Table A1: PDB IDs of bound antigens on the test set along with the PDB IDs of analogous unbound antigens, total number of epitopic residues on the unbound antigen and the residue numbers of these residues.

|  |  |  |  |
| --- | --- | --- | --- |
| **Bound\_Antigen\_PDB\_ID** | **Unbound\_Antigen\_PDB\_ID** | **Number of Epitope Residues** | **Epitope Residue Numbers on the Unbound Antigen** |
| 7DUO | 2EF1 | 18 | 120+121+135+139+141+142+202+203+205+236+237+239+241+272+273+274+275+276 |
| 5BO1 | 2VJ2 | 18 | 190+201+202+203+204+205+206+207+209+211+219+221+222+224+246+247+250+252 |
| 3O2D | 1WIO | 18 | 3+94+96+120+122+123+124+125+126+127+140+141+142+162+163+164+165+166 |
| 6P50 | 3UP1 | 15 | 52+54+55+59+61+62+84+85+86+88+93+94+95+98+100 |
| 4RRP | 1WG3 | 23 | 17+18+19+20+21+22+23+24+27+28+30+32+35+67+68+69+70+73+77+78+79+80+82 |
| 3LDB | 3K2O | 13 | 53+55+57+58+61+62+65+158+291+319+320+322+323 |
| 7LFA | 7L6K | 8 | 124+125+127+128+130+132+133+137 |
| 5DHV | 6BSY | 13 | 11+14+15+18+21+22+48+51+55+58+59+62+63 |
| 5H35 | 5WTR | 21 | 1+2+5+6+9+55+57+59+62+107+110+111+113+114+115+164+168+169+172+173+176 |
| 4KUC | 4Q2V | 13 | 53+92+98+99+101+102+105+106+109+112+113+114+116 |
| 4CMH | 6EDR | 25 | 75+76+79+107+108+110+111+112+113+114+115+116+117+118+119+148+150+194+195+196+198+199+201+233+234 |
| 3PGF | 5EDU | 23 | 195+198+199+200+201+203+206+218+367+409+410+413+416+417+429+432+433+435+436+437+438+439+440 |
| 4JR9 | 4U4W | 11 | 12+15+16+17+19+24+25+27+28+29+32 |
| 4OII | 4OIE | 21 | 232+235+236+237+239+240+253+256+257+258+260+261+262+264+265+289+293+294+314+315+351 |
| 3LEV | 3LES | 9 | 107+108+109+110+111+112+113+116+244 |
| 5CBA | 7JNY | 14 | 20+23+24+26+27+28+29+30+48+50+61+64+65+68 |
| 3MXW | 3M1N | 21 | 44+45+87+123+125+126+131+132+133+134+135+136+147+153+155+174+176+177+178+179+180 |
| 3NH7 | 2K3G | 21 | 43+60+62+64+67+74+77+78+79+80+81+84+86+90+91+92+93+94+95+96+97 |
| 5JQ6 | 1N67 | 21 | 408+428+429+431+432+433+434+460+463+464+465+466+467+468+473+477+479+481+510+512+518 |
| 4ETQ | 4ETQ | 22 | 5+39+40+41+44+174+175+176+177+178+179+204+205+215+217+219+220+221+223+224+226+227 |
| 3KS0 | 1LDC | 10 | 30+63+64+65+66+67+68+69+70+72 |
| 3LD8 | 6MEV | 13 | 53+55+57+58+61+62+65+158+291+319+320+322+326 |
| 3WKM | 3WKL | 24 | 116+117+161+162+165+195+198+200+207+215+216+242+246+250+276+277+278+279+280+281+282+283+288+289 |
| 5FB8 | 1I16 | 19 | 38+39+40+42+43+44+45+46+51+53+63+65+66+94+95+96+97+99+102 |
| 2JEL | 1HDN | 15 | 1+2+3+4+34+41+64+66+67+68+70+71+72+75+76 |
| 2VXQ | 1BMW | 15 | 32+34+39+40+41+43+65+67+68+75+76+77+78+79+80 |
| 4U6V | 6U49 | 16 | 173+179+181+182+183+185+186+187+188+189+190+191+200+263+264+266 |
| 3LIZ | 1YG9 | 18 | 199+200+201+232+233+234+235+236+237+248+250+251+253+254+256+257+270+272 |
| 5MES | 5KU9 | 12 | 174+205+208+308+309+310+311+313+317+318+320+322 |