody Lineage From Immunization Of Rhesus Macaques	2.49
5dd5	Crystal Structures In An Anti-HIV Antibody Lineage From Immunization Of Rhesus Macaques	1.9
5dr5	Crystal Structure Of The Sclerostin-Neutralizing Fab Abd09097	1.85
5drw	Crystal Structure Of The BCR Fab Fragment From Subset #4 Case CLL183	2.27
5drz	Crystal Structure Of Anti-HIV-1 Antibody F240 Fab In Complex With Gp41 Peptide	2.54
5dum	Crystal Structure Of Influenza A Virus H5 Hemagglutinin Globular Head In Complex With The Fab Of Antibody 65C6	3
5dur	Influenza A Virus H5 Hemagglutinin Globular Head In Complex With Antibody 100F4	2.82
5e8e	Crystal Structure Of Thrombin Bound To An Exosite 1-Specific Iga Fab	1.9

5ea0	Structure Of The Antibody 7968 With Human Complement Factor H-Derived Peptide	2
5eii	Structural Determination Of An Protein Complex Of A Fab With Increased Solubility	2.44
5esv	Crystal Structure Of Broadly Neutralizing Antibody CH03, Isolated From Donor CH0219, In Complex With Scaffolded Trimeric HIV-1 Env V1V2 Domain From The Clade C Superinfecting Strain Of Donor CAP256.	3.11
5eu7	Crystal Structure Of HIV-1 Integrase Catalytic Core In Complex With Fab	2.64
5f3h	Structure Of Myostatin In Complex With Humanized RK35 Antibody	2.7
5f6h	Crystal Structure Of Tier 2 Neutralizing Antibody DH427 From A Rhesus Macaque	2.66
5f6i	Crystal Structure Of Tier 2 Neutralizing Antibody DH428 From A Rhesus Macaque	2.32
5f72	De Novo Design And Crystallographic Validation Of Antibodies Targeting A Pre-Selected Epitope	1.85
5f96	Crystal Structure Of Broadly Neutralizing VH1-46 Germline-Derived CD4-Binding Site-Directed Antibody CH235.12 In Complex With HIV-1 Clade A/E 93TH057 Gp120	2.24
5f9o	Crystal Structure Of Broadly Neutralizing VH1-46 Germline-Derived CD4-Binding Site-Directed Antibody CH235.09 In Complex With HIV-1 Clade A/E 93TH057 Gp120	1.86
5f9w	Crystal Structure Of Broadly Neutralizing VH1-46 Germline-Derived CD4-Binding Site-Directed Antibody CH235 In Complex With HIV-1 Clade A/E 93TH057 Gp120	2.89
5fcu	Crystal Structure Of The Inner Domain Of Clade A/E Hiv-1 Gp120 In Complex With The Adcc-Potent Rhesus Macaque Antibody Jr4	1.85
5feh	Crystal Structure Of PCT64_35B, A Broadly Neutralizing Anti-HIV Antibody	3.1
5fha	Crystal Structure Of Protective Ebola Virus Antibody 114	1.97
5fhb	Crystal Structure Of Protective Ebola Virus Antibody 100	1.97
5fuz	Extending The Half-Life Of A Fab Fragment Through Generation Of A Humanised Anti-Human Serum Albumin (HSA) Fv Domain: An Investigation Into The Correlation Between Affinity And Serum Half-Life	2.68
5g64	The Complex Between Human Ige-Fc And Two Anti-Ige Fab Fragments	3.71
5ggq	Crystal Structure Of Nivolumab Fab Fragment	1.9
5ggs	PD-1 In Complex With Pembrolizumab Fab	2

5ggt	PD-L1 In Complex With BMS-936559 Fab	2.8
5ggv	CTLA-4 In Complex With Tremelimumab Fab	2
5gks	Crystal Structure Of SLE Patient-Derived Anti-DNA Antibody	2.05
5gmq	Structure Of MERS-Cov RBD In Complex With A Fully Human Antibody MCA1	2.7
5gru	Structure Of Mono-Specific Diabody	1.96
5grv	Crystal Structure Of Homo-Specific Diabody	2.3
5grw	Crystal Structure Of Homo-Specific Diabody	2.8
5grx	Crystal Structure Of Disulfide-Bonded Diabody	2
5gry	Crystal Structure Of Disulfide-Bonded Diabody	1.64
5grz	Crystal Structure Of Disulfide-Bonded Diabody	2.7
5gs1	Crystal Structure Of Homo-Specific Diabody	2
5gzo	Structure Of Neutralizing Antibody Bound To Zika Envelope Protein	2.76
5hi4	Binding Site Elucidation And Structure Guided Design Of Macrocyclic IL-17A Antagonists	1.8
5i15	Crystal Structure Of Human Germline Antibody Ighv1-69/Igkv1-39	2.6
5i16	Crystal Structure Of Human Germline Antibody Ighv1-69/Igkv3-11	1.9
5i17	Crystal Structure Of Human Germline Antibody Ighv1-69/Igkv3-20	3.3
5i19	Crystal Structure Of Human Germline Antibody Ighv3-23/Igkv1-39	2.8
5i1a	Crystal Structure Of Human Germline Antibody Ighv3-23/Igkv3-11	2
5i1c	Crystal Structure Of Human Germline Antibody Ighv3-23/Igkv3-20	2.25
5i1d	Crystal Structure Of Human Germline Antibody Ighv3-23/Igkv4-1	2
5i1e	Crystal Structure Of Human Germline Antibody Ighv3-53/Igkv1-39	2.7
5i1g	Crystal Structure Of Human Germline Antibody Ighv3-53/Igkv3-11	2.3
5i1h	Crystal Structure Of Human Germline Antibody Ighv3-53/Igkv3-20	2.22
5i1i	Crystal Structure Of Human Germline Antibody Ighv3-53/Igkv4-1	2.5
5i1l	Crystal Structure Of Human Germline Antibody Ighv5-51/Igkv4-1	1.95
5i8c	Crystal Structure Of HIV-1 Clade A BG505 Fusion Peptide (Residue 512-520) In Complex With Broadly Neutralizing Antibody VRC34.01 Fab	1.54
5ibt	UCA Fab (Unbound) From 6515 Lineage	2.4
5ibu	6652 Fab (Unbound)	1.71

5ifh	Crystal Structure Of The BCR Fab Fragment From Subset #2 Case P11475	2.29
5ig7	Crystal Structure Of Anti-Gliadin 1002-1E01 Fab Fragment In Complex Of Peptide PLQPQQPFP	1.97
5igx	Crystal Structure Of NIH45-46 Fab Germline Precursor In Complex With 426c.TM1deltaV1-3 Gp120	3.39
5ik3	Crystal Structure Of Anti-Gliadin 1002-1E03 Fab Fragment	1.65
5iq7	Crystal Structure Of 10E8-S74W Fab In Complex With An HIV-1 Gp41 Peptide.	3.29
5iq9	Crystal Structure Of 10E8v4 Fab In Complex With An HIV-1 Gp41 Peptide.	2.4
5it2	Structure Of A Transglutaminase 2-Specific Autoantibody 693-10-B06 Fab Fragment	1.7
5itb	Crystal Structure Of The Anti-RSV F Fab 14N4	2
5iwl	CD47-Diabody Complex	2.8
5j13	Structural Basis For TSLP Antagonism By The Therapeutic Antibody Tezepelumab (MEDI9929 / AMG-157)	2.3
5j75	Fluorogen Activating Protein AM2.2 In Complex With ML342	2
5jo4	Antibody Fab Fragment Complex	2.53
5jof	Crystal Structure Of VRC03 Ghvglv Antigen-Binding Fragment.	3.21
5jr1	Crystal Structure Of 10E8 Ghv-Maturel Antigen-Binding Fragment.	1.6
5jrp	Crystal Structure Of Monoclonal Antibody MR78 Fab	2
5jw5	Structure Of MEDI8852 Fab Fragment	1.9
5jz7	NGF IN COMPLEX WITH MEDI578 Scfv	3.4
5k59	Crystal Structure Of Lukgh From Staphylococcus Aureus In Complex With A Neutralising Antibody	2.84
5k9j	Crystal Structure Of Multidonor HV6-1-Class Broadly Neutralizing Influenza A Antibody 56.A.09 Isolated Following H5 Immunization.	1.9
5kg9	Crystal Structure Of The Gp120 V2 Antibody RE505-22 Fab From IGH- And IGK-Humanized Mouse	2.3
5kn5	Tgfalpha/Epiregulin Complex With Neutralizing Antibody LY3016859	2.8
5kw9	Structural Basis For Norovirus Neutralization By A HBGA Blocking Human Iga Antibody	2.3
5l6y	Il13 In Complex With Tralokinumab	1.99
5lbs	Structural Basis Of Zika And Dengue Virus Potent Antibody Cross-Neutralization	2.41

5lsp	107_A07 Fab In Complex With Fragment Of The Met Receptor	2.61
5mes	Mcl1 Fab Complex In Complex With Compound 29	2.24
5mvz	Fab 4AB007 Bound To Interleukin-1-Beta	2.15
5n2k	Structure Of Unbound Briakinumab Fab	2.22
5n4g	Human Fab Fragment 12E1 Against NHBA From Neisseria Meningitidis	2.75
5n4j	Human Fab Fragment 10C3 Against NHBA From Neisseria Meningitidis	1.5
5nb5	Principles For Computational Design Of Antibodies	3
5nhw	Crystal Structure Of The Bimagrumab Fab	1.78
5ob5	Fab Complex With Grobeta. Abvance: Increasing Our Knowledge Of Antibody Structural Space To Enable Faster And Better Decision-Making In Antibody Drug Discovery.	1.65
5ogi	Complex Of A Binding Protein And Human Adenovirus C 5 Hexon	2.8
5sx5	Crystal Structure Of Panitumumab In Complex With Epidermal Growth Factor Receptor Domain 3 Mutant S468R.	2.5
5sy8	Crystal Structure Of The Complex Of 10E8 Fab Light Chain Mutant1 And T117v2 HIV-1 MPER Scaffold	1.62
5t29	Crystal Structure Of 10E8 Fab Light Chain Mutant3, Against The MPER Region Of The HIV-1 Env, In Complex With The MPER Epitope Scaffold T117v2	2.03
5t4z	Structure Of The Anti-Hiv Antibody Dh501 That Binds Gp120 V3 Glycan And The Base Of V3 With Free Man9 Glycan	1.99
5t5b	Crystal Structure Of The Complex Of 10e8 Fab Light Chain Mutant5 And T117v2 Hiv-1 Mper Scaffold	2.07
5t6l	Crystal Structure Of 10E8 Fab In Complex With The MPER Epitope Scaffold T117v2	2.1
5tdn	Crystal Structure Of The Fab Fragment Of Anti-HER2 Antibody 4D5 With Redesigned Heavy And Light Chain Interfaces	1.63
5tdo	Crystal Structure Of The Fab Fragment Of Anti-HER2 Antibody 4D5 With Redesigned Heavy And Light Chain Interfaces	1.61
5te7	Crystal Structure Of Broadly Neutralizing VRC01-Class Antibody N6 In Complex With HIV-1 Clade C Strain DU172.17 Gp120 Core	2.15
5tf1	Structure Of Chimeric 02-CC Fab, A VRC01-Like Germline Antibody	1.86
5tfs	Structure Of Chimeric 02-K Fab, A VRC01-Like Germline Antibody	2.32

5tfw	Crystal Structure Of 10E8 Fab Light Chain Mutant2 Against The MPER Region Of The HIV-1 Env, In Complex With T117v2 Epitope Scaffold	2.17
5tgb	Structure Of Chimeric 02-CB Fab, A VRC01-Like Germline Antibody	2.74
5tpl	Crystal Structure Of DH270.3 (Unliganded) From The DH270 Broadly Neutralizing N332-Glycan Dependent Lineage	2.5
5trp	Crystal Structure Of The Unliganded DH270 Cooperating Lineage Member DH272	2.69
5tru	Structure Of The First-In-Class Checkpoint Inhibitor Ipilimumab Bound To Human CTLA-4	3
5ty6	Crystal Structure Of The Broadly Neutralizing Influenza A Antibody VRC 315 13-1b02 Fab.	1.36
5tz2	Crystal Structure Of Human CD47 ECD Bound To Fab Of C47B222	2.3
5tzt	Crystal Structure Of Human CD47 ECD Bound To Fab Of C47B161	2.89
5u0r	Crystal Structure Of DH270.UCA1 (Unliganded) From The DH270 Broadly Neutralizing N332-Glycan Dependent Lineage	3.3
5u0u	Crystal Structure Of DH270.1 (Unliganded, Single-Chain Fv) From The DH270 Broadly Neutralizing N332-Glycan Dependent Lineage	3.43
5u15	Crystal Structure Of DH270.UCA3 (Unliganded) From The DH270 Broadly Neutralizing N332-Glycan Dependent Lineage	2.26
5u3j	Crystal Structure Of DH511.1 Fab In Complex With HIV-1 Gp41 MPER Peptide	2.74
5u3l	Crystal Structure Of DH511.2 Fab In Complex With HIV-1 Gp41 MPER 670-683 Peptide	2.16
5u3o	Crystal Structure Of DH511.2_K3 Fab In Complex With HIV-1 Gp41 MPER Peptide	1.76
5u3p	Crystal Structure Of DH511.4 Fab	1.5
5u4r	Crystal Structure Of The Broadly Neutralizing Influenza A Antibody VRC 315 53-1A09 Fab.	1.76
5u68	Structural Basis For Antibody Cross-Neutralization Of Respiratory Syncytial Virus And Human Metapneumovirus	3.08
5u7o	Crystal Structure Of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound To Small Molecule HIV-1 Entry Inhibitor BMS-626529 In Complex With Human Antibodies PGT122 And 35O22 At 3.8 Angstrom	3.03
5uby	Fab Structure Of Anti-HIV-1 Gp120 Mab 1A8	2.6
5ubz	Fab Structure Of HIV Gp120 Specific Mab 1E12	2.75

5ucb	Structure Of Antigen-Fab Complex With Engineered Switch Residue Region.	1.52
5udc	Crystal Structure Of RSV F A2 Bound To MEDI8897	3.45
5uea	Structure Of Antigen-Fab Complex With Histone Chaperone ASF1	1.7
5uek	Structure Of Antigen-Fab 12E Complex With Histone Chaperone ASF1	1.7
5uem	Crystal Structure Of 354NC37 Fab In Complex With HIV-1 Clade AE Strain 93TH057 Gp120	2.7
5ukn	Structure Of Unliganded Anti-Gp120 CD4bs Antibody DH522UCA Fab	1.75
5uko	Structure Of Unliganded Anti-Gp120 CD4bs Antibody DH522IA Fab	2.3
5ukp	Structure Of Unliganded Anti-Gp120 CD4bs Antibody DH522.1 Fab	2
5ukq	Structure Of Unliganded Anti-Gp120 CD4bs Antibody DH522.2 Fab	2.1
5uoe	Crystal Structure Analysis Of Elbow-Engineered-Fab-Bound Human Insulin Degrading Enzyme (IDE)	3.8
5ur8	Human Antibody Fragment (Fab) To Meningococcal Factor H Binding Protein	1.76
5ush	Structure Of Vaccinia Virus D8 Protein Bound To Human Fab Vv66	2.3
5usi	Structure Of Vaccinia Virus D8 Protein Bound To Human Fab Vv138	2.9
5usl	Structure Of Vaccinia Virus D8 Protein Bound To Human Fab Vv304	2.9
5v7r	Cyrstal Structure Of Anti-Tau Antibody CBTAU-7.1 Fab	2.3
5v7u	Cyrstal Structure Of Anti-Tau Antibody CBTAU-22.1 Fab	1.64
5vag	Crystal Structure Of H7-Specific Antibody M826 In Complex With The HA1 Domain Of Hemagglutinin From H7N9 Influenza Virus	1.9
5veb	Crystal Structure Of A Fab Binding To Extracellular Domain 5 Of Cadherin-6	2.34
5vf6	Crystal Structure Of Single Chain Variable Fragment (Scfv45).	1.63
5vic	Crystal Structure Of Anti-Zika Antibody Z004 Bound To DENV-1 Envelope Protein DIII	3
5vig	Crystal Structure Of Anti-Zika Antibody Z006 Bound To Zika Virus Envelope Protein DIII	3
5vl7	PCSK9 Complex With Fab33	3.5
5vob	Crystal Structure Of HCMV Pentamer In Complex With Neutralizing Antibody 8I21	3.02
5vsi	CH1/Ckappa Fab Mutant 15.1	1.51
5vvf	Crystal Structure Of 354BG1 Fab	2

5w05	Anti-Tissue Factor Antibody M59, A Humanized Version Of 10h10	1.64
5w06	Human Tissue Factor In Complex With Antibody M1587	2.6
5w08	A/Texas/50/2012(H3N2) Influenza Hemagglutinin In Complex With K03.12 Fab	2.6
5w6c	UCA Fab (Unbound) From 6649 Lineage	1.63
5w6g	Human Antibody 6649 In Complex With Influenza Hemagglutinin H1 Solomon Islands	2.79
5waw	Fcabvance: Increasing Our Knowledge Of Antibody Structural Space To Enable Faster And Better Decision-Making In Antibody Drug Discovery	2.25
5wca	Crystal Structure Of The Broadly Neutralizing Influenza A Antibody VRC 315 27-1C08 Fab.	1.37
5wcd	Crystal Structure Of The Broadly Neutralizing Influenza A Antibody VRC 315 04-1D02 Fab.	1.81
5whj	Crystal Structure Of Fab Fragment Of Anti-Fcrn Antibody DX-2507	2.15
5wk2	Crystal Structure Of Anti-Ccl17 Antibody M116	1.5
5wuv	Crystal Structure Of Certolizumab Fab	1.95
5wym	Crystal Structure Of An Anti-Connexin26 Scfv	2.65
5x8m	PD-L1 In Complex With Durvalumab	2.66
5xaj	Structural Mimicry Of The Dengue Virus Envelope Glycoprotein Revealed By The Crystallographic Study Of An Idiotype-Anti-Idiotype Fab Complex.	2.5
5xhv	Crystal Structure Of Fab S40 In Complex With Influenza Hemagglutinin, HA1 Subunit.	3.35
5xku	Crystal Structure Of Hemagglutinin Globular Head From An H7N9 Influenza Virus In Complex With A Neutralizing Antibody Hnigga6	1.78
5xxy	Crystal Structure Of PD-L1 Complexed With Atezolizumab Fab At 2.9A	2.9
5y11	SFTSV GN With Neutralizing Antibody Mab4-5	2.1
5y9k	Structure Of The Belimumab Fab Fragment	1.9
5yax	Crystal Structure Of A Human Neutralizing Antibody Bound To A HBV Pres1 Peptide	2.5
6axk	Crystal Structure Of Fab311 Complex	2.1
6axl	Crystal Structure Of Fab317 Complex	2.4
6ayz	Crystal Structure Of Asf1-Fab 12E Complex	2.1
6az2	Crystal Structure Of Asf1-Fab 12E Complex	2.48

6azm	Crystal Structure Of The 580 Germline Antibody Bound To Circumsporozoite Protein NANP 5-Mer	1.6
6azx	Crystal Structure Of The Neutralizing Anti-Circumsporozoite Protein 663 Antibody	2.1
6azz	Crystal Structure Of Pfs25 In Complex With The Transmission Blocking Antibody 1190	2.4
6b08	Crystal Structure Of Pfs25 In Complex With The Transmission Blocking Antibody 1276	2.2
6b0a	Crystal Structure Of Pfs25 In Complex With The Transmission Blocking Antibody 1269	2.5
6b0e	Crystal Structure Of Pfs25 In Complex With The Transmission Blocking Antibody 1260	3.3
6b0g	Crystal Structure Of Pfs25 In Complex With The Transmission Blocking Antibody 1245	1.9
6b0h	Crystal Structure Of Pfs25 In Complex With The Transmission Blocking Antibody 1262	2.7
6b0w	Crystal Structure Of The Anti-Circumsporozoite Protein 1710 Antibody	1.9
6b14	Crystal Structure Of Spinach RNA Aptamer In Complex With Fab BL3-6S97N	1.64
6b3d	Crystal Structure Of Anti-HIV Antibody PGT128 In Complex With A Bacterially Derived Synthetic Mimetic Of Man9.	2.27
6b3k	Crystal Structure Of Mutant Spinach RNA Aptamer In Complex With Fab BL3-6	2.09
6be3	Crystal Structure Of A Polysaccharide-Binding Human Fab (F598) In Complex With N-Acetyl-D-Glucosamine (Glcnac)	1.6
6bhz	Trastuzumab Fab D185a (Light Chain) Mutant.	1.75
6bp2	Therapeutic Human Monoclonal Antibody MR191 Bound To A Marburgvirus Glycoprotein	3.17
6c6z	Crystal Structure Of Potent Neutralizing Antibody CDC2-C2 In Complex With MERS-Cov S1 RBD	2.1
6ehw	Scfv Abvance: Increasing Our Knowledge Of Antibody Structural Space To Enable Faster And Better Decision Making In Drug Discovery	2.19
6ehx	Scfv Abvance: Increasing Our Knowledge Of Antibody Structural Space To Enable Faster And Better Decision Making In Drug Discovery	2.2
6ehy	Scfv Abvance: Increasing Our Knowledge Of Antibody Structural Space To Enable Faster And Better Decision Making In Drug Discovery	2.25

6erx	Crystal Structure Of Human BAFF In Complex With Fab Fragment Of Anti-BAFF Antibody Belimumab	2.9
8fab	Crystal Structure Of The Fab Fragment From The Human Myeloma Immunoglobulin Igg Hil At 1.8 Angstroms Resolution	1.8

Table S2: Antibody Benchmark Set

PDB-ID	Name	Resolution (Å)	H3 loop length
1adq	Crystal Structure Of A Human Igm Rheumatoid Factor Fab In Complex With Its Autoantigen Igg Fc	3.15	14
1afv	Hiv-1 Capsid Protein (P24) Complex With Fab25.3	3.7	11
1egj	Domain 4 Of The Beta Common Chain In Complex With An Antibody	2.8	10
1eo8	Influenza Virus Hemagglutinin Complexed With A Neutralizing Antibody	2.8	9
1hez	Antibody-Antigen Complex	2.7	12
1i9r	Structure Of Cd40l In Complex With The Fab Fragment Of Humanized 5c8 Antibody	3.1	9
1iqd	Human Factor VIII C2 Domain Complexed To Human Monoclonal BO2C11 Fab.	2	8
1kb5	Murine T-Cell Receptor Variable Domain/Fab Complex	2.5	10
1ken	Influenza Virus Hemagglutinin Complexed With An Antibody That Prevents The Hemagglutinin Low Ph Fusogenic Transition	3.5	11
1ncb	Crystal Structures Of Two Mutant Neuraminidase-Antibody Complexes With Amino Acid Substitutions In The Interface	2.5	11
1nmb	The Structure Of A Complex Between The Nc10 Antibody And Influenza Virus Neuraminidase And Comparison With The Overlapping Binding Site Of The Nc41 Antibody	2.2	13
1nsn	The Crystal Structure Of Antibody N10-Staphylococcal Nuclease Complex At 2.9 Angstroms Resolution	2.8	4
1ob1	Crystal Structure Of A Fab Complex Whith Plasmodium Falciparum MSP1-19	2.9	11
1orq	X-Ray Structure Of A Voltage-Dependent Potassium Channel In Complex With An Fab	3.2	9
1osp	Crystal Structure Of Outer Surface Protein A Of Borrelia Burgdorferi Complexed With A Murine Monoclonal Antibody Fab	1.95	12
1qfu	Influenza Virus Hemagglutinin Complexed With A Neutralizing Antibody	2.8	13
1rjl	Structure Of The Complex Between Ospb-CT And Bactericidal Fab-H6831	2.6	11

1yjd	Crystal Structure Of Human CD28 In Complex With The Fab Fragment Of A Mitogenic Antibody (5.11A1)	2.7	11
1yqv	The Crystal Structure Of The Antibody Fab Hyhel5 Complex With Lysozyme At 1.7A Resolution	1.7	7
1ztx	West Nile Virus Envelope Protein DIII In Complex With Neutralizing E16 Antibody Fab	2.5	10
2adf	Crystal Structure And Paratope Determination Of 82D6A3, An Antithrombotic Antibody Directed Against The Von Willebrand Factor A3-Domain	1.9	9
2arj	CD8alpha-Alpha In Complex With YTS 105.18 Fab	2.88	9
2hmi	Hiv-1 Reverse Transcriptase/Fragment Of Fab 28/Dna Complex	2.8	13
2i9l	Structure Of Fab 7D11 From A Neutralizing Antibody Against The Poxvirus L1 Protein	3.1	10
2jel	Jel42 Fab/Hpr Complex	2.5	9
2nyy	Crystal Structure Of Botulinum Neurotoxin Type A Complexed With Monoclonal Antibody CR1	2.61	9
2nz9	Crystal Structure Of Botulinum Neurotoxin Type A Complexed With Monoclonal Antibody AR2	3.79	9
2q8b	Structure Of The Malaria Antigen AMA1 In Complex With A Growth-Inhibitory Antibody	2.3	3
2qr0	Structure Of VEGF Complexed To A Fab Containing TYR And SER In The Cdrs	3.5	9
2r29	Neutralization Of Dengue Virus By A Serotype Cross-Reactive Antibody Elucidated By Cryoelectron Microscopy And X-Ray Crystallography	3	7
2r56	Crystal Structure Of A Recombinant Ige Fab Fragment In Complex With Bovine Beta-Lactoglobulin Allergen	2.8	12
2xra	Crystal Structure Of The HK20 Fab In Complex With A Gp41 Mimetic 5- Helix	2.3	13
2ypv	Crystal Structure Of The Meningococcal Vaccine Antigen Factor H Binding Protein In Complex With A Bactericidal Antibody	1.8	10
2zch	Crystal Structure Of Human Prostate Specific Antigen Complexed With An Activating Antibody	2.83	13
2zuq	Crystal Structure Of Dsbb-Fab Complex	3.3	6
3b9k	Crystal Structure Of CD8alpha-Beta In Complex With YTS 156.7 FAB	2.7	9

3bgf	X-Ray Crystal Structure Of The SARS Coronavirus Spike Receptor Binding Domain In Complex With F26G19 Fab	3	12
3d85	Crystal Structure Of IL-23 In Complex With Neutralizing FAB	1.9	6
3eff	The Crystal Structure Of Full-Length Kcsa In Its Closed Conformation	3.8	15
3fmg	Structure Of Rotavirus Outer Capsid Protein VP7 Trimer In Complex With A Neutralizing Fab	3.4	12
3ks0	Crystal Structure Of The Heme Domain Of Flavocytochrome B2 In Complex With Fab B2B4	2.7	9
3liz	Crystal Structure Of Bla G 2 Complexed With Fab 4C3	1.8	10
3opz	Crystal Structure Of Trans-Sialidase In Complex With The Fab Fragment Of A Neutralizing Monoclonal Igg Antibody	3.4	10
3q3g	Crystal Structure Of A-Domain In Complex With Antibody	2.7	13
3r1g	Structure Basis Of Allosteric Inhibition Of BACE1 By An Exosite-Binding Antibody	2.8	10
3rkd	Hepatitis E Virus E2s Domain (Genotype I) In Complex With A Neutralizing Antibody	1.9	14
3ubx	Crystal Structure Of The Mouse CD1d-C20:2-Agalcer-L363 Mab Fab Complex	3.1	11
3v7a	Structural Basis For Broad Detection Of Genogroup II Noroviruses By A Monoclonal Antibody That Binds To A Site Occluded In The Viral Particle	3.297	11
3vg9	Crystal Structure Of Human Adenosine A2A Receptor With An Allosteric Inverse-Agonist Antibody At 2.7 A Resolution	2.7	15
3vrl	Crystal Structure Of BMJ4 P24 Capsid Protein In Complex With A10F9 Fab	3.2	13
3wfd	Reduced And Acetaldoxime-Bound Cytochrome C-Dependent Nitric Oxide Reductase (Cnor) From Pseudomonas Aeruginosa In Complex With Antibody Fragment	2.3	15
4ag4	Crystal Structure Of A DDR1-Fab Complex	2.8	7
4bz1	Structure Of Dengue Virus EDIII In Complex With Fab 3e31	2.15	8
4bz2	Structure Of Dengue Virus EDIII In Complex With Fab 2D73	2.03	12
4cad	Mechanism Of Farnesylated CAAX Protein Processing By The Integral Membrane Protease Rce1	2.5	16

4cmh	Crystal Structure Of CD38 With A Novel CD38-Targeting Antibody SAR650984	1.53	11
4ffv	Crystal Structure Of Dipeptidyl Peptidase IV (DPP4, DPP-IV, CD26) In Complex With 11A19 Fab	2.4	8
4h88	Structure Of POM1 FAB Fragment Complexed With Mouse Prpc Fragment 120-230	1.9	10
4ht1	Human TWEAK In Complex With The Fab Fragment Of A Neutralizing Antibody	2.498	11
4jr9	Crystal Structure Of Nitrate/Nitrite Exchanger Nark	2.6	9
4jzj	Crystal Structure Of Receptor-Fab Complex	2.801	11
4k2u	Crystal Structure Of Pfeba-175 F1 In Complex With R218 Antibody Fab Fragment	2.45	12
4lvn	Crystal Structure Of Pfsub1-Prodomain-NIMP.M7 Fab Complex	2.25	11
4np4	Clostridium Difficile Toxin B CROP Domain In Complex With FAB Domains Of Neutralizing Antibody Bezlotoxumab	2.89	10
4plj	Hepatitis E Virus E2s Domain (Genotype IV) In Complex With A Neutralizing Antibody 8G12	2.3	14
4q6i	Crystal Structure Of Murine 2D5 Fab, A Potent Anti-CD4 HIV-1-Neutralizing Antibody In Complex With CD4	3.65	11
4qww	Crystal Structure Of The Fab410-Bfache Complex	2.7	14
4rdq	Calcium-Activated Chloride Channel Bestrophin-1, From Chicken, In Complex With Fab Antibody Fragments, Chloride And Calcium	2.85	7
4rgm	Structure Of Staphylococcal Enterotoxin B Bound To The Neutralizing Antibody 20B1	2.689	12
4rgo	Structure Of Staphylococcal Enterotoxin B Bound To The Neutralizing Antibody 14G8	1.8	12
4tnw	C. Elegans Glutamate-Gated Chloride Channel (Glucl) In Complex With Fab And Popc In A Lipid-Modulated Conformation	3.2	13
4uao	Crystal Structure Of Apical Membrane Antigen 1 From Plasmodium Knowlesi In Complex With An Invasion Inhibitory Antibody	3.1	12
4zpt	Structure Of MERS-Coronavirus Spike Receptor-Binding Domain (England1 Strain) In Complex With Vaccine-Elicited Murine Neutralizing Antibody D12 (Crystal Form 1)	2.591	7
5bv7	Crystal Structure Of Human LCAT (L4F, N5D) In Complex With Fab Of An Agonistic Antibody	2.45	16

5czx	Crystal Structure Of Notch3 NRR In Complex With 20358 Fab	2.1	10
5dfv	Crystal Structure Of Human Cd81 Large Extracellular Loop In Complex With Murine Fab Fragment K04	2.8	12
5hbt	Complex Structure Of Fab35 And Human Nachr Alpha1	2.61	12
5kvf	Zika Specific Antibody, ZV-64, Bound To ZIKA Envelope DIII	1.4	10
5lqb	Complex Structure Of Human IL2 Mutant, Proleukin, With Fab Fragment Of NARA1 Antibody	1.95	12
5mhr	T3D Reovirus Sigma1 Complexed With 9BG5 Fab Fragments	3	12
5t5f	Neisseria Meningitidis Factor H Binding Protein In Complex With Monoclonal Antibody JAR5	2.98	13
5ush	Structure Of Vaccinia Virus D8 Protein Bound To Human Fab Vv66	2.3	13
5usl	Structure Of Vaccinia Virus D8 Protein Bound To Human Fab Vv304	2.9	15
5veb	Crystal Structure Of A Fab Binding To Extracellular Domain 5 Of Cadherin-6	2.34	9
5y9c	Crystal Structure Of HPV58 Pentamer In Complex With The Fab Fragment Of Antibody A12A3	3.443	11
5y9f	Crystal Structure Of HPV59 Pentamer In Complex With The Fab Fragment Of Antibody 28F10	3.35	14
6bpa	Plasmodium Vivax Reticulocyte Binding Protein 2b (Pvrbp2b) Bound To Monoclonal Antibody 3E9	2.53	11

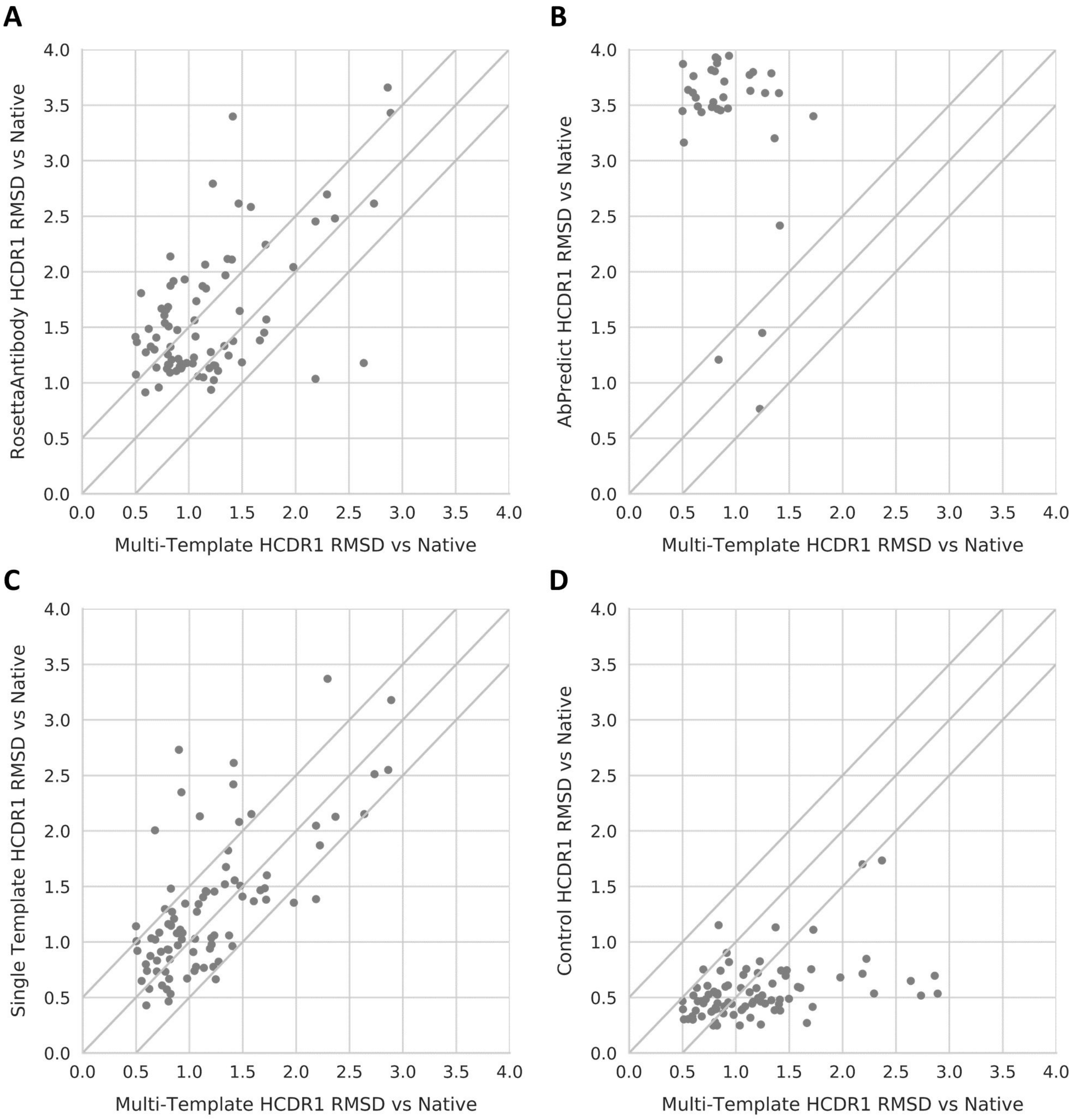

Figure S1: Comparison of antibody HCDR1 modeling performance for the best models produced by each method to the best multi-template models. The performance of RosettaAntibody (A), AbPredict (B), Single Template (C), and our control method (D) were each individually compared to our multi-template method by graphing that method's median RMSD against our multi-template method's median RMSD for each antibody. Each chart has a line at y=x representing equal performance between methods. Points above the line represent cases where our multi-template method outperformed another method, whereas points below the line represent the opposite case.

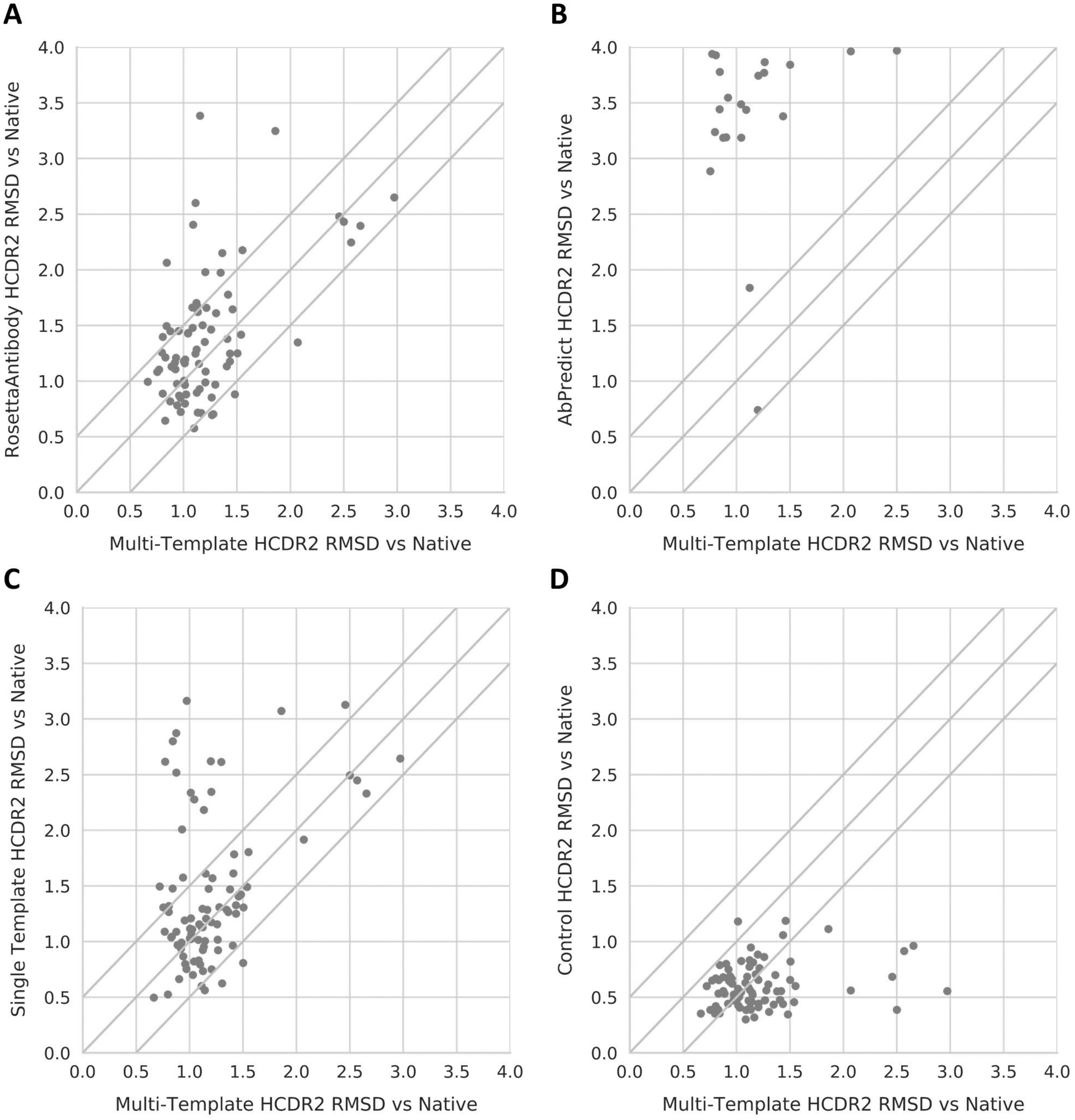

Figure S2: Comparison of antibody HCDR2 modeling performance for the best models produced by each method to the best multi-template models. The performance of RosettaAntibody (A), AbPredict (B), Single Template (C), and our control method (D) were each individually compared to our multi-template method by graphing that method's median RMSD against our multi-template method's median RMSD for each antibody. Each chart has a line at y=x representing equal performance between methods. Points above the line represent cases where our multi-template method outperformed another method, whereas points below the line represent the opposite case.

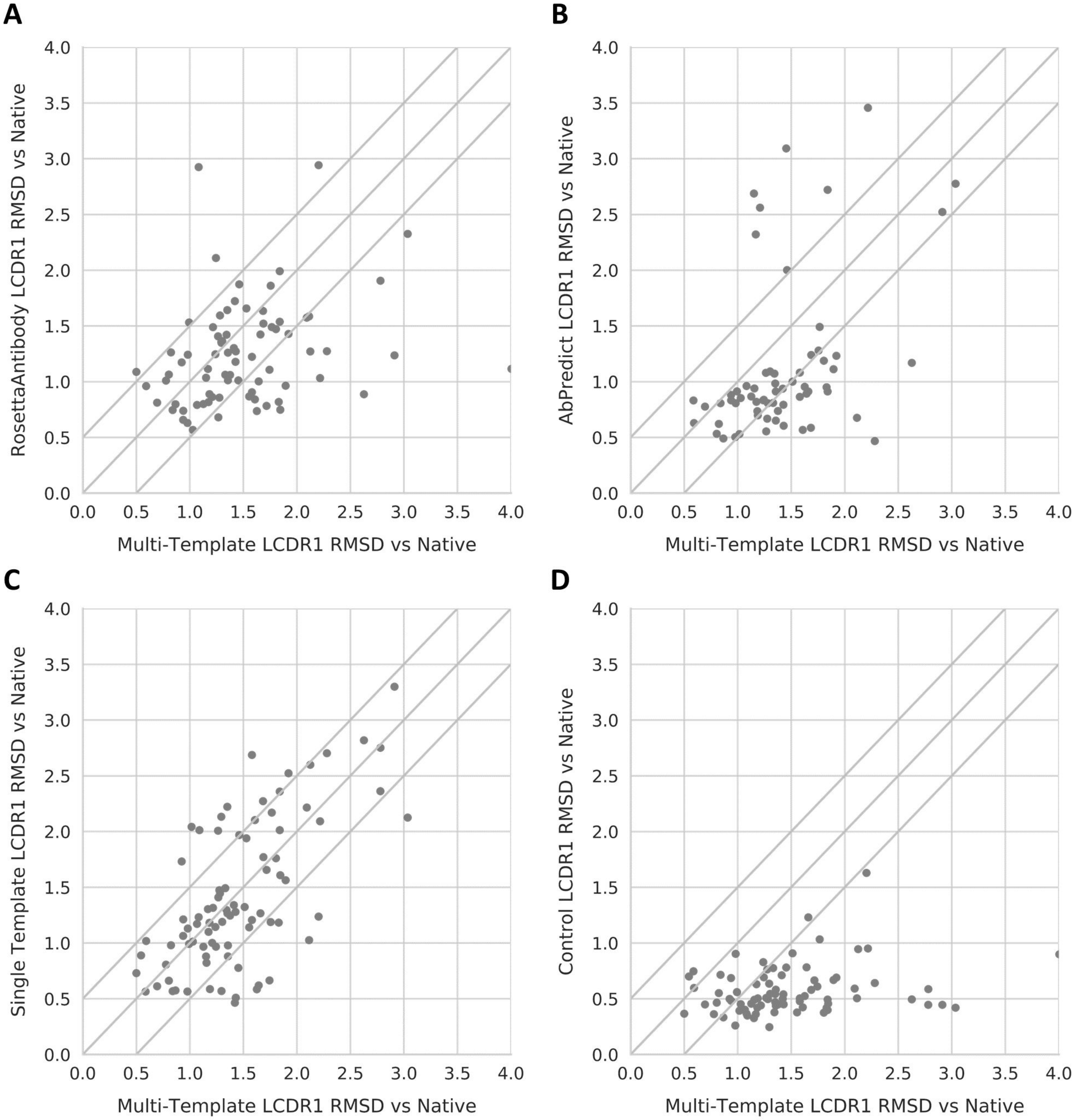

Figure S3: Comparison of antibody LCDR1 modeling performance for the best models produced by each method to the best multi-template models. The performance of RosettaAntibody (A), AbPredict (B), Single Template (C), and our control method (D) were each individually compared to our multi-template method by graphing that method's median RMSD against our multi-template method's median RMSD for each antibody. Each chart has a line at y=x representing equal performance between methods. Points above the line represent cases where our multi-template method outperformed another method, whereas points below the line represent the opposite case.

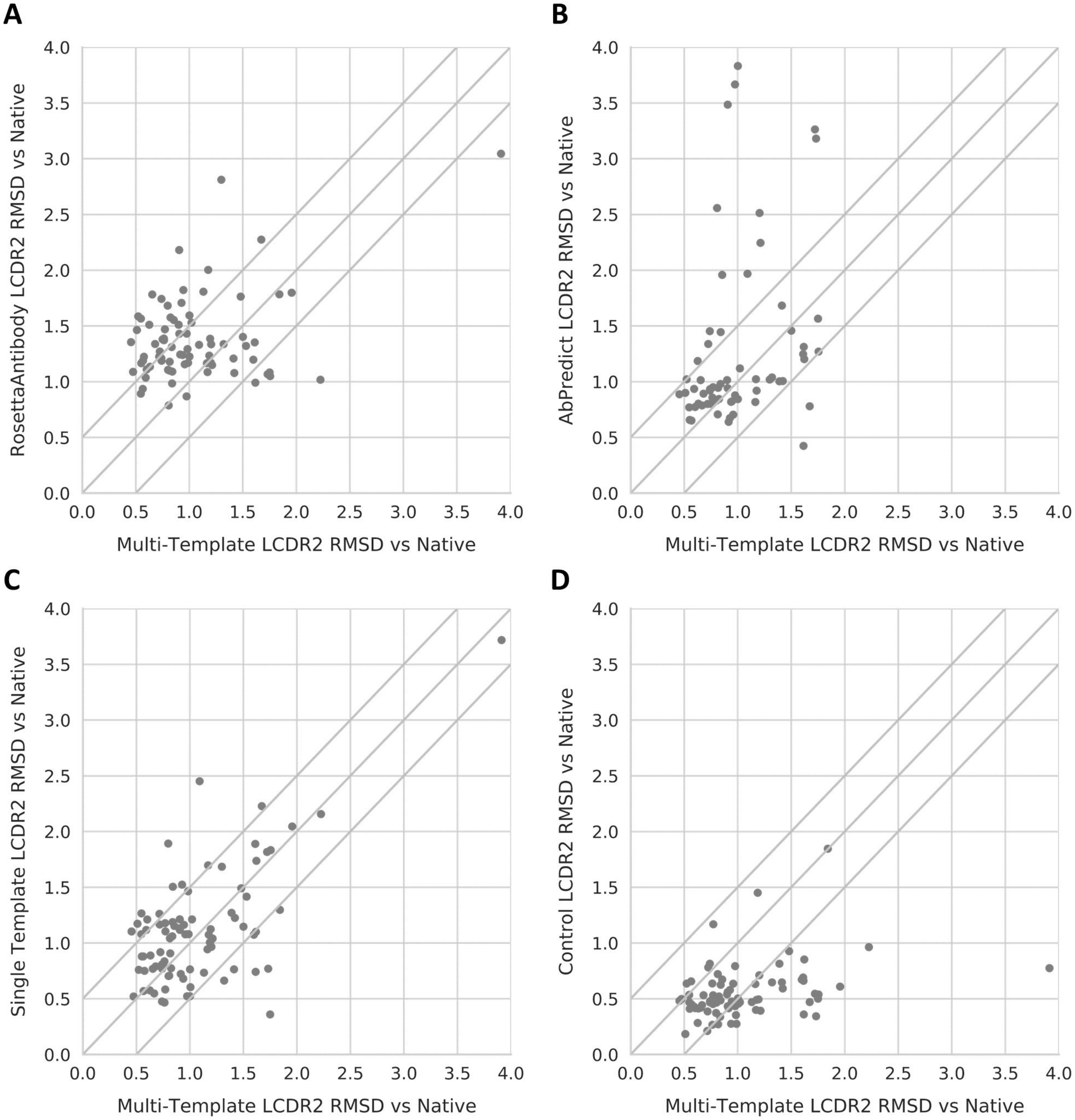

Figure S4: Comparison of antibody LCDR2 modeling performance for the best models produced by each method to the best multi-template models. The performance of RosettaAntibody (A), AbPredict (B), Single Template (C), and our control method (D) were each individually compared to our multi-template method by graphing that method's median RMSD against our multi-template method's median RMSD for each antibody. Each chart has a line at y=x representing equal performance between methods. Points above the line represent cases where our multi-template method outperformed another method, whereas points below the line represent the opposite case.

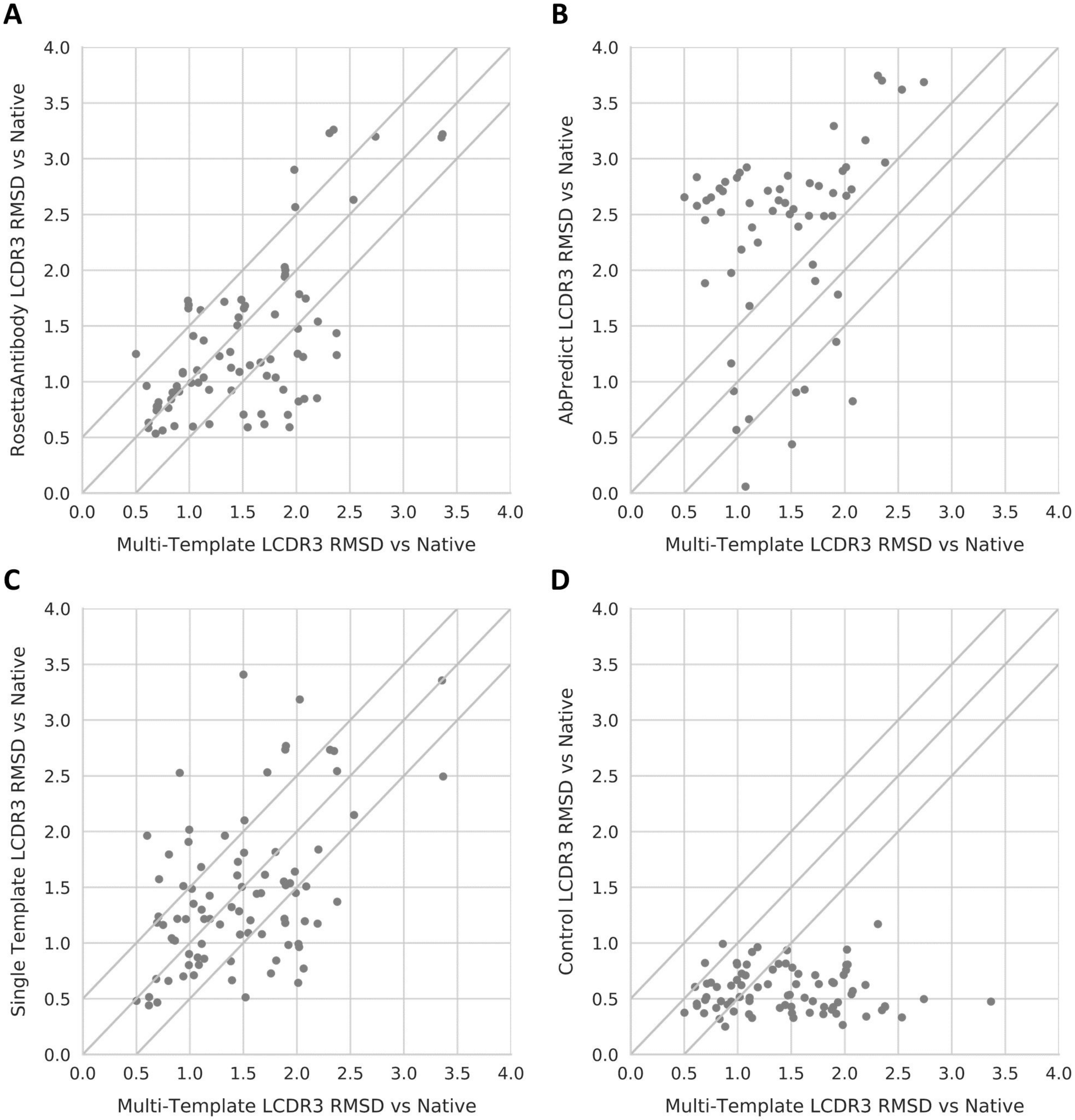

Figure S5: Comparison of antibody LCDR3 modeling performance for the best models produced by each method to the best multi-template models. The performance of RosettaAntibody (A), AbPredict (B), Single Template (C), and our control method (D) were each individually compared to our multi-template method by graphing that method's median RMSD against our multi-template method's median RMSD for each antibody. Each chart has a line at y=x representing equal performance between methods. Points above the line represent cases where our multi-template method outperformed another method, whereas points below the line represent the opposite case.

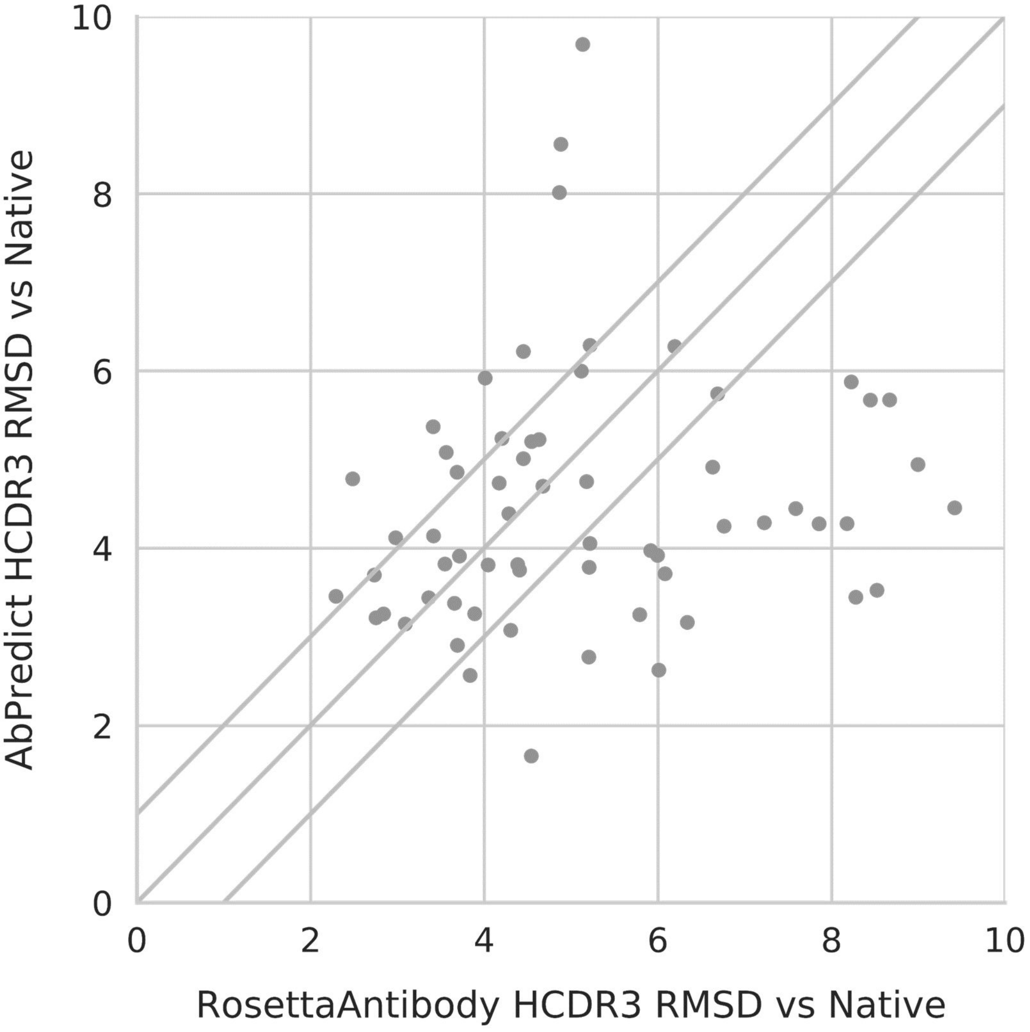

Figure S6: Comparison of antibody HCDR3 modeling performance for the bets models produced by AbPredict against RosettaAntibody. Each method's median RMSD was graphed against each other for each antibody. The cart has a line at y=x representing equal performance between methods. Points above the line represent cases where RosettaAntibody outperformed AbPredict, whereas points below the line represent the opposite case.

The following example commands have been executed to model the human IGM rheumatoid factor Fab and can be used for any other Fab.

Homology Modeling of Human IGM Rheumatoid Factor Fab using RosettaCM

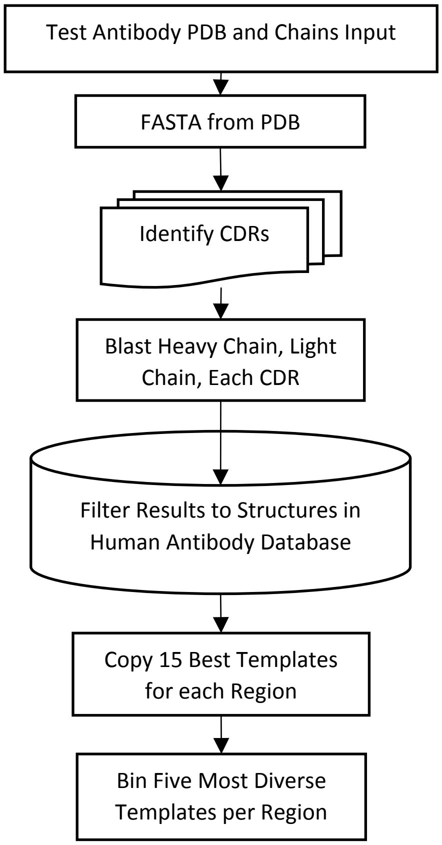

Figure S7: RosettaCM Template selection

Structure and input preparation

For all RosettaCM modeling, Rosetta-3.7 was used

Identification of CDRs:

```
def IdentifyCDRs(light_chain, heavy_chain):
	""" Determination of loops in both light and heavy chains

	light_chain -- string representation of light chain
	heavy_chain -- string representation of heavy chain
	"""

	L1_pattern=r'C[A-Z]{1,17}(WYL|WLQ|WFQ|WYQ|WYH|WVQ|WVR|WWQ|WVK|WYR|WLL|WFL|WVF|WIQ|WYR|WNQ|WHL|WHQ|WYM|WYY)'
	L3_pattern=r'C[A-Z]{1,15}(L|F|V|S)G[A-Z](G|Y)'
```

```
        H1_pattern=r'C[A-Z]{1,16}(W)(I|V|F|Y|A|M|L|N|G)(R|K|Q|V|N|C|G)(Q|K|H|E|L|R)' # Jeff's mod
for ATHM set
  #H1_pattern=r'C[A-Z]{1,16}(W)(I|V|F|Y|A|M|L|N|G)(R|K|Q|V|N|C)(Q|K|H|E|L|R)'
        H3_pattern=r'C[A-Z]{1,33}(W)(G|A|C)[A-Z]{1,2}(Q|S|G|R)'

        ''' Identify CDR region and return them as dict with keys: 'FR_H1', 'FR_H2', 'FR_H3', 'FR_H4',
'FR_L1', 'FR_L2', 'FR_L3', 'FR_L4', 'H1', 'H2', 'H3', 'L1', 'L2', 'L3'
        '''
        light_first = light_chain[:65] if len(light_chain) > 130 else light_chain[:60]
        heavy_first = heavy_chain[:70] if len(heavy_chain) > 140 else heavy_chain[:60]
        len_FR_L1=0
        res = re.search(L1_pattern,light_first)
        FR_L1 = L1 = False
        if res:
                L1 = res.group()[1:-3]
                L1_start = light_chain.index(L1)
                L1_end = L1_start + len(L1) - 1
                print(("L1 detected: %s (%d residues at positions %d to %d)" % (L1, len(L1), L1_start,
L1_end)))
                FR_L1 = light_chain[:L1_start]
                if len(FR_L1) >  24:
                        len_FR_L1 = len(FR_L1) - 24
                        FR_L1 = light_chain[len_FR_L1:L1_start]
        else:
                print("L1 detected: False")

        light_second = light_chain[L1_end+16+7:L1_end+16+7+80] if len(light_chain) > 130 else
light_chain[L1_end+16+7:]

        ## L3
        L3 = False
        res = re.search(L3_pattern,light_second)
        if res:
                L3 = res.group()[1:-4]
                L3_start = light_chain.index(L3)
                L3_end = L3_start + len(L3) - 1
                print(("L3 detected: %s ( %d residues at positions %d to %d)" % (L3, len(L3), L3_start,
L3_end)))
        else:
                print("L3 detected: False")
        if L1 and L3:
                #L1_start = light_chain.index(L1)
                #L1_end = L1_start + len(L1) - 1

                L2_start = L1_end + 16
                L2_end = L2_start + 7 - 1
```

```
        L2 = light_chain[L2_start:L2_start+7]  # L2 is identified here. Current implementation can
deal with only 7-resiue L2
        print(("L2 detected: %s (%d residues at positions %d to %d)" % (L2, len(L2), L2_start,
L2_end)))

        #FR_L1 = light_chain[:L1_start]
        FR_L2 = light_chain[ L1_end + 1  :  L1_end + 1 + 15
    ]
        FR_L3 = light_chain[ L2_end + 1  :  L2_end + 1 + L3_start - L2_end - 1 ]
        FR_L4 = light_chain[ L3_end + 1  :  L3_end + 1 + 12
    ]

        print(("FR_L1: ", FR_L1))
        print(("FR_L2: ", FR_L2))
        print(("FR_L3: ", FR_L3))
        print(("FR_L4: ", FR_L4))
        print(("L segments: ",FR_L1,L1,FR_L2,L2,FR_L3,L3,FR_L4))
    # HH EE AA VV YY
    ## H1
    res = re.search(H1_pattern, heavy_first)
    H1 = False
    len_FR_H1 = 0
    if res:
        H1 = res.group()[4:-4]
        H1_start = heavy_chain.index(H1)
        H1_end = H1_start + len(H1) - 1
        print(("H1 detected: %s (%d residues at positions %d to %d)" % (H1, len(H1), H1_start,
H1_end)))
        FR_H1 = heavy_chain[:H1_start]
        if len(FR_H1) >  25:
            len_FR_H1 = len(FR_H1) - 25
            FR_H1 = heavy_chain[len_FR_H1:H1_start]
    else:
        print("H1 detected: False")

    heavy_second = heavy_chain[H1_end+33+15:H1_end+33+15+95+len_FR_H1] if
len(heavy_chain) > 140 else heavy_chain[H1_end+33+15:]

    ## H3
    H3 = False #H3_and_stem=False
    res = re.search(H3_pattern,heavy_second)
    if res:
        H3 = res.group()[3:-4] #H3_and_stem = res.group()[0:-4]
        H3_start = heavy_chain.index(H3)
        H3_end = H3_start + len(H3) - 1
        print(("H3 detected: %s (%d residues at positions %d to %d)" % (H3, len(H3), H3_start,
H3_end)))
```

```
    else:
        print("H3 detected: False")
    if H1 and H3:
        #H1_start = heavy_chain.index(H1)
        #H1_end = H1_start + len(H1) - 1
        H2_start = H1_end + 15
        H2_end = H3_start - 33
        H2 = heavy_chain[H2_start:H2_start + H2_end-H2_start+1]
        print(("H2 detected: %s (%d residues at positions %d to %d)" % (H2, len(H2), H2_start,
H2_end)))
        #FR_H1 = heavy_chain[:H1_start]
        #if len(FR_H1) >  26:
        #       FR_H1 = light_chain[20:H1_start]
        FR_H2 = heavy_chain[H1_end + 1: H1_end + 1 + H2_start - H1_end - 1]
        FR_H3 = heavy_chain[H2_end + 1: H2_end + 1 + H3_start - H2_end - 1]
        FR_H4 = heavy_chain[H3_end + 1: H3_end + 1 + 12]
        print(("FR_H1: ", FR_H1))
        print(("FR_H2: ", FR_H2))
        print(("FR_H3: ", FR_H3))
        print(("FR_H4: ", FR_H4))
        print(("H segments: ",FR_H1,H1,FR_H2,H2,FR_H3,H3,FR_H4))
    if not (L1 and L3 and H1 and H3):
        if not L1: print(('ERROR: CDR L1 cannot be recognized !!!  L1 pattern: %s' %
L1_pattern))
#C[A-Z]{1,17}(WYL|WLQ|WFQ|WYQ|WYH|WVQ|WVR|WWQ|WVK|WYR|WLL|WFL|WVF|WIQ|W
YR|WNQ|WHL|WHQ|WYM|WYY)'
        if not L3: print(('ERROR: CDR L3 cannot be recognized !!!  L3 pattern: %s' %
L3_pattern)) # C[A-Z]{1,15}(L|F|V|S)G[A-Z](G|Y)
        if not H1: print(('ERROR: CDR H1 cannot be recognized !!!  H1 pattern: %s' %
H1_pattern)) # C[A-Z]{1,16}(W)(I|V|F|Y|A|M|L|N|G)(R|K|Q|V|N|C)(Q|K|H|E|L|R)
        if not H3: print(('ERROR: CDR H3 cannot be recognized !!!  H3 pattern: %s' %
H3_pattern)) # C[A-Z]{1,33}(W)(G|A|C)[A-Z](Q|S|G|R)
        sys.exit(1)
    res = dict(L1=L1, L2=L2, L3=L3, H1=H1, H2=H2, H3=H3,  FR_L1=FR_L1, FR_L2=FR_L2,
FR_L3=FR_L3, FR_L4=FR_L4,  FR_H1=FR_H1, FR_H2=FR_H2, FR_H3=FR_H3, FR_H4=FR_H4)
    #if Options.verbose: print 'L1: %(L1)s\nL2: %(L2)s\nL3: %(L3)s\nH1: %(H1)s\nH2: %(H2)s\nH3:
%(H3)s' % res
    return res
```

Selection of template structures using Blast:

```
def Blast(folder, folderall, minscore, maxscore, threshold):
    os.system('mkdir ' + folder)
    if os.path.exists('./' + folder +'/results.html'): #Skip Blast if Blast results already exist
        pass
    else: #Submit fragment to Blast and download results
        Blasturl = urllib.request.Request('https://blast.ncbi.nlm.nih.gov/Blast.cgi?')
```

```
        BlastFile = open('./' + folderall +'/' + folder + '.fasta', 'rb')
        BlastuploadText = BlastFile.read()
        BlastFile.close()
        Blastdata = urllib.parse.urlencode({'QUERY': BlastuploadText,'PROGRAM':
'blastp','DATABASE': 'pdb','MAX_NUM_SEQ': '5000','HITLIST_SIZE': '100','DESCRIPTIONS':
'5000','ALIGNMENTS': '100', 'SHORT_QUERY_ADJUST': 'on', 'CMD': 'Put'}).encode('utf-8')
        BlastIDresults = urllib.request.urlopen(Blasturl, Blastdata)
        with open('./' + folder +'/IDresults.html', 'wb') as f:
            f.write(BlastIDresults.read())
            f.close
        BlastResultsFile = open('./' + folder +'/IDresults.html', 'r')
        HTMLresults = BlastResultsFile.read()
        start = 0
        if HTMLresults.find('<input name="RID" value="', start) > 0:
            idx = HTMLresults.find('<input name="RID" value="', start)
            closing_anchor = HTMLresults.find('"', idx+25)
            scoreID = HTMLresults[idx+25:closing_anchor]
        time.sleep(10)
        Blastdata = urllib.parse.urlencode({'CMD': 'Get','RID': scoreID,'DESCRIPTIONS':
'5000',}).encode('utf-8')
        Blastresults = urllib.request.urlopen(Blasturl, Blastdata)
        with open('./' + folder +'/results.html', 'wb') as f:
            f.write(Blastresults.read())
            f.close()

    with open('./' + folder +'/results.html', 'rb') as f:
        text = f.read().decode('utf-8')

    start = 0
    while text.find('Status=WAITING', start) > 0: #Check if Blast is finished
        print('Not Ready')
        time.sleep(10)
        f.close()
        Blastresults = urllib.request.urlopen(Blasturl, Blastdata)
        with open('./' + folder +'/results.html', 'wb') as f:
            f.write(Blastresults.read())
            f.close
        with open('./' + folder +'/results.html', 'rb') as f:
            text = f.read().decode('utf-8')
        start = 0

    start = 0
    q = []
    added = 0
    while text.find('<td class="c1 l lim">', start) > 0: #Look through results file for list of PDBs and
score
        idx = text.find('<td class="c1 l lim">', start)
```

```
        closing_anchor = text.find('</a>', idx)
        title = text[closing_anchor-6:closing_anchor]
        title = title.replace('_', ' ')
        altidx = text.find('c7', idx - 65)
        altclose = text.find('%', altidx)
        score = int(float(text[altidx+4:altclose]))
        dr = ''
        if title[0:4].lower() in antibody_list and title[0:4].lower != folderall[0:4].lower: # Filter by database
            print(title[0:4].lower() )
            if folder == 'heavy' and len(score_list[title[0:4].lower()]) == 0:
                score_list[title[0:4].lower()].append(score)
            if folder == 'light' and len(score_list[title[0:4].lower()]) == 1:
                score_list[title[0:4].lower()].append(score)
            if minscore < score < maxscore and added < threshold: #Check if score is within range and less than the threshold number of files have been downloaded
                with gzip.open('./templates/' + title[0:4].lower() + '.pdb.gz', 'rb') as f_in:
                    with open('./' + folder +'/' + title[0:4].lower() + '.pdb', 'wb') as f_out:
                        shutil.copyfileobj(f_in, f_out)
                os.system('python pdb2fasta.py ' + './' + folder +'/' + title[0:4].lower() + '.pdb > '+ './' + folder +'/' + title[0:4].lower() + '.fasta')
                print('python pdb2fasta.py ' + './' + folder +'/' + title[0:4].lower() + '.pdb > '+ './' + folder +'/' + title[0:4].lower() + '.fasta')
                time.sleep(0.05)
                added += 1
        start = idx + 40
    #Run clustering off of grouped files
    p = subprocess.Popen('clustalw.py ' + folder + ' ' + folderall, shell=True)
    q.append(p)
    exitcodes = [p.wait() for p in q]
```

Preparation of input structures using RosettaRelax:

```
../rosetta-3.7/main/source/bin/relax.default.linuxgccrelease -s 1aqk.pdb @relax.options -nstruct 1
```

RosettaRelax options:

```
-relax:fast
-default_max_cycles 200
-constrain_relax_to_start_coords true
-out:file:fullatom
-out:pdb_gz
```

Command used for partial thread:

```
../rosetta-3.7/main/source/bin/partial_thread.default.linuxgccrelease -in:file:fasta 1adq.fasta -in:file:alignment 1adq_1aqk.grishin -in:file:template_pdb 1aqk.pdb
```

Construction of Human IGM Rheumatoid Factor Fab using RosettaCM

Command used for RosettaCM:

```
#SBATCH --output=all_%a.out
#SBATCH --array=0-99%50
../rosetta-3.7/main/source/bin/rosetta_scripts.default.linuxgccrelease @rosetta_cm.options -nstruct 10 -
out:prefix ${SLURM_ARRAY_TASK_ID}_
```

RosettaCM Protocol:

```
<dock_design>
   <TASKOPERATIONS>
   </TASKOPERATIONS>
   <SCOREFXNS>
       <stage1 weights=score3 symmetric=0>
           <Reweight scoretype=atom_pair_constraint weight=0.5/>
           </stage1>
           <stage2 weights=score4_smooth_cart symmetric=0>
           <Reweight scoretype=atom_pair_constraint weight=0.5/>
            </stage2>
           <fullatom weights=talaris2013_cart symmetric=0>
           <Reweight scoretype=atom_pair_constraint weight=0.5/>
           </fullatom>
   </SCOREFXNS>
   <FILTERS>
   </FILTERS>
   <MOVERS>
       <Hybridize name=hybridize stage1_scorefxn=stage1 stage2_scorefxn=stage2 fa_scorefxn=fullatom
batch=1 stage1_increase_cycles=1.0 stage2_increase_cycles=1.0 linmin_only=1>
           <Template pdb="1aqk.pdb.pdb" cst_file="AUTO" weight=   0.6862745098039216 />
            <Template pdb="1dfb.pdb.pdb" cst_file="AUTO" weight=   0.6509803921568628 />
            <Template pdb="1mim.pdb.pdb" cst_file="AUTO" weight=   0.5294117647058824 />
            <Template pdb="1w72.pdb.pdb" cst_file="AUTO" weight=   0.8588235294117647 />
            <Template pdb="3ghe.pdb.pdb" cst_file="AUTO" weight=   0.6313725490196078 />
            <Template pdb="3giz.pdb.pdb" cst_file="AUTO" weight=   0.6862745098039216 />
            <Template pdb="3lmj.pdb.pdb" cst_file="AUTO" weight=   0.6078431372549019 />
            <Template pdb="3piq.pdb.pdb" cst_file="AUTO" weight=   0.7843137254901961 />
            <Template pdb="3ujj.pdb.pdb" cst_file="AUTO" weight=   0.615686274509804 />
            <Template pdb="3uls.pdb.pdb" cst_file="AUTO" weight=   0.6784313725490196 />
            <Template pdb="3wd5.pdb.pdb" cst_file="AUTO" weight=   0.6666666666666666 />
            <Template pdb="4fql.pdb.pdb" cst_file="AUTO" weight=   0.6588235294117647 />
            <Template pdb="4fqq.pdb.pdb" cst_file="AUTO" weight=   0.7137254901960784 />
            <Template pdb="4g5z.pdb.pdb" cst_file="AUTO" weight=   0.6431372549019608 />
            <Template pdb="4hf5.pdb.pdb" cst_file="AUTO" weight=   0.6588235294117647 />
            <Template pdb="4hk0.pdb.pdb" cst_file="AUTO" weight=   0.7294117647058823 />
            <Template pdb="4hpy.pdb.pdb" cst_file="AUTO" weight=   0.7843137254901961 />
            <Template pdb="4iml.pdb.pdb" cst_file="AUTO" weight=   0.7176470588235294 />
```

```
        <Template pdb="4jzn.pdb.pdb" cst_file="AUTO" weight=   0.7294117647058823 />
        <Template pdb="4m5y.pdb.pdb" cst_file="AUTO" weight=   0.7254901960784313 />
        <Template pdb="4m6o.pdb.pdb" cst_file="AUTO" weight=   0.6705882352941176 />
        <Template pdb="4npy.pdb.pdb" cst_file="AUTO" weight=   0.7019607843137254 />
        <Template pdb="4qci.pdb.pdb" cst_file="AUTO" weight=   0.7686274509803922 />
        <Template pdb="4v1d.pdb.pdb" cst_file="AUTO" weight=   0.6470588235294118 />
        <Template pdb="4wuk.pdb.pdb" cst_file="AUTO" weight=   0.7294117647058823 />
        <Template pdb="4yk4.pdb.pdb" cst_file="AUTO" weight=   0.5450980392156862 />
        <Template pdb="5fgc.pdb.pdb" cst_file="AUTO" weight=   0.7411764705882353 />
        <Template pdb="5j13.pdb.pdb" cst_file="AUTO" weight=   0.8156862745098039 />

    </Hybridize>
      <FastRelax name=relax scorefxn=fullatom/>
  </MOVERS>
  <APPLY_TO_POSE>
  </APPLY_TO_POSE>
  <PROTOCOLS>
    <Add mover=hybridize/>
      <Add mover=relax/>
  </PROTOCOLS>
  <OUTPUT scorefxn=talaris2014 />
</dock_design>
```

RosettaCM Options:

```
# i/o
-in:file:fasta 1adq.fasta
-parser:protocol rosetta_cm.xml
-out:pdb_gz

# relax options
-relax:constrain_relax_to_start_coords true
-default_max_cycles 500
-dualspace

# reduce memory footprint
-chemical:exclude_patches LowerDNA  UpperDNA Cterm_amidation SpecialRotamer VirtualBB
ShoveBB VirtualDNAPhosphate VirtualNTerm CTermConnect sc_orbitals pro_hydroxylated_case1
pro_hydroxylated_case2 ser_phosphorylated thr_phosphorylated  tyr_phosphorylated tyr_sulfated
lys_dimethylated lys_monomethylated  lys_trimethylated lys_acetylated glu_carboxylated cys_acetylated
tyr_diiodinated N_acetylated C_methylamidated MethylatedProteinCterm
```

RosettaRelax of Human IGM Rheumatoid Factor Fab

Command for RosettaRelax:

```
#SBATCH --output=allrelax_%a.out
#SBATCH --array=0-99%100
```

```
../rosetta-3.7/main/source/bin/relax.default.linuxgccrelease @relax.options -l
"${SLURM_ARRAY_TASK_ID}_score.txt" -out:prefix relax -nstruct 1
```

RosettaRelax Options:

```
-relax:fast
-default_max_cycles 200
-constrain_relax_to_start_coords true
-out:file:fullatom
-out:pdb_gz
```

Homology Modeling of Human IGM Rheumatoid Factor Fab using RosettaAntibody

Structure and Input Preparation

For all RosettaAntibody modeling, Rosetta 2019.06+release.4d8c807 was used

Command used for grafting:

```
../Rosetta_AB/main/source/bin/antibody.linuxgccrelease -fasta 1ADQ.fasta -antibody::grafting_database
../Rosetta_AB/tools/antibody/ -antibody::blastp /dors/meilerlab/apps/Linux2/x86_64/blast/2.7.1/bin/blastp
-antibody:n_multi_templates 1 -exclude_pdb 1ADQ -allow_omega_mismatches_for_north_clusters
```

H3 Loop *de novo* Modeling

Command used for H3 loop modeling:

```
#SBATCH --output=PATHL_%a.out
#SBATCH --array=0-99
../Rosetta_AB/main/source/bin/antibody_H3.linuxgccrelease @abH3.flags -in:file:s ../grafting/model-
0.relaxed.pdb -nstruct 10 -antibody:auto_generate_kink_constraint -
antibody:all_atom_mode_kink_constraint -out:file:scorefile ../H3_modeling_scores.fasc -out:path:pdb
../H3_modeling/ -out:prefix ${SLURM_ARRAY_TASK_ID}_
```

RosettaAntibody Options:

```
#how to run antibody mode -- these are the current best-practices
-antibody::remodel            perturb_kic
-antibody::snugfit            true
-antibody::refine             refine_kic
-antibody::cter_insert        false
-antibody::flank_residue_min  true
-antibody::bad_nter           false
-antibody::h3_filter          false
-antibody::h3_filter_tolerance 5
-antibody:constrain_vlvh_qq

#more standard settings, for packages used by antibody_H3
-ex1
-ex2
-extrachi_cutoff 0
```

```
#these are standard settings for kic/ngk
-loops:legacy_kic false
-loops:kic_min_after_repack true
-loops:kic_omega_sampling
-loops:allow_omega_move true    ### remove 'true' and loop::?
-kic_bump_overlap_factor 0.36
-loops:ramp_fa_rep
-loops:ramp_rama
-loops:refine_outer_cycles 5

#These enable the kink constraints.  Increase the weight if you want tighter kink constraints.
-antibody:constrain_cter
-constraints:cst_weight 1.0
```

RosettaRelax of Human IGM Rheumatoid Factor Fab

Command for RosettaRelax:

```
#SBATCH --output=allrelax_%a.out
#SBATCH --array=0-99%100
../rosetta-3.7/main/source/bin/relax.default.linuxgccrelease @relax.options -l
"${SLURM_ARRAY_TASK_ID}_score.txt" -out:prefix relax -nstruct 1
```

RosettaRelax Options:

```
-relax:fast
-default_max_cycles 200
-constrain_relax_to_start_coords true
-out:file:fullatom
-out:pdb_gz
```

Homology Modeling of Human IGM Rheumatoid Factor Fab using AbPredict

Structure and Input Preparation

For all AbPredict modeling, Rosetta-3.12 was used

Command used for template selection:

```
./create_run.sh 66 12 75 17
```

Command used for sequence preparation:

```
./prepare.sh 1ADQ.fasta
```

Construction of Human IGM Rheumatoid Factor Fab using AbPredict

Command used for AbPredict:

```
#SBATCH --output=1ADQ_HL_%a.out
#SBATCH --array=0-99
```

```
filename='segment_lengths_script_vars'
line_no=$(cat ${filename} | wc -l)
line_no=$((line_no-1))
line_no=$((line_no/40))
nstruct=$((1000/${line_no}))

array_index=$((SLURM_ARRAY_TASK_ID/4))

readarray -t myarray < ${filename}

/dors/meilerlab/apps/rosetta/rosetta-3.12/main/source/bin/rosetta_scripts.default.linuxgccrelease @flags -
-database /dors/meilerlab/apps/rosetta/rosetta-3.12/main/database/ -nstruct ${nstruct} -out:prefix
${SLURM_ARRAY_TASK_ID}_ ${myarray[${array_index}]}
sequence=YVLTQPPSVSVAPGQTARITCGGNNIGKSVHWYQQKPGQAPVLVVYDDSDRPPGIPER
FSGSNSGNTATLTISRVEAGDEADYYCQVWDSSSDHAVFGGGTKLTVQLVESGGGLVQPGRSLR
LSCVTSGFTFDDYAMHWVRQSPGKGLEWVSGISWNTGTIIYADSVGRFIISRDNAKNSLYLQMN
SLRVEDTALYYCAKTRSYVVAAEYYFHYWGQGILVTVS
```

AbPredict Templates:

```
-parser:script_vars entry_H1_H2=2HRPN entry_L1_L2=3G6JG entry_H3=4ODSH entry_L3=3U2SB
-parser:script_vars entry_H1_H2=5BVJH entry_L1_L2=3ESVG entry_H3=5DSCA entry_L3=3MUGE
-parser:script_vars entry_H1_H2=4HG4T entry_L1_L2=1FNSL entry_H3=3QCUI entry_L3=4UTAL
-parser:script_vars entry_H1_H2=4QEXH entry_L1_L2=1B4JL entry_H3=3RHWI entry_L3=4ODWL
-parser:script_vars entry_H1_H2=3FMGH entry_L1_L2=4OIIL entry_H3=4JPWH entry_L3=4F58N
-parser:script_vars entry_H1_H2=2DBLH entry_L1_L2=3QPQL entry_H3=3RI5H entry_L3=4NKIL
-parser:script_vars entry_H1_H2=2OTUD entry_L1_L2=4DKFL entry_H3=4TNWU entry_L3=5C9KB
-parser:script_vars entry_H1_H2=4RRPJ entry_L1_L2=4MA7L entry_H3=3RHWI entry_L3=4QHNB
-parser:script_vars entry_H1_H2=2FR4H entry_L1_L2=4XWOP entry_H3=5F9WB entry_L3=4AIXC
-parser:script_vars entry_H1_H2=3ZE1H entry_L1_L2=1YY9C entry_H3=1IBGH entry_L3=5ACOL
-parser:script_vars entry_H1_H2=4GXUQ entry_L1_L2=3CFEA entry_H3=4UIKH entry_L3=4TRPL
-parser:script_vars entry_H1_H2=4TNVH entry_L1_L2=2BDNL entry_H3=1IBGH entry_L3=1MCKB
-parser:script_vars entry_H1_H2=4OQTH entry_L1_L2=1FGVL entry_H3=4QTHH entry_L3=3MLYM
-parser:script_vars entry_H1_H2=4OCWH entry_L1_L2=1L7IL entry_H3=4EDWH entry_L3=3EYFC
-parser:script_vars entry_H1_H2=3CFEH entry_L1_L2=1RIHL entry_H3=4UINH entry_L3=3B5GA
-parser:script_vars entry_H1_H2=3MLSH entry_L1_L2=3UBXL entry_H3=4TNWF entry_L3=4QHLB
-parser:script_vars entry_H1_H2=5ANMH entry_L1_L2=3BGFL entry_H3=3MCKB entry_L3=4UNUB
-parser:script_vars entry_H1_H2=2EXYE entry_L1_L2=2XRAL entry_H3=3Q3GB entry_L3=4DQOL
-parser:script_vars entry_H1_H2=15C8H entry_L1_L2=1QP1B entry_H3=4KZDH entry_L3=1MCFB
-parser:script_vars entry_H1_H2=4WFEE entry_L1_L2=2BX5O entry_H3=4ODVH entry_L3=3G6AA
-parser:script_vars entry_H1_H2=2VXSH entry_L1_L2=1E4WL entry_H3=3W9DA entry_L3=3MLYL
-parser:script_vars entry_H1_H2=3MLSJ entry_L1_L2=2DQHL entry_H3=4QTHA entry_L3=4XWGL
-parser:script_vars entry_H1_H2=3HMXH entry_L1_L2=4ODUL entry_H3=5DSCH entry_L3=4TRPL
-parser:script_vars entry_H1_H2=1HEZB entry_L1_L2=4D9RD entry_H3=3TNMA entry_L3=4F58O
-parser:script_vars entry_H1_H2=4F9LC entry_L1_L2=2DQFD entry_H3=5DQJA entry_L3=4YC2L
-parser:script_vars entry_H1_H2=3DETC entry_L1_L2=4GW1A entry_H3=3G6AB entry_L3=4JAMB
```

```
-parser:script_vars entry_H1_H2=4H0GA entry_L1_L2=3HMXL entry_H3=4YBLB entry_L3=3V6FL
-parser:script_vars entry_H1_H2=4XWOQ entry_L1_L2=1YY8A entry_H3=4TNVH entry_L3=1AQKL
-parser:script_vars entry_H1_H2=2HT3C entry_L1_L2=1FL5L entry_H3=5DUBH entry_L3=3U2SL
-parser:script_vars entry_H1_H2=4GMTH entry_L1_L2=3EYFC entry_H3=4TNVH entry_L3=3V6FB
-parser:script_vars entry_H1_H2=4RDQO entry_L1_L2=3IY0L entry_H3=3CX5J entry_L3=4TRPL
-parser:script_vars entry_H1_H2=3ZE0H entry_L1_L2=1BWWB entry_H3=2NTFH entry_L3=3MLYL
-parser:script_vars entry_H1_H2=4YO0A entry_L1_L2=1RZ7L entry_H3=3IFPE entry_L3=5C9KG
-parser:script_vars entry_H1_H2=3FKUX entry_L1_L2=4GMSN entry_H3=3SDYH entry_L3=4TUOB
-parser:script_vars entry_H1_H2=5CIPA entry_L1_L2=2ITDB entry_H3=1P84J entry_L3=4TUKL
-parser:script_vars entry_H1_H2=4F9LC entry_L1_L2=1BWWA entry_H3=4QHKO entry_L3=4K9EL
-parser:script_vars entry_H1_H2=2ZJSH entry_L1_L2=4CMHC entry_H3=2IPTH entry_L3=2MCG1
-parser:script_vars entry_H1_H2=4R96B entry_L1_L2=1J5OL entry_H3=4TNVH entry_L3=4HH9C
-parser:script_vars entry_H1_H2=5CSZA entry_L1_L2=3HI6L entry_H3=4PB9H entry_L3=5E8EA
-parser:script_vars entry_H1_H2=2VDRH entry_L1_L2=3S36L entry_H3=5DQJA entry_L3=2FL5C
```

AbPredict Options:

```
-nodelay
-use_input_sc
-ignore_unrecognized_res
-overwrite
-out:file:fullatom
-s 2BRR.ppk_ideal.pdb
-parser:protocol AbPredict_xsd.xml
-parser:script_vars template_pdb=2BRR.ppk_ideal.pdb
-pdb_comments true

-parser:script_vars H1_H2.db=../AB_db_files/H1_H2.db H3.db=../AB_db_files/H3.db
L3.db=../AB_db_files/L3.db L1_L2.db=../AB_db_files/L1_L2.db
```

RosettaRelax of Human IGM Rheumatoid Factor Fab

Command for RosettaRelax:

```
#SBATCH --output=PATHL_%a.out
#SBATCH --array=0-99
#exclude=bf21,bf22,bf23,bf24
/dors/meilerlab/apps/rosetta/rosetta-3.7/main/source/bin/relax.default.linuxgccrelease @./relax.options -
in:file:s ${SLURM_ARRAY_TASK_ID}_2BRR.ppk_ideal_0001.pdb -out:prefix relax -nstruct 1
```

RosettaRelax Options:

```
-relax:fast
-default_max_cycles 200
-constrain_relax_to_start_coords true
-out:file:fullatom
-out:pdb_gz
```

Data Analysis

Calculation of RMSD to native structure

```
pymol.cmd.load(path + '/' + folder + '/native.pdb.gz', 'Native')
pymol.cmd.do('run findseq.py')
#rmsd = get_RMSD('Test', rootx + '/' + pdbFile + '.pdb.gz', folder, path + '/' + folder + '/temp.pdb.gz', CDRs['heavy'], CDRs['light'])
alignrmsd = pymol.cmd.align('Test', 'Native', cycles=5)[0]
superrmsd = pymol.cmd.super('Test & backbone', 'Native & backbone', cycles=0)[0]

pymol.cmd.do('findseq ' + CDRs['H1'] + ', Native, NativeH1')
pymol.cmd.do('findseq ' + CDRs['H1'] + ', Test, TestH1')
pymol.cmd.do('alter NativeH1, chain="H"')
pymol.cmd.do('alter TestH1, chain="H"')
pymol.cmd.do('alter TestH1 & chain H, resi=str(1)')
pymol.cmd.do('alter NativeH1 & chain H, resi=str(1)')
H1RMS = pymol.cmd.rms_cur('TestH1 & backbone', 'NativeH1 & backbone')
```