

**CBR1**  
NP\_001748.1  
[277 aa]

6 151

**Domain:** Short Chain Dehydrogenase (PF16152)  
**Active Site Proton Acceptor:** Y194  
**Important Residue (NADP-binding):** N90  
**Important Residue (Glutathione-binding):** Q106

**CG11200**  
NP\_611471.1  
[355 aa]

21 68 68 252

**Domain:** Short Chain Dehydrogenase (PF16152)  
**Predicted Active Site Proton Acceptor:** Y233  
**Predicted Important Residue (NADP-binding):** N154

**B.**

CG11200/1-355

1 10 20 30 40 50

β1 β2 α1 β3 β4

CG11200/1-355  
3BHJ/2-276

..MLGTLLWIFFVGLLLCAFLFSKTTKEFPKSWFEWKTEFRYQYLGIVGLVHDAQYKARD  
SG.....

CG11200/1-355

60 70 80 90 100 110

β5 α2 β6 α3

CG11200/1-355  
3BHJ/2-276

RVALYKQPDRIAVITG.GNRGIGIRIVKLLACD.MTVVVGVRDPKIAETAVASIVDLNA  
.....IHVALVITG.G.NKGIGIRIVRDLCRLFSGDVVLTARDVTRGQAAVQQLQAEG.

CG11200/1-355

120 130 140 150 160

β7 α4 β8

CG11200/1-355  
3BHJ/2-276

TKGKLICEOLDVGDILKSVKAFALIKERY.S.KVDMLLNAGIMF....AP...F...KLT  
..LSPRFHOLDIDLQSERALRDFLRKE.YGGLDVLVNNAGIAFKVADP.TPFHIQA...

CG11200/1-355

170 180 190 200 210

α5 α6 β9 η1

CG11200/1-355  
3BHJ/2-276

ADGYESHFAINFLGHFLTLHLLEQLRAAGKEGRNSRIVNVSSCVN.LT.....  
....EVTMKTNEFGGTRDVCTELLELILK...P...Q.GRVNVSSIMSVRALKSCSPELQQK

CG11200/1-355

220 230 240

T..T TT α7

CG11200/1-355  
3BHJ/2-276

.....GRINY..KDINGT.KH.....YYPGTAYSQSKLQAQILFTRH  
FRSETITEEELVG....LMNK.F..VEDTKKGVHQKEGWPS....SAYGVTKLGVTVLSRI

CG11200/1-355

250 260 270 280 290

β10 α8 α9

CG11200/1-355  
3BHJ/2-276

LQTLDAE.K.KSHVQVNVVHPGIV.....DTDLEHSAATTSVPPIF.KKLFCKT.PEFGS  
HARKLSEQRKGDKILLNACCPCGVVVRTDMAG.....PK.AT.....KSPEEGA

CG11200/1-355

300 310 320 330 340

α10 α11

CG11200/1-355  
3BHJ/2-276

RTVVFANIDP....SIE...GQGGTYLSNGGKGPFFHPDAKKPAKCEQLFQSCDLLKIQ  
ETPVYIALLPDAEG.PHGQFV...SE..K.RVEQW.....

CG11200/1-355

350

CG11200/1-355  
3BHJ/2-276

QYNGNEY  
.....

C.

CG11200/1-355 1 - -MLGTLTWIFFVGLLLCAFLFSKTTKEFPKSWFEWKTEFRYQYLGI VGLVHDAQYKARDRVALYKQPDRIAVIT73  
3BHJ/2-276 2 SG-----I HVALVT10

CG11200/1-355 74 G-GNRGIGLRIVEKLLACD-MTVVMGVVDPKIAETAVASIVDLNATKGKLCEDLDVGDLSVKAFQALIKERYYS146  
3BHJ/2-276 11 GG-NKGIGLAIVRDLCLRFSGDVVLTAADVTRGQAAVQQLQAEG---LSRFRHQLDIDDLQSI RALRDFLRKE-Y80

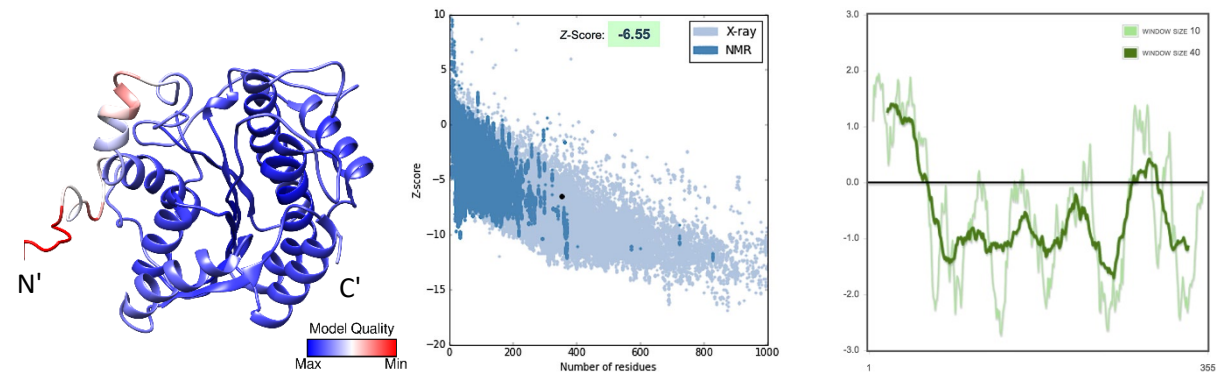
CG11200/1-355 147 -KVDLLLNNAGIMF-----AP---F--KLTADGYESHFAINFLGHFLTHLLPQLRAAGKEGRNSRIVNVSSCV210  
3BHJ/2-276 81 GGLDVLVNNAGIAFKVADP-TPFHIQA-----EVTMKTNFFGTRDVCTELLPLIK--P---Q-GRVNVSSIM141

CG11200/1-355 211 N-LI-----GRINY--KDINGT-KH-----YYPGTAYSQSKLAQILFTRH246  
3BHJ/2-276 142 SVRALKSCSP ELQQKFRSETITEELVG---LMNKF--VEDTKKG VHQKEGWS---SAYGVTKIGVTVLSRI206

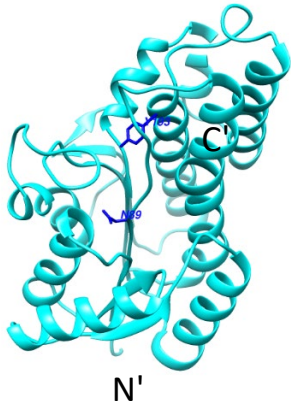

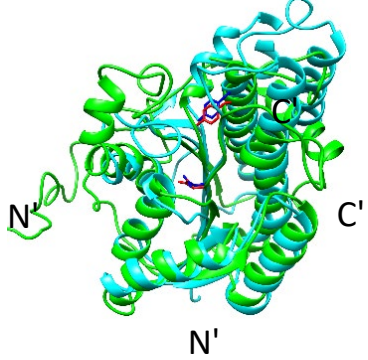
CG11200/1-355 247 LQTLLDAE-K-SHVQVNVVHPGIV-----DTDLEHFSATTSVP I F-KKLFFKT-PERGSRTVVFAAIDP-----S307  
3BHJ/2-276 207 HARKLSECRKGDKILLNACCPGWVRTMAG-----PK-AT-----KSP EEGAETPVYLALLPPDAEG262

CG11200/1-355 308 I E---GQGGTYLSNGGKGPFFHDAKKPAKCEQLQFSCDLLKIQQYGNGEY 355  
3BHJ/2-276 263 -PHGQFV---SE-K-VEQW----- 276

D.



E.

CBR1 Structure	<i>D. melanogaster</i> Model	Superimposed
		

F.	Length (AA)	Domain Architecture (Pfam, range)	Functional Residues (aligned matches in <i>D. melanogaster</i> )	Sequence ID%	Structural Overlap (RMSD)
Carbonyl reductase 1 (CBR1, NP_001748.1, PDB: 3BHJ)	277	Short chain dehydrogenase domain (PF16152) 6-151	N90 and Y194	20% ID 33% SIM	1.153 Å
CBR (CG11200, NP_611471.1)	355	Short chain dehydrogenase domain (PF16152) 68-252	N154 and Y233		

**S11 Fig. Sequence and structural details of the modeled fly CBR1 candidate.** A. Domain architecture of CBR1 and CG11200 and known/predicted functional residues B. Pairwise alignment of CG11200 and 3BHJ generated from structural superposition showing shared secondary structure elements and known/predicted functional residues ( marked with red asterisks) C. Pairwise alignment of CG11200 and 3BHJ generated from structural superposition with conserved residues highlighted using the physiochemical color scheme (CLUSTALX) D. Validation of the CG11200 model: ProQ2 quality score mapped to a 3D model of CG11200 (left); ProSA global quality score ranking (middle) and per-residue quality graph (right) E. CPA1 (3BHJ, cyan-blue) superimposed on the predicted structure of CG11200 (green-red) with potential matches for conserved functional residues highlighted F. Summary of features shared by CBR1 and potential *D. melanogaster* ortholog CG11200.