Structure Assessment

Help   Examples ▾

IcGABBA-TM-seqRdl; Model 01;
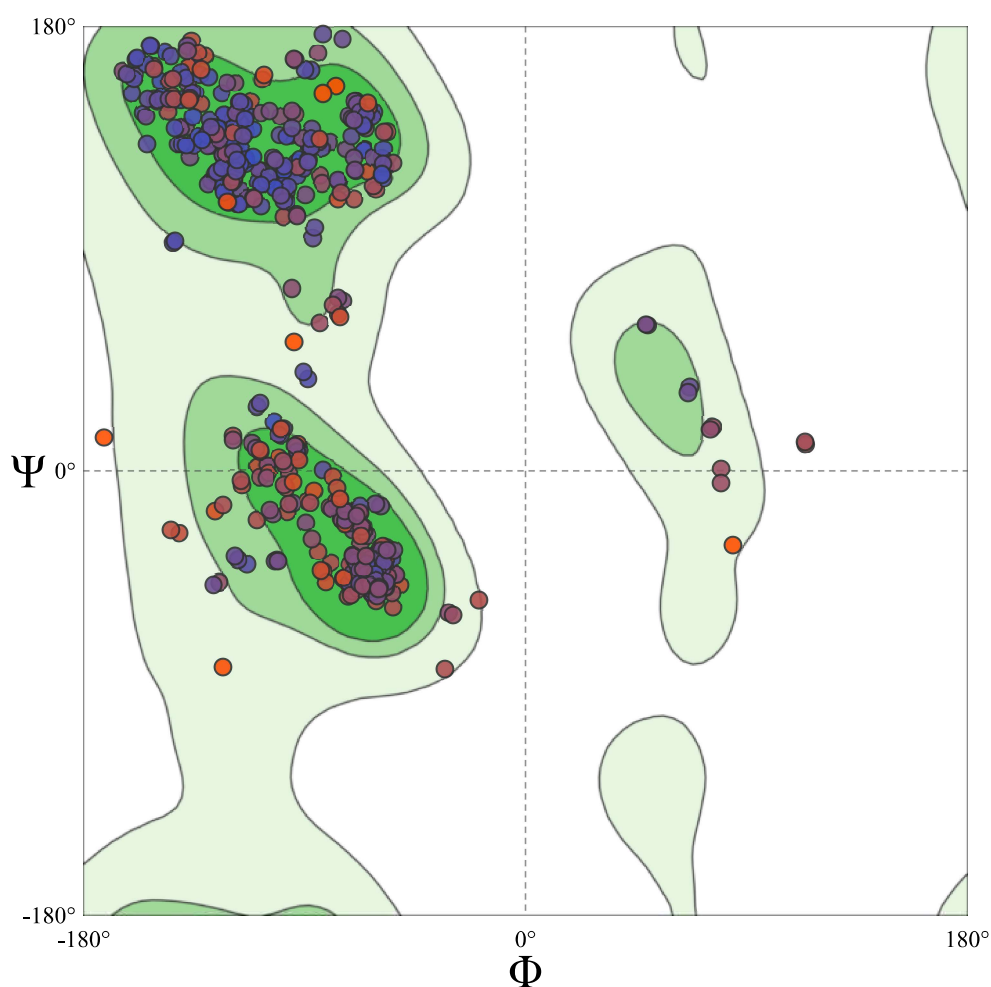
Project Data ▾   ☰ ☑ *Compare* ⧉

Created: Fri 17th Dec, 18:29;

Membrane annotation has been transferred from template. ❷
☑ Show / Hide

Ramachandran Plots   ⌃

General | Glycine | Proline | Pre-Proline   All selected (2) ▾   📷

MolProbity Results   ⌃

MolProbity Score	1.36
☐ Clash Score	1.50

	Ramachandran Favoured	95.61%	
☐	Ramachandran Outliers	1.21%	B69 PRO, A79 GLU, B75 SER, A75 SER, A170 VAL, B170 VAL, A163 GLU, B163 GLU
☐	Rotamer Outliers	1.67%	B195 THR, B178 GLN, B71 VAL, A73 THR, A274 ILE, B50 LEU, A97 SER, B274 ILE, A199 SER, B199 SER
☐	C-Beta Deviations	5	A46 MET, B46 MET, B170 VAL, A103 THR, A170 VAL
	Bad Bonds	0 / 5480	
☐	Bad Angles	45 / 7450	A73 THR, (B240 THR-B241 PRO), B51 ASP, B91 PHE, B156 ASP, B99 PHE, (B68 ARG-B69 PRO), (A220 ILE-A221 PRO), A80 PHE, (A305 THR-A306 PRO), B47 ASP, (B220 ILE-B221 PRO), A91 PHE, (B305 THR-B306 PRO), (A240 THR-A241 PRO), A47 ASP, (A162 ASN-A163 GLU), B54 PHE, (B162 ASN-B163 GLU), A103 THR, (B198 TYR-B199 SER), (A78 SER-A79 GLU), (A198 TYR-A199 SER), A310 ASP, (B317 PHE-B318 PRO), (A317 PHE-A318
☐	Cis Non-Proline	2 / 632	(A102 ALA-A103 THR), (B102 ALA-B103 THR)
☐	Cis Prolines	2 / 30	(A136 PHE-A137 PRO), (B136 PHE-B137 PRO)
☐	Twisted Non-Proline	1 / 632	(A79 GLU-A80 PHE)

Results obtained using MolProbity version 4.4

Quality Estimate ⌃

QMEANDisCo Global: 0.70   ± 0.05 ❓

QMEANDisCo Local

Local Quality Estimate

QMEAN Z-Scores

QMEAN		-3.67
Cβ		-3.00
All Atom		0.25
solvation		-0.75
torsion		-2.91

Comparison with Non-redundant Set of PDB Structures

Residue Quality ⌃

QMEAN

Chain:A   V N I S A I L D S F S V S Y D K R V R P N Y G G P P V E V G V T M Y V L S I S S   40

QMEAN   40

Chain:B   V N I S A I L D S F S V S Y D K R V R P N Y G G P P V E V G V T M Y V L S I S S

template_upload.1.A   - F V K E T V D K L L K G Y D I R L R P D F G G P P V C V G M N I D I A S I D M   40

QMEAN

Chain:A   L S E V K M D F T L D F Y F R Q F R T D P R L A Y R K R P - G V E T L S V G S E   79

QMEAN   79

Chain:B   L S E V K M D F T L D F Y F R Q F R T D P R L A Y R K R P - G V E T L S V G S E

template_upload.1.A   V S E V N M D Y T L T M Y F Q Q Y W R D K R L A Y S G I P L N L T L D N R V - -   78

QMEAN

Chain:A   F I K N I W V P D T F F V N E K Q S Y F H I A T T S N E F I R V H H S G S I T R   119

QMEAN   119

Chain:B   F I K N I W V P D T F F V N E K Q S Y F H I A T T S N E F I R V H H S G S I T R

template_upload.1.A   - A D Q L W V P D T Y F L N D K K S F V H G V T V K N R M I R L H P D G T V L Y   117

QMEAN

Chain:A   S I R L T I T A S C P M N L Q Y F P M D R Q L C H I E I E S F G Y T M R D I R Y   159

QMEAN   159

Chain:B   S I R L T I T A S C P M N L Q Y F P M D R Q L C H I E I E S F G Y T M R D I R Y

template_upload.1.A   G L R I T T T A A C M M D L R R Y P L D E Q N C T L E I E S Y G Y T T D D I E F   157

QMEAN

Chain:A   K W N E G P N S V G V S N E V S L P Q F K V L G H R Q R A M E I S L T T G N Y S   199

QMEAN   199

Chain:B   K W N E G P N S V G V S N E V S L P Q F K V L G H R Q R A M E I S L T T G N Y S

template_upload.1.A   Y W R G G D K A V T G V E R I E L P Q F S I V E H R L V S R N V V F A T G A Y P   197

QMEAN

`- C H H H H H H H H T T C C S S S C T T T T S S C E E E E E E E E E E E E`
Chain:A `R I (A C E I Q F V R S) M G Y Y L I Q I Y I P S G L I (V V I S W V S F W L N R N A)` 239

QMEAN

`- C H H H H H H H H T T C C T T S C T T T T S S C E E E E E E E E E E E E E`
Chain:B `R I (A C E I Q F V R S) M G Y Y L I Q I Y I P S G L I (V V I S W V S F W L N R N A)` 239
template_upload.1.A `A R (L S L S F R L K R N) I G Y F I L Q T Y M P S I L I (T I L S W V S F W I N Y D A)` 237

QMEAN

`E E T T T T E E E E E E E E E E E C G G G C C S S C C - S E E C C T T S T T`
Chain:A `T P A R V A L G V T T V L T M T T L M S S T N A A L P K I S Y V K S I D V Y L G` 279

QMEAN

`E E T T T T E E E E E E E E E E E C G G G C C S S C C - C E E E C T T T T S`
Chain:B `T P A R V A L G V T T V L T M T T L M S S T N A A L P K I S Y V K S I D V Y L G` 279
template_upload.1.A `S A A R V A L G I T T V L T M T T I N T H L R E T L P K I P Y V K A I D M Y L M` 277

QMEAN

`T T S S C C C C E E E T T E E E E E C C S S S C S E E E E E C T T S E E E E`
Chain:A `A C F V M V F A S L L E Y A T V G Y M A K L L G I T P S D I D K Y S R I V F P V` 319

QMEAN

`T T T S S C C C C E E E T T E E E E E C C S S S C S E E E E E C T T S E E E E`
Chain:B `A C F V M V F A S L L E Y A T V G Y M A K L L G I T P S D I D K Y S R I V F P V` 319
template_upload.1.A `G C F V F V F L A L L E Y A F V N Y I F F S Q P A R A A A I D R W S R I V F P F` 317

QMEAN

`E E E E E E E E C C C C C T T T T S C E E E E E E E E E E E S S C C T T T E E E`
Chain:A `C F V C F N L M Y W I I Y L H V` 335

QMEAN

`E E E E E E E E C C C C C T T T T S C E E E E E E E E E E E S S C C T T T E E E`
Chain:B `C F V C F N L M Y W I I Y L H V` 335
template_upload.1.A `T F S L F N L V Y W L Y Y V - -` 331

`E E T T G G G S E E C G G G C C C S S E E E E E E E E E E E E E E E T T E E E`

`E E T T G G G S E E C G G G C C C S S E E E E E E E E E E E E E E E T T E E E`

`E E E E E E E E E C S H H H I I I I I H H H H H H H H H G G G S C T T C`

E E E E E E E E E C S H H H I I I I H H H H H H H H G G G G S C T T C

H H H H H H H H H H H H H H H H H H H H T S T C S C C H H H H H

H H H H H H H H H H H H H H H H H H H H H T S C C S C C H H H H H

H H H H H H H H H H H H H H H H H H T T T C S H H H H H H H H H H

H H H H H H H H H H H H H H H H H H T T T C S H H H H H H H H H H

H H H H H H H H H H H H C - -

H H H H H H H H H H H H C - -