

MySQL [scop]> select * from pdb_local where pdb_release_id in (163177,179179,184515,224659,229883,233426,253494,261357,265096,323899,369478,397188);				
pdb_release_id	pdb_path	xml_path	is_raf_calculated	snapshot_date
163177	/lab/db/pdb/data/090323/files/hash/ld/pdb1ldt.ent.gz	/lab/db/pdb/data/090323/files/xml-hash/ld/lldt.xml.gz	1	2009-03-23
179179	/lab/db/pdb/data/090323/files/hash/uc/pdb1lucy.ent.gz	/lab/db/pdb/data/090323/files/xml-hash/uc/lucy.xml.gz	1	2009-03-23
184515	/lab/db/pdb/data/090323/files/hash/xq/pdb1xq5.ent.gz	/lab/db/pdb/data/090323/files/xml-hash/xq/lxq5.xml.gz	1	2009-03-23
224659	/lab/db/pdb/data/110713/files/hash/ay/pdb1ay6.ent.gz	/lab/db/pdb/data/110713/files/xml-hash/ay/lay6.xml.gz	1	2011-07-13
229883	/lab/db/pdb/data/110713/files/hash/fk/pdb1fk5.ent.gz	/lab/db/pdb/data/110713/files/xml-hash/fk/1fk5.xml.gz	1	2011-07-13
233426	/lab/db/pdb/data/110713/files/hash/ih/pdb1ihs.ent.gz	/lab/db/pdb/data/110713/files/xml-hash/ih/1ihs.xml.gz	1	2011-07-13
253494	/lab/db/pdb/data/111228/files/hash/zj/pdb2zjp.ent.gz	/lab/db/pdb/data/111228/files/xml-hash/zj/2zjp.xml.gz	1	2011-12-28
261357	/lab/db/pdb/data/120523/files/hash/o9/pdb2o9m.ent.gz	/lab/db/pdb/data/120523/files/xml-obs-hash/o9/2o9m.xml.gz	1	2012-05-23
265096	/lab/db/pdb/data/120815/files/hash/av/pdb4awz.ent.gz	/lab/db/pdb/data/120815/files/xml-hash/av/4awz.xml.gz	1	2012-08-15
323899	/lab/db/pdb/data/150527/files/hash/ry/pdb4ryz.ent.gz	/lab/db/pdb/data/150527/files/xml-hash/ry/4ryz.xml.gz	1	2015-05-27
369478	/lab/db/pdb/data/170628/files/hash/cu/pdb3cup.ent.gz	/lab/db/pdb/data/170628/files/xml-hash/cu/3cup.xml.gz	1	2017-06-28
397188	/lab/db/pdb/data/171101/files/hash/ef/pdb1efr.ent.gz	/lab/db/pdb/data/171101/files/xml-hash/ef/1efr.xml.gz	1	2017-11-01

12 rows in set (0.00 sec)

163177 : ins code mismatch, 1-46 but actually 1l ~ 46l

debug: chain L entity 2

rafBody: 1lkk 2lkk 3lvv 4lcc 5laa 6lcc 7lpp 8lkk 9lii  
 10lli 11lkk 12lpp 13lvv 14lcc 15lgg 16lss 17lld 18lgg 19lrr  
 20ltt 21lly 22laa 23lnn 24lss 25lcc 26lii 27laa 28lrr 29lcc  
 30lnn 31lgg 32lvv 33lss 34lii 35lkk 36lss 37lee 38lgg  
 39lss 40lcc 41lpp 42ltt 43lgg 44lii 45lli 46lnn

2

dbStart: 1

dbEnd: 46

pdbStart: 1

pdbEnd: 46

ps: -1

pe: -1

seqadvs: null

check enter:b

check enter:d

Pdbfile inspection:

ATOM	1668	N	LYS	L	1I	59.751	49.132	43.657	1.00	41.62	N
ATOM	1669	CA	LYS	L	1I	58.955	48.837	42.446	1.00	35.24	C
ATOM	1670	C	LYS	L	1I	57.533	49.341	42.638	1.00	38.01	C
ATOM	1671	O	LYS	L	1I	57.229	50.490	42.311	1.00	56.90	O
ATOM	1672	CB	LYS	L	1I	58.914	47.324	42.164	1.00	33.06	C
ATOM	1673	CG	LYS	L	1I	60.262	46.653	41.946	1.00	47.03	C
ATOM	1674	CD	LYS	L	1I	60.375	45.385	42.823	1.00	41.57	C
ATOM	1675	CE	LYS	L	1I	61.790	44.772	42.823	1.00	31.48	C
ATOM	1676	NZ	LYS	L	1I	61.829	43.462	43.561	1.00	53.19	N
ATOM	1677	N	LYS	L	2I	56.738	48.529	43.331	1.00	49.69	N
ATOM	1678	CA	LYS	L	2I	55.308	48.744	43.567	1.00	39.82	C
ATOM	1679	C	LYS	L	2I	54.677	48.216	42.305	1.00	34.57	C
ATOM	1680	O	LYS	L	2I	54.322	48.960	41.385	1.00	44.70	O
ATOM	1681	CB	LYS	L	2I	54.894	50.198	43.791	1.00	35.71	C
ATOM	1682	CG	LYS	L	2I	53.472	50.318	44.364	1.00	39.17	C
ATOM	1683	CD	LYS	L	2I	53.343	49.640	45.759	1.00	44.53	C
ATOM	1684	CE	LYS	L	2I	53.037	48.123	45.692	1.00	40.36	C
ATOM	1685	NZ	LYS	L	2I	53.040	47.438	47.032	1.00	45.84	N
ATOM	1686	N	VAL	L	3I	54.737	46.899	42.209	1.00	32.73	N
ATOM	1687	CA	VAL	L	3I	54.197	46.154	41.101	1.00	26.23	C
ATOM	1688	C	VAL	L	3I	52.900	45.559	41.653	1.00	42.24	C
ATOM	1689	O	VAL	L	3I	52.766	45.329	42.868	1.00	30.30	O
ATOM	1690	CB	VAL	L	3I	55.209	45.062	40.604	1.00	30.95	C

DBREF	1LDT	T	16	245	UNP	P00761	TRYP_PIG	9	231
DBREF	1LDT	L	1	46	UNP	P80424	LDTI_HIRME	1	46

179179 : start mismatch due to ACE

debug: chain I entity 4

rafBody: 7 dd 8 ff 9 || 10 aa 11 ee 12 gg 13 gg 14 gg 15 vv

16 rr 18 pp 19 rr

5

dbStart: 6

dbEnd: 16

pdbStart: 6

pdbEnd: 16

ps: -1

pe: 9

Pdbfile inspection:

DBREF	1UCY	L	1H	15	UNP	P00735	THR_BOVIN	318	366
DBREF	1UCY	H	16	149A	UNP	P00735	THR_BOVIN	367	516
DBREF	1UCY	E	149B	247	UNP	P00735	THR_BOVIN	517	625
DBREF	1UCY	F	6	16	UNP	P12803	FIBA_MACFU	6	16
DBREF	1UCY	J	1H	15	UNP	P00735	THR_BOVIN	318	366
DBREF	1UCY	K	16	247	UNP	P00735	THR_BOVIN	367	625
DBREF	1UCY	G	6	16	UNP	P12803	FIBA_MACFU	6	16
DBREF	1UCY	M	1H	15	UNP	P00735	THR_BOVIN	318	366
DBREF	1UCY	N	16	247	UNP	P00735	THR_BOVIN	367	625
DBREF	1UCY	I	6	16	UNP	P12803	FIBA_MACFU	6	16

SEQADV	1UCY	ACE	F	6	UNP	P12803	GLY	6	CONFLICT
SEQADV	1UCY	OPR	F	16	UNP	P12803	ARG	16	CONFLICT
SEQADV	1UCY	ACE	G	6	UNP	P12803	GLY	6	CONFLICT
SEQADV	1UCY	OPR	G	16	UNP	P12803	ARG	16	CONFLICT
SEQADV	1UCY	ACE	I	6	UNP	P12803	GLY	6	CONFLICT
SEQADV	1UCY	OPR	I	16	UNP	P12803	ARG	16	CONFLICT

184515 start mismatch due to ACE

rafBody: 1 ss 2 ll 3 ss 4 ss 5 kk 6 dd 7 kk 8 dd 9 tt 10  
 vv 11 kk 12 aa 13 ll 14 ww 15 gg 16 kk 17 ii 18 aa 19 dd 20  
 kk 21 aa 22 ee 23 ee 24 ii 25 gg 26 ss 27 dd 28 aa 29 ll 30  
 ss 31 rr 32 mm 33 ll 34 aa 35 vv 36 yy 37 pp 38 qq 39 tt  
 40 kk 41 tt 42 yy 43 ff 44 ss 45 hh 46 ww 47 kk 48 dd 49  
 ll 50 ss 51 pp 52 gg 53 ss 54 aa 55 pp 56 vv 57 nn 58 kk  
 59 hh 60 gg 61 kk 62 tt 63 ii 64 mm 65 gg 66 gg 67 ii 68  
 vv 69 dd 70 aa 71 vv 72 aa 73 ss 74 ii 75 dd 76 dd 77 ll 78  
 nn 79 aa 80 gg 81 ll 82 ll 83 aa 84 ll 85 ss 86 ee 87 ll 88  
 hh 89 aa 90 ff 91 tt 92 ll 93 rr 94 vv 95 dd 96 pp 97 aa 98  
 nn 99 ff 100 kk 101 ii 102 ll 103 ss 104 hh 105 cc 106 ii 107 ll 108  
 vv 109 ll 110 ll 111 aa 112 vv 113 kk 114 ff 115 pp 116 kk 117 dd 118  
 ff 119 tt 120 pp 121 ee 122 vv 123 hh 124 ii 125 ss 126 yy 127 dd  
 128 kk 129 ff 130 ff 131 ss 132 aa 133 ll 134 aa 135 rr 136 aa 137  
 ll 138 aa 139 ee 140 kk 141 yy 142 rr

2

dbStart: 2

dbEnd: 143

pdbStart: 0

pdbEnd: 141

ps: -1

pe: 140

REMARK 359 INTO ANY SEQUENCE DATABASE									
DBREF	1XQ5	A	0	141	UNP	A8HTG8	A8HTG8_PERFV	2	143
DBREF	1XQ5	B	1	146	PDB	1XQ5	1XQ5	1	146
DBREF	1XQ5	C	0	141	UNP	A8HTG8	A8HTG8_PERFV	2	143
DBREF	1XQ5	D	1	146	PDB	1XQ5	1XQ5	1	146

HET	ACE	A	0	3
HET	ACE	C	0	3
HET	HEM	A	143	43
HET	HEM	B	148	43
HET	HEM	C	143	43
HET	HEM	D	148	43

224659: ins code mismatch, The corresponding insertion is not documented in ATOM

rafBody: -3.t -2.f -1.g 0.s 1Dgg 1Cee 1Baa 1Add 1cc  
2 gg 3 ll 4 rr 5 pp 6 ll 7 ff 8 ee 9 kk 10 kk 11 ss 12 ll 13  
ee 14 dd 14Akk 14Btt 14Cee 14Drr 14Eee 14Fll 14Gll 14Hee  
14Iss 14Jyy 14Kii 15.d 16.g 17.r

3

dbStart: 328

dbEnd: 363

pdbStart: 1H

pdbEnd: 14N

ps: -1

pe: -1

DBREF	1AY6	L	1H	14N	UNP	P00734	THRΒ_HUMAN	328	363
DBREF	1AY6	H	16	247	UNP	P00734	THRΒ_HUMAN	364	622
DBREF	1AY6	I	55	64	UNP	P01050	ΙΤΗΒ_ΗΙΡΜΕ	55	64
SEQADV	1AY6	ACE	I	52	UNP	P01050	INSERTION		
SEQADV	1AY6	ASN	I	53	UNP	P01050	INSERTION		
SSEQADV	1AY6	GLU	T	54	UNP	P01050	TNSERTTQN		

ATOM	216	N	TYR	L	14J	1.280	5.336	36.527	1.00	32.80	N
ATOM	217	CA	TYR	L	14J	2.353	6.204	37.110	1.00	33.97	C
ATOM	218	C	TYR	L	14J	1.692	6.837	38.315	1.00	37.51	C
ATOM	219	O	TYR	L	14J	1.572	8.041	38.530	1.00	37.84	O
ATOM	220	CB	TYR	L	14J	2.806	7.165	36.050	1.00	29.30	C
ATOM	221	CG	TYR	L	14J	3.140	6.748	34.673	1.00	30.31	C
ATOM	222	CD1	TYR	L	14J	3.586	5.413	34.439	1.00	29.96	C
ATOM	223	CD2	TYR	L	14J	3.079	7.566	33.525	1.00	27.41	C
ATOM	224	CE1	TYR	L	14J	3.945	4.946	33.186	1.00	28.64	C
ATOM	225	CE2	TYR	L	14J	3.551	7.123	32.296	1.00	28.63	C
ATOM	226	CZ	TYR	L	14J	3.992	5.839	32.100	1.00	29.72	C
ATOM	227	OH	TYR	L	14J	4.284	5.364	30.829	1.00	28.54	O
ATOM	228	N	ILE	L	14K	1.053	5.921	39.025	1.00	41.23	N
ATOM	229	CA	ILE	L	14K	0.101	6.133	40.141	1.00	44.03	C
ATOM	230	C	ILE	L	14K	-0.209	7.582	40.468	1.00	46.08	C
ATOM	231	O	ILE	L	14K	-1.025	8.365	39.863	1.00	47.35	O
ATOM	232	CB	ILE	L	14K	0.575	5.229	41.349	1.00	44.44	C
ATOM	233	CG1	ILE	L	14K	2.118	5.438	41.364	1.00	45.94	C
ATOM	234	CG2	ILE	L	14K	0.090	3.797	41.189	1.00	45.07	C
ATOM	235	CD1	ILE	L	14K	2.393	7.004	41.391	1.00	45.89	C
TER	236		ILE	L	14K						
ATOM	237	N	ILE	H	16	4.830	-9.441	18.372	1.00	22.53	N
ATOM	238	CA	ILE	H	16	4.109	-9.070	19.569	1.00	24.67	C

SCALE2	0.000000	0.013862	0.000000		0.000000						
SCALE3	0.000000	0.000000	0.013980		0.000000						
ATOM	1	N	GLY	L	1D	16.219	15.929	14.612	1.00	50.00	N
ATOM	2	CA	GLY	L	1D	14.998	16.623	15.045	1.00	50.00	C
ATOM	3	C	GLY	L	1D	14.519	16.583	16.473	1.00	50.00	C
ATOM	4	O	GLY	L	1D	13.419	17.110	16.881	1.00	50.00	O
ATOM	5	N	GLU	L	1C	15.252	15.831	17.290	1.00	50.00	N
ATOM	6	CA	GLU	L	1C	14.888	15.751	18.754	1.00	50.00	C
ATOM	7	C	GLU	L	1C	14.852	17.213	19.253	1.00	50.00	C
ATOM	8	O	GLU	L	1C	15.961	17.838	19.199	1.00	50.00	O
ATOM	9	CB	GLU	L	1C	15.985	14.913	19.417	1.00	50.00	C
ATOM	10	CG	GLU	L	1C	16.024	14.645	20.917	1.00	50.00	C
ATOM	11	CD	GLU	L	1C	15.971	13.134	21.277	1.00	50.00	C
ATOM	12	OE1	GLU	L	1C	15.557	12.270	20.442	1.00	46.82	O
ATOM	13	OE2	GLU	L	1C	16.330	13.074	22.511	1.00	45.83	O
ATOM	14	N	ALA	L	1B	13.733	17.770	19.654	1.00	48.66	N
ATOM	15	CA	ALA	L	1B	13.498	19.175	20.008	1.00	45.36	C
ATOM	16	C	ALA	L	1B	11.958	19.336	20.081	1.00	42.82	C
ATOM	17	O	ALA	L	1B	11.267	19.908	20.923	1.00	42.54	O
ATOM	18	CB	ALA	L	1B	13.949	20.050	18.861	1.00	45.74	C
ATOM	19	N	ASP	L	1A	11.460	18.661	19.059	1.00	39.74	N
ATOM	20	CA	ASP	L	1A	10.053	18.363	18.846	1.00	37.24	C
ATOM	21	C	ASP	L	1A	9.813	16.843	19.212	1.00	32.80	C

261357: Whole chain mismatch: Every chain should restart index but doesn't

debug: chain E entity 1

rafBody: 801 mm 802 dd 803 ii 804 vv 805 ff 806 ii 807 ee 808 qq 809 ll 810 ss 811 vv 812 ii 813 tt 814 tt 815 ii 816 gg 817 vv 818 yy 819 dd 820 ww 821 ee 822 qq 823 tt 824 ii 825 ee 826 qq 827 kk 828 ll 829 vv 830 ff 831 dd 832 ii 833 ee 834 mm 835 aa 836 ww 837 dd 838 nn 839 rr 840 kk 841 aa 842 aa 843 kk 844 ss 845 dd 846 dd 847 vv 848 aa 849 dd 850 cc 851 ll 852 ss 853 yy 854 aa 855 dd 856 ii 857 aa 858 ee 859 tt 860 vv 861 vv 862 ss 863 hh 864 vv 865 ee 866 gg 867 aa 868 rr 869 ff 870 aa 871 ll 872 vv 873 ee 874 rr 875 vv 876 aa 877 ee 878 ee 879 vv 880 aa 881 ee 882 ll 883 ll 884 ll 885 aa 886 rr 887 ff 888 nn 889 ss 890 pp 891 ww 892 vv 893 rr 894 ii 895 kk 896 ll 897 ss 898 kk 899 pp 900 gg 901 aa 902 vv 903 aa 904 rr 905 aa 906 aa 907 nn 908 vv 909 gg 910 vv 911 ii 912 ii 913 ee 914 rr 915 gg 916 nn 917 nn 918 ll 919 .k 920 .e 921 .n

922 .n

1

dbStart: 1

dbEnd: 122

pdbStart: 1

pdbEnd: 122

ps: -1

pe: -1

rafBody: 1001 mm1002 dd1003 ii1004 vv1005 ff1006 ii1007  
ee1008 qq1009 ll1010 ss1011 vv1012 ii1013 tt1014 tt1015 ii1016  
gg1017 vv1018 yy1019 dd1020 ww1021 ee1022 qq1023 tt1024  
ii1025 ee1026 qq1027 kk1028 ll1029 vv1030 ff1031 dd1032  
ii1033 ee1034 mm1035 aa1036 ww1037 dd1038 nn1039 rr1040  
kk1041 aa1042 aa1043 kk1044 ss1045 dd1046 dd1047 vv1048  
aa1049 dd1050 cc1051 ll1052 ss1053 yy1054 aa1055 dd1056  
ii1057 aa1058 ee1059 tt1060 vv1061 vv1062 ss1063 hh1064  
vv1065 ee1066 gg1067 aa1068 rr1069 ff1070 aa1071 ll1072  
vv1073 ee1074 rr1075 vv1076 aa1077 ee1078 ee1079 vv1080  
aa1081 ee1082 ll1083 ll1084 ll1085 aa1086 rr1087 ff1088  
nn1089 ss1090 pp1091 ww1092 vv1093 rr1094 ii1095 kk1096  
ll1097 ss1098 kk1099 pp1100 gg1101 aa1102 vv1103 aa1104  
rr1105 aa1106 aa1107 nn1108 vv1109 gg1110 vv1111 ii1112 ii1113  
ee1114 rr1115 gg1116 nn1117 nn1118 ll1119 kk1120  
ee1121 .n1122 .n

1

dbStart: 1

dbEnd: 122

pdbStart: 1

pdbEnd: 122

ps: -1

pe: -1

DBREF	209M A	1	122	UNP	P0AC16	FOLB_ECOLI	1	122
DBREF	209M B	1	122	UNP	P0AC16	FOLB_ECOLI	1	122
DBREF	209M C	1	122	UNP	P0AC16	FOLB_ECOLI	1	122
DBREF	209M D	1	122	UNP	P0AC16	FOLB_ECOLI	1	122
DBREF	209M E	1	122	UNP	P0AC16	FOLB_ECOLI	1	122
DBREF	209M F	1	122	UNP	P0AC16	FOLB_ECOLI	1	122
DBREF	209M G	1	122	UNP	P0AC16	FOLB_ECOLI	1	122
DBREF	209M H	1	122	UNP	P0AC16	FOLB_ECOLI	1	122

HET	PH2	A	131	14
HET	PH2	A	731	14
HET	PH2	C	331	14
HET	PH2	D	531	14
HET	PH2	E	931	14
HET	PH2	G	1131	14
HET	PH2	H	1331	14
HET	PH2	H	1531	14

SEQRES	1 A	122	MET ASP ILE VAL PHE ILE GLU GLN LEU SER VAL ILE THR
SEQRES	2 A	122	THR ILE GLY VAL TYR ASP TRP GLU GLN THR ILE GLU GLN
SEQRES	3 A	122	LYS LEU VAL PHE ASP ILE GLU MET ALA TRP ASP ASN ARG
SEQRES	4 A	122	LYS ALA ALA LYS SER ASP ASP VAL ALA ASP CYS LEU SER
SEQRES	5 A	122	TYR ALA ASP ILE ALA GLU THR VAL VAL SER HIS VAL GLU
SEQRES	6 A	122	GLY ALA ARG PHE ALA LEU VAL GLU ARG VAL ALA GLU GLU
SEQRES	7 A	122	VAL ALA GLU LEU LEU ALA ARG PHE ASN SER PRO TRP
SEQRES	8 A	122	VAL ARG ILE LYS LEU SER LYS PRO GLY ALA VAL ALA ARG
SEQRES	9 A	122	ALA ALA ASN VAL GLY VAL ILE ILE GLU ARG GLY ASN ASN
SEQRES	10 A	122	LEU LYS GLU ASN ASN
SEQRES	1 B	122	MET ASP ILE VAL PHE ILE GLU GLN LEU SER VAL ILE THR
SEQRES	2 B	122	THR ILE GLY VAL TYR ASP TRP GLU GLN THR ILE GLU GLN
SEQRES	3 B	122	LYS LEU VAL PHE ASP ILE GLU MET ALA TRP ASP ASN ARG
SEQRES	4 B	122	LYS ALA ALA LYS SER ASP ASP VAL ALA ASP CYS LEU SER
SEQRES	5 B	122	TYR ALA ASP ILE ALA GLU THR VAL VAL SER HIS VAL GLU
SEQRES	6 B	122	GLY ALA ARG PHE ALA LEU VAL GLU ARG VAL ALA GLU GLU
SEQRES	7 B	122	VAL ALA GLU LEU LEU ALA ARG PHE ASN SER PRO TRP
SEQRES	8 B	122	VAL ARG ILE LYS LEU SER LYS PRO GLY ALA VAL ALA ARG
SEQRES	9 B	122	ALA ALA ASN VAL GLY VAL ILE ILE GLU ARG GLY ASN ASN
SEQRES	10 B	122	LEU LYS GLU ASN ASN

323899: start mismatch due to ACE

rafBody: 2 ss 3 ss 4 qq 5 vv 6 ee 7 hh 8 pp 9 aa 10 gg  
11 gg 12 yy 13 kk 14 kk 15 ll 16 ff 17 ee 18 tt 19 vv 20 ee 21  
ee 22 ll 23 ss 24 ss 25 pp 26 ll 27 tt 28 aa 29 hh 30 vv 31  
tt 32 gg 33 rr 34 ii 35 pp 36 ll 37 ww 38 ll 39 tt 40 gg 41  
ss 42 ll 43 ll 44 rr 45 cc 46 gg 47 pp 48 gg 49 ll 50 ff 51  
ee 52 vv 53 gg 54 ss 55 ee 56 pp 57 ff 58 yy 59 hh 60 ll  
61 ff 62 dd 63 gg 64 qq 65 aa 66 ll 67 ll 68 hh 69 kk 70 ff  
71 dd 72 ff 73 kk 74 ee 75 gg 76 hh 77 vv 78 tt 79 yy 80 hh  
81 rr 82 rr 83 ff 84 ii 85 rr 86 tt 87 dd 88 aa 89 yy 90 vv  
91 rr 92 aa 93 mm 94 tt 95 ee 96 kk 97 rr 98 ii 99 vv 100 ii  
101 tt 102 ee 103 ff 104 gg 105 tt 106 cc 107 aa 108 ff 109 pp  
110 .d 111 .p 112 .c 113 .k 114 .n 115 .i 116 .f 117 .s 118 .r 119 .f  
120 .f 121 .s 122 .y 123 .f 124 .r 125 .g 126 .v 127 ee 128 vv 129 tt  
130 dd 131 nn 132 aa 133 ll 134 vv 135 nn 136 ii 137 yy 138 pp  
139 vv 140 gg 141 ee 142 dd 143 yy 144 yy 145 aa 146 cc 147 tt  
148 ee 149 tt 150 nn 151 ff 152 ii 153 tt 154 kk 155 vv 156 nn 157  
pp 158 ee 159 tt 160 ll 161 ee 162 tt 163 ii 164 kk 165 qq 166 vv  
167 dd 168 ll 169 cc 170 nn 171 yy 172 vv 173 ss 174 vv 175 nn  
176 gg 177 aa 178 tt 179 aa 180 hh 181 pp 182 hh 183 ii 184 ee  
185 nn 186 dd 187 gg 188 tt 189 vv 190 yy 191 nn 192 ii 193 gg  
194 nn 195 cc 196 ff 197 .g 198 .k 199 .n 200 .f 201 .s 202 ii 203  
aa 204 yy 205 nn 206 ii 207 vv 208 kk 209 ii 210 pp 211 pp 212  
ll 213 qq 214 aa 215 dd 216 kk 217 ee 218 dd 219 pp 220 ii 221  
ss 222 kk 223 ss 224 ee 225 ii 226 vv 227 vv 228 qq 229 ff 230  
pp 231 cc 232 ss 233 dd 234 rr 235 ff 236 kk 237 pp 238 ss  
239 yy 240 vv 241 hh 242 ss 243 ff 244 gg 245 ll 246 tt 247 pp  
248 nn 249 yy 250 ii 251 vv 252 ff 253 vv 254 ee 255 tt 256 pp  
257 vv 258 kk 259 ii 260 nn 261 ll 262 ff 263 kk 264 ff 265 ll  
266 ss 267 ss 268 ww 269 ss 270 ll 271 ww 272 gg 273 aa 274  
nn 275 yy 276 mm 277 dd 278 cc 279 ff 280 ee 281 ss 282 nn  
283 ee 284 tt 285 mm 286 gg 287 vv 288 ww 289 ll 290 hh 291

ii 292 aa 293 dd 294 kk 295 kk 296 rr 297 kk 298 kk 299 yy  
300 ii 301 nn 302 nn 303 kk 304 yy 305 rr 306 tt 307 ss 308 pp  
309 ff 310 nn 311 ll 312 ff 313 hh 314 hh 315 ii 316 nn 317 tt 318  
yy 319 ee 320 dd 321 hh 322 ee 323 ff 324 ll 325 ii 326 vv 327  
dd 328 ll 329 cc 330 cc 331 ww 332 kk 333 gg 334 ff 335 ee  
336 ff 337 vv 338 yy 339 nn 340 yy 341 ll 342 yy 343 ll 344 aa  
345 nn 346 ll 347 rr 348 ee 349 nn 350 ww 351 ee 352 ee 353  
vv 354 kk 355 kk 356 nn 357 aa 358 rr 359 kk 360 aa 361 pp  
362 qq 363 pp 364 ee 365 vv 366 rr 367 rr 368 yy 369 vv 370  
ll 371 pp 372 ll 373 nn 374 ii 375 dd 376 kk 377 aa 378 dd 379 tt  
380 gg 381 kk 382 nn 383 ll 384 vv 385 tt 386 ll 387 pp 388 nn  
389 tt 390 tt 391 aa 392 tt 393 aa 394 ii 395 ll 396 cc 397 ss  
398 dd 399 ee 400 tt 401 ii 402 ww 403 ll 404 ee 405 pp 406  
ee 407 vv 408 ll 409 ff 410 ss 411 gg 412 pp 413 rr 414 qq 415  
aa 416 ff 417 ee 418 ff 419 pp 420 qq 421 ii 422 nn 423 yy 424  
qq 425 kk 426 yy 427 gg 428 gg 429 kk 430 pp 431 yy 432 tt  
433 yy 434 aa 435 yy 436 gg 437 ll 438 gg 439 ll 440 nn 441  
hh 442 ff 443 vv 444 pp 445 dd 446 rr 447 ll 448 cc 449 kk  
450 ll 451 nn 452 vv 453 kk 454 tt 455 kk 456 ee 457 tt 458  
ww 459 vv 460 ww 461 qq 462 ee 463 pp 464 dd 465 ss 466  
yy 467 pp 468 ss 469 ee 470 pp 471 ii 472 ff 473 vv 474 ss 475  
hh 476 pp 477 dd 478 aa 479 ll 480 ee 481 ee 482 dd 483 dd  
484 gg 485 vv 486 vv 487 ll 488 ss 489 vv 490 vv 491 vv 492  
ss 493 pp 494 gg 495 aa 496 gg 497 qq 498 kk 499 pp 500 aa  
501 yy 502 ll 503 ll 504 ii 505 ll 506 nn 507 aa 508 kk 509 dd  
510 ll 511 ss 512 ee 513 vv 514 aa 515 rr 516 aa 517 ee 518 vv  
519 ee 520 ii 521 nn 522 ii 523 pp 524 vv 525 tt 526 ff 527 hh  
528 gg 529 ll 530 ff 531 kk 532 kk 533 ss

1

dbStart: 1

dbEnd: 533

pdbStart: 1

pdbEnd: 533

ps: -1

pe: 531

## Pdb Inspection:

DBREF	4RYZ A	1	533	UNP	Q28175	RPE65_BOVIN	1	533
DBREF	4RYZ B	1	533	UNP	Q28175	RPE65_BOVIN	1	533
SEQADV	4RYZ ACE A	1	UNP	Q28175	MET	1 ACETYLATION		
SEQADV	4RYZ LEU A	341	UNP	Q28175	SER	341 CONFLICT		
SEQADV	4RYZ ACE B	1	UNP	Q28175	MET	1 ACETYLATION		
SEQADV	4RYZ LEU B	341	UNP	Q28175	SER	341 CONFLICT		
SEQRES	1 A 533 ACE	SER SER GLN VAL GLU HIS PRO ALA GLY GLY TYR LYS						
SEQRES	2 A 533 LYS LEU PHE GLU THR VAL GLU GLU LEU SER SER PRO LEU							
SEQRES	3 A 533 THR ALA HIS VAL THR GLY ARG ILE PRO LEU TRP LEU THR							
SEQRES	4 A 533 GLY SER LEU LEU ARG CYS GLY PRO GLY LEU PHE GLU VAL							
SEQRES	5 A 533 GLY SER GLU PRO PHE TYR HIS LEU PHE ASP GLY GLN ALA							
SEQRES	6 A 533 LEU LEU HIS LYS PHE ASP PHE LYS GLU GLY HIS VAL THR							

397188: Start mismatch due to ACE

debug: chain Q entity 4

rafBody: 1 xx 2 aa 3 xx 4 aa 5 aa 6 || 7 aa 8 gg 9 aa  
10 aa 11 xx 12 aa 13 gg 14 || 15 aa 16 xx

4

dbStart: 1

dbEnd: 17

pdbStart: 0

pdbEnd: 16

ps: -1

pe: 15

## Pdb Inspection:

DBREF	1EFR A	2	510	UNP	P19483	ATP0_BOVIN	45	553
DBREF	1EFR B	2	510	UNP	P19483	ATP0_BOVIN	45	553
DBREF	1EFR C	2	510	UNP	P19483	ATP0_BOVIN	45	553
DBREF	1EFR D	-3	478	UNP	P00829	ATPB_BOVIN	47	528
DBREF	1EFR E	-3	478	UNP	P00829	ATPB_BOVIN	47	528
DBREF	1EFR F	-3	478	UNP	P00829	ATPB_BOVIN	47	528
DBREF	1EFR G	1	272	UNP	P05631	ATPG_BOVIN	26	297
DBREF	1EFR Q	0	16	PDB	1EFR	1EFR	1	17

SEQRES	1	Q	17	ACE YCP AIB YCP AIB AIB LEU BAL GLY AIB AIB YCP AIB
SEQRES	2	Q	17	GLY LEU AIB TLX

229883: ins code not found in RAF

debug: chain B entity 1

rafBody: 43 .r 44 .r 45Pgg 46Pss 47Pff 48Pvv 1 ee 2 mm  
3 vv 4 dd 5 nn 6 ll 7 rr 8 gg 9 kk 10 ss 11 gg 12 qq 13  
gg 14 yy 15 yy 16 vv 17 ee 18 mm 19 tt 20 vv 21 gg 22 ss  
23 pp 24 pp 25 qq 26 tt 27 ll 28 nn 29 ii 30 ll 31 vv 32 dd  
33 tt 34 gg 35 ss 36 ss 37 nn 38 ff 39 aa 40 vv 41 gg 42  
aa 45 hh 46 pp 47 ff 48 ll 49 hh 50 rr 51 yy 52 yy 53 qq  
54 rr 55 qq 56 ll 57 ss 58 ss 59 tt 60 yy 61 rr 62 dd 63 ll  
64 rr 65 kk 66 gg 67 vv 68 yy 69 vv 70 pp 71 yy 72 tt 73  
qq 74 gg 75 kk 76 ww 77 ee 78 gg 79 ee 80 ll 81 gg 82 tt  
83 dd 84 ll 85 vv 86 ss 87 ii 88 pp 89 hh 90 gg 91 pp 92  
nn 93 vv 94 tt 95 vv 96 rr 97 aa 98 nn 99 ii 100 aa 101 aa  
102 ii 103 tt 104 ee 105 ss 106 dd 107 kk 108 ff 109 ff 110 ii 111  
nn 112 gg 113 ss 114 nn 115 ww 116 ee 117 gg 118 ii 119 ll 120 gg  
121 ll 122 aa 123 yy 124 aa 125 ee 126 ii 127 aa 128 rr 129 pp 130  
dd 131 dd 132 ss 133 ll 134 ee 135 pp 136 ff 137 ff 138 dd 139 ss  
140 ll 141 vv 142 kk 143 qq 144 tt 145 hh 146 vv 147 pp 148 nn  
149 ll 150 ff 151 ss 152 ll 153 qq 154 ll 155 cc 156 gg 157 aa 158  
gg 159 ff 160 pp 161 ll 162 nn 163 qq 164 ss 165 ee 166 vv 167 ll  
168 aa 169 ss 170 vv 171 gg 172 gg 173 ss 174 mm 175 ii 176 ii  
177 gg 178 gg 179 ii 180 dd 181 hh 182 ss 183 ll 184 yy 185 tt  
186 gg 187 ss 188 ll 189 ww 190 yy 191 tt 192 pp 193 ii 194 rr  
195 rr 196 ee 197 ww 198 yy 199 yy 200 ee 201 vv 202 ii 203 ii  
204 vv 205 rr 206 vv 207 ee 208 ii 209 nn 210 gg 211 qq 212 dd  
213 ll 214 kk 215 mm 216 dd 217 cc 218 kk 219 ee 220 yy 221 nn  
222 yy 223 dd 224 kk 225 ss 226 ii 227 vv 228 dd 229 ss 230  
gg 231 tt 232 tt 233 nn 234 ll 235 rr 236 ll 237 pp 238 kk 239  
kk 240 vv 241 ff 242 ee 243 aa 244 aa 245 vv 246 kk 247 ss  
248 ii 249 kk 250 aa 251 aa 252 ss 253 ss 254 tt 255 ee 256 kk

257 ff 258 pp 259 dd 260 gg 261 ff 262 ww 263 ll 264 gg 265  
ee 266 qq 267 ll 268 vv 269 cc 270 ww 271 qq 272 aa 273 gg  
274 tt 275 tt 276 pp 277 ww 278 nn 279 ii 280 ff 281 pp 282 vv  
283 ii 284 ss 285 ll 286 yy 287 ll 288 mm 289 gg 290 ee 291 vv  
292 tt 293 nn 294 qq 295 ss 296 ff 297 rr 298 ii 299 tt 300 ii  
301 ll 302 pp 303 qq 304 qq 305 yy 306 ll 307 rr 308 pp 309 vv  
310 ee 311 dd 312 vv 313 aa 314 tt 315 ss 316 qq 317 dd 318 dd  
319 cc 320 yy 321 kk 322 ff 323 aa 324 ii 325 ss 326 qq 327 ss  
328 ss 329 tt 330 gg 331 tt 332 vv 333 mm 334 gg 335 aa 336  
vv 337 ii 338 mm 339 ee 340 gg 341 ff 342 yy 343 vv 344 vv  
345 ff 346 dd 347 rr 348 aa 349 rr 350 kk 351 rr 352 ii 353 gg  
354 ff 355 aa 356 vv 357 ss 358 aa 359 cc 360 hh 361 vv 362  
hh 363 dd 364 ee 365 ff 366 rr 367 tt 368 aa 369 aa 370 vv  
371 ee 372 gg 373 pp 374 ff 375 vv 376 tt 377 ll 378 dd 379  
mm 380 ee 381 dd 382 cc 383 gg 384 yy 385 nn

2

dbStart: 46

dbEnd: 436

pdbStart: 43P

pdbEnd: 385

ps: -1

pe: 388

seqadvs: null

check enter:b

check enter:d

tmp :CD

debug: chain C entity 2

Pdb inspection: Chain B does not have 43 and start with 45[ ]  
whereas chain A do can be mapped correctly

DBREF	1FKN	A	43P	385	UNP	P56817	BACE1_HUMAN	46	436
DBREF	1FKN	B	43P	385	UNP	P56817	BACE1_HUMAN	46	436
DBREF	1FKN	C	1	7	PDB	1FKN	1FKN	1	7
DBREF	1FKN	D	1	7	PDB	1FKN	1FKN	1	7

ATOM	3077	N	GLY	B	45P	64.691	25.969	49.731	1.00	61.03	N
ATOM	3078	CA	GLY	B	45P	65.083	27.376	49.996	1.00	62.72	C
ATOM	3079	C	GLY	B	45P	65.106	27.574	51.489	1.00	64.30	C
ATOM	3080	O	GLY	B	45P	65.763	28.482	52.006	1.00	66.26	O
ATOM	3081	N	SER	B	46P	64.361	26.697	52.159	1.00	64.03	N
ATOM	3082	CA	SER	B	46P	64.231	26.646	53.606	1.00	62.37	C
ATOM	3083	C	SER	B	46P	63.316	27.684	54.247	1.00	60.15	C
ATOM	3084	O	SER	B	46P	63.790	28.674	54.813	1.00	59.43	O
ATOM	3085	CB	SER	B	46P	65.614	26.707	54.249	1.00	64.92	C
ATOM	3086	OG	SER	B	46P	66.406	25.616	53.821	1.00	67.47	O
ATOM	3087	N	PHE	B	47P	62.005	27.453	54.151	1.00	55.61	N
ATOM	3088	CA	PHE	B	47P	60.992	28.333	54.761	1.00	51.72	C
ATOM	3089	C	PHE	B	47P	59.884	27.413	55.260	1.00	50.80	C
ATOM	3090	O	PHE	B	47P	58.694	27.675	55.067	1.00	49.72	O
ATOM	3091	CB	PHE	B	47P	60.425	29.338	53.747	1.00	47.77	C
ATOM	3092	CG	PHE	B	47P	61.344	30.497	53.454	1.00	44.96	C

233426 : raf start offset due to ACE

debug: chain I entity 3

rafBody: 1 ff 2 pp 3 rr 67 qq 68 ss 69 hh 70 nn 71 dd 72  
gg 73 dd 74 ff 75 ee 76 ee 77 ii 78 pp 79 ee 80 ee 81 yy 82  
ii 83 qq

3

dbStart: 49

dbEnd: 65

**pdbStart:** 0

**pdbEnd:** 83

ps: -1

pe: 19

seqadvs: null

check enter:b

check enter:d

DBREF	1IHS	L	1H	14N	UNP	P00734	THRΒ_HUMAN	328	363
DBREF	1IHS	H	16	247	UNP	P00734	THRΒ_HUMAN	364	622
DBREF	1IHS	I	0	83	UNP	P28504	HIR2_HIRME	49	65

SEQADV	1IHS	ACE	I	0	UNP	P28504		INSERTION
SEQADV	1IHS	DPN	I	1	UNP	P28504		INSERTION
SEQADV	1IHS	PRO	I	2	UNP	P28504		INSERTION
SEQADV	1IHS	OPR	I	3	UNP	P28504		INSERTION

253494 : raf end offset : The last one is a NH2

debug: chain 5 entity 5

rafBody: 1 ss 2 xx 3 tt 4 aa 5 xx 6 xx 7 xx 8 cc 9 xx  
10 xx 11 xx 12 aa

31

dbStart: 38

dbEnd: 50

pdbStart: 1

pdbEnd: 13

ps: 0

pe: -1

DBREF	2ZJP	O	1	100	UNP	Q9RY64	RL21_DEIRA	1	100
DBREF	2ZJP	P	1	134	UNP	Q9RXJ7	RL22_DEIRA	1	134
DBREF	2ZJP	Q	1	95	UNP	Q9RXK0	RL23_DEIRA	1	95
DBREF	2ZJP	R	1	115	UNP	Q9RXJ1	RL24_DEIRA	1	115
DBREF	2ZJP	S	1	237	UNP	Q9RX88	RL25_DEIRA	1	237
DBREF	2ZJP	T	1	91	UNP	Q9RY65	RL27_DEIRA	1	91
DBREF	2ZJP	U	1	81	UNP	Q9RRG8	RL28_DEIRA	1	81
DBREF	2ZJP	V	1	67	UNP	Q9RXJ4	RL29_DEIRA	1	67
DBREF	2ZJP	W	1	55	UNP	Q9RSL0	RL30_DEIRA	1	55
DBREF	2ZJP	Y	1	60	UNP	P49228	RL32_DEIRA	1	60
DBREF	2ZJP	1	1	55	UNP	Q9RSS4	RL33_DEIRA	1	55
DBREF	2ZJP	2	1	47	UNP	Q9RSW2	RL34_DEIRA	1	47
DBREF	2ZJP	3	1	66	UNP	Q9RSW6	RL35_DEIRA	1	66
DBREF	2ZJP	4	1	37	UNP	Q9RSK0	RL36_DEIRA	1	37
DBREF	2ZJP	5	1	13	UNP	C6FX52	NOSM_STRAS	38	50

SEQRES	1	5	13	SER	BB9	THR	DBU	BB9	3GL	BB9	CYS	BB9	MH6	BB9	DHA	NH2
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265096 : This one is confusing since the residue number is not consistent 1~303 VS 2~319 also how 3199.p is generated?

debug: chain C entity 1

rafBody: 2.m 3.k 4.r 5.r 6.f 7.t 8.l 9.l 10.g 11.s  
12.v 13.v 14.a 15.l 16.a 17.l 18.s 19.s 20.t 21.a 22.l  
23.a 24.s 25.d 26.a 27.p 28.aa 29.ss 30.rr 31.gg 32.cc  
33.aa 34.dd 35.dd 36.aa 37.gg 38.ww 39.nn 40.dd 41.pp  
42.aa 43.mm 44.pp 45.ll 47.rr 48.vv 49.yy 50.gg 51.nn 52.  
tt 53.ww 54.yy 55.vv 56.gg 57.tt 66.cc 67.gg 68.ii 69.ss  
70.aa 71.ll 72.ll 73.vv 74.tt 75.ss 76.dd 78.aa 79.gg 80.hh  
81.ii 82.ll 83.vv 84.dd 85.aa 86.aa 87.tt 89.pp 90.qq 91.aa  
92.gg 93.pp 94.qq 95.ii 96.ll 97.aa 98.nn 99.ii 100.rr 101.aa  
102.ll 103.gg 104.ff 105.rr 106.pp 107.ee 108.dd 109.vv 110.rr 111.  
aa 112.ii 113.vv 114.ff 115.ss 116.hh 117.ee 118.hh 119.ff 120.dd  
121.hh 122.aa 123.gg 124.ss 125.ll 126.aa 127.ee 128.ll 129.qq  
130.rr 131.aa 132.tt 133.gg 134.aa 135.pp 136.vv 137.yy 138.aa  
139.rr 140.aa 141.pp 142.aa 143.ii 144.dd 145.tt 146.ll 147.rr 148.  
gg 149.gg 150.ll 151.pp 152.dd 153.rr 154.tt 155.dd 156.pp 157.qq  
158.ff 159.ee 160.vv 161.aa 162.ee 163.pp 164.vv 165.aa 166.pp  
168.vv 169.aa 170.nn 171.ii 172.vv 173.tt 174.ll 175.aa 176.dd 177.  
dd 178.gg 179.vv 180.vv 181.ss 182.vv 183.gg 184.pp 185.ll 186.  
aa 187.ll 188.tt 189.aa 190.vv 191.aa 193.ss 194.pp 195.gg 196.  
hh 197.tt 198.pp 199.gg 200.gg 201.tt 202.ss 203.ww 204.tt  
205.ww 206.rr 207.ss 208.cc 209.ee 210.gg 211.dd 212.dd 213.  
cc 214.rr 215.qq 216.mm 217.vv 218.yy 219.aa 220.dd 221.ss  
222.ll 223.tt 224.aa 225.ii 226.ss 227.dd 227.dd 227.vv 228.ff  
229.rr 230.yy 231.ss 232.dd 233.dd 234.aa 235.aa 236.hh 237.  
pp 238.gg 239.yy 240.ll 241.aa 242.aa 243.ff 244.rr 245.nn 246.  
tt 247.ll 248.aa 249.rr 250.vv 251.aa 252.aa 254.ll 255.dd 256.  
cc 257.dd 258.ii 259.ll 260.vv 261.tt 262.pp 263.hh 264.pp 265.  
ss 266.aa 267.ss 268.gg 269.ll 270.ww 271.nn 272.rr 273.ii 274.  
gg 275.pp 276.rr 277.aa 281.aa 282.aa 283.pp 284.ll 285.mm  
286.dd 287.tt 288.tt 289.aa 290.cc 291.rr 292.rr 293.yy 294.aa

295 qq 296 gg 297 aa 298 rr 299 qq 300 rr 301 ll 302 ee 303  
kk 304 rr 305 ll 306 aa 307 ee 308 ee 309 aa 310 aa 311 tt  
3122.s 313.p 3144.s 3155.s 3166.g 3177.a 3188.r 3199.p

1

dbStart: 1

dbEnd: 303

pdbStart: 2

pdbEnd: 319

ps: 0

pe: -1

DBREF	4AWZ A	2	319	UNP	B5DCA0	B5DCA0_PSEAI	1	303
DBREF	4AWZ B	2	319	UNP	B5DCA0	B5DCA0_PSEAI	1	303
DBREF	4AWZ C	2	319	UNP	B5DCA0	B5DCA0_PSEAI	1	303

ATOM	6125	OE2	GLU	C	308	57.180	-18.116	43.392	1.00	12.97	0
ATOM	6126	N	ALA	C	309	59.465	-16.876	49.750	1.00	20.00	N
ATOM	6127	CA	ALA	C	309	59.967	-17.321	51.065	1.00	22.09	C
ATOM	6128	C	ALA	C	309	59.241	-16.567	52.173	1.00	24.20	C
ATOM	6129	O	ALA	C	309	59.022	-17.117	53.245	1.00	25.62	O
ATOM	6130	CB	ALA	C	309	61.488	-17.119	51.192	1.00	21.40	C
ATOM	6131	N	ALA	C	310	58.859	-15.321	51.893	1.00	26.01	N
ATOM	6132	CA	ALA	C	310	58.184	-14.462	52.849	1.00	27.76	C
ATOM	6133	C	ALA	C	310	56.678	-14.721	52.989	1.00	29.41	C
ATOM	6134	O	ALA	C	310	56.033	-14.071	53.819	1.00	30.02	O
ATOM	6135	CB	ALA	C	310	58.412	-12.995	52.471	1.00	27.91	C
ATOM	6136	N	THR	C	311	56.104	-15.627	52.188	1.00	30.48	N
ATOM	6137	CA	THR	C	311	54.654	-15.855	52.221	1.00	31.86	C
ATOM	6138	C	THR	C	311	54.273	-17.337	52.332	1.00	31.90	C
ATOM	6139	O	THR	C	311	54.870	-18.183	51.669	1.00	32.82	O
ATOM	6140	CB	THR	C	311	53.980	-15.253	50.979	1.00	31.85	C
ATOM	6141	OG1	THR	C	311	54.473	-15.917	49.818	1.00	34.39	O
ATOM	6142	CG2	THR	C	311	54.271	-13.758	50.857	1.00	32.56	C
TER	6143										

369478: pdbStart: null case unmet before  
rafBody: 215 .g 216 .s 217 .h 218 .s 219 .r 220 .g 221 .l 222 kk  
223 kk 224 mm 225 rr 226 ee 227 ii 228 ii 229 gg 230 ww 231

pp 232 gg 233 gg 234 ss 235 gg 236 gg 237 .s 238 .g 239 .s  
240 .g 241 .s 242 .g 243 .d 244 .s 245 ee 246 rr 247 hh 248 ff  
249 vv 250 hh 251 qq 252 ff 253 kk 254 gg 255 ee 256 cc 257  
yy 258 ff 259 tt 260 nn 261 gg 262 tt 263 qq 264 rr 265 ii 266  
rr 267 ll 268 vv 269 tt 270 rr 271 yy 272 ii 273 yy 274 nn 275 rr  
276 ee 277 ee 278 yy 279 ll 280 rr 281 ff 282 dd 283 ss 284 dd  
285 vv 286 gg 287 ee 288 yy 289 rr 290 aa 291 vv 292 tt 293  
ee 294 ll 295 gg 296 rr 297 hh 298 ss 299 aa 300 ee 301 yy  
302 yy 303 nn 304 kk 305 qq 306 yy 307 ll 308 ee 309 rr 310 tt  
311 rr 312 aa 313 ee 314 ll 315 dd 316 tt 317 aa 318 cc 319 rr  
320 hh 321 nn 322 yy 323 ee 324 ee 325 tt 326 ee 327 vv 328  
pp 329 tt 330 ss 331 ll 332 rr 333 rr 334 ll 335 ee 336 qq 337  
pp 338 nn 339 vv 340 aa 341 ii 342 ss 343 ll 344 ss 345 .r  
346 .t 347 .e 348 .a 349 .l 350 .n 351 .h 352 .h 353 .n 354 tt  
355 ll 356 vv 357 cc 358 ss 359 vv 360 tt 361 dd 362 ff 363 yy  
364 pp 365 aa 366 kk 367 ii 368 kk 369 vv 370 rr 371 ww 372  
ff 373 .r 374 .n 375 .g 376 .q 377 .e 378 ee 379 tt 380 vv 381 gg  
382 vv 383 ss 384 ss 385 tt 386 qq 387 ll 388 ii 389 rr 390 nn  
391 gg 392 dd 393 ww 394 tt 395 ff 396 qq 397 vv 398 ll 399  
vv 400 mm 401 ll 402 .e 403 .m 404 .t 405 .p 406 .h 407 .q  
408 .g 409 .e 410 .v 411 yy 412 tt 413 cc 414 hh 415 vv 416 ee  
417 hh 418 pp 419 ss 420 ll 421 kk 422 ss 423 pp 424 ii 425 tt  
426 vv 427 ee 428 ww 429 .s 430 .s 431 .a 432 .d 433 .l 434 .v  
435 .p 436 .r

2

dbStart: 47

dbEnd: 61

pdbStart: 221

pdbEnd: 235

ps: 6

pe: 20

dbStart: 28

dbEnd: 214

pdbStart: null

pdbEnd: 428

ps: -1

pe: 213

## Pdb inspection:

Chain B's numbering issue