

Table S1: Conditions that yielded crystals for wild type chicken γ S-crystallin. Related to STAR methods section “Crystallization”.

Index Screen:

- 3** 0.1 M Sodium acetate trihydrate pH 4.5, 2.0 M Ammonium Sulfate
6 0.1 M Tris pH 8.5, 2.0 M Ammonium Sulfate
19 1.344 M Potassium phosphate dibasic, pH 8.2, 0.056 M Sodium phosphate monobasic monohydrate,
21 1.8 M Ammonium citrate tribasic, pH 7.0
29 60% v/v Tascimate, pH 7.0
44 0.1 M HEPES, pH 7.7, 25% PEG 3350
45 0.1 M Tris pH 8.5, 25% PEG 3350
46 0.1 M Bis-Tris, pH 6.5, 20% PEG MME 5,000
55 0.1 M HEPES, pH 7.5, 30% PEG MME 55, 0.05 M Magnesium chloride hexahydrate
59 0.1 M HEPES, pH 7.5, 22% Poly(acrylic acid sodium salt) 5,100, 0.02 M Magnesium chloride hexahydrate,
60 0.1 M Tris, pH 8.5, 20% Polyvinylpyrrolidone K15, 0.01 M Cobalt(II) chloride hexahydrate
79 0.1 M Bis-Tris pH 6.5, 25% PEG 3350, 0.2 M Ammonium acetate
80 0.1 M HEPES pH 7.5, 25% PEG 335, 0.2 M Ammonium acetate
81 0.1 M Tris pH 8.5, 25% PEG 3350, 0.2 M Ammonium Sulfate
83 0.1 M Bis-Tris, pH 6.5, 25% PEG 3350, 0.2 M Magnesium chloride hexahydrate
84 0.1 M HEPES, pH 7.5, 25% PEG 3350, 0.2 M Magnesium chloride hexahydrate
90 20% PEG 3350, 0.2 M Sodium formate
91 20% PEG 3350, 0.15 M DL-Malic acid pH 7.0
92 15% PEG 3350, 0.1 M Magnesium formate dehydrate
95 30% PEG MME 2,000, 0.1 M Potassium thiocyanate
96 30% PEG MME 2,000, 0.15 M Potassium bromide

Peg/Ion Screen:

- 1** 0.1 M Sodium fluoride pH 7.3, 20% PEG 3350
2 0.1 M Potassium fluoride pH 7.3, 20% PEG 3350
3 0.2 M Ammonium fluoride pH 6.2, 20% PEG 3350
4 0.2 M Lithium chloride pH 6.8, 20% PEG 3350
5 0.2 M Magnesium chloride hexahydrate pH 5.9, 20% PEG 3350
6 0.2 M Sodium chloride pH 6.9, 20% PEG 3350
8 0.2 M Potassium chloride pH 7.0, 20% PEG 3350
13 0.2 M Sodium thiocyanate pH 6.9, 20% PEG 3350
14 0.2 M Potassium thiocyanate pH 7.0, 20% PEG 3350
15 0.2 M Lithium nitrate pH 7.1, 20% PEG 3350
17 0.2 M Sodium nitrate pH 6.8, 20% PEG 3350
18 0.2 M Potassium nitrate pH 6.8, 20% PEG 3350
20 0.2 M Magnesium formate dihydrate pH 7.0, 20% PEG 3350
21 0.2 M Sodium formate, pH 7.2, 20% PEG 3350
22 0.2 M Potassium formate pH 7.3, 20% PEG 3350
23 0.2 M Ammonium formate pH 6.6, 20% PEG 3350
24 0.2 M Lithium acetate dihydrate pH 7.9, 20% PEG 3350
25 0.2 M Magnesium acetate tetrahydrate pH 7.9, 20% PEG 3350
27 0.2 M Sodium acetate trihydrate pH 8.0, 20% PEG 3350
28 0.2 M Calcium acetate hydrate pH 7.5, 20% PEG 3350
30 0.2 M Ammonium acetate, pH 7.1, 20% PEG 3350

Peg/Ion Screen2:

- 20** 0.2 M Succinic acid pH 7.0, 20% PEG 3350
25 0.1 M Sodium acetate trihydrate pH 7.0, 12% PEG 3350
26 0.2 M Sodium acetate trihydrate pH 7.0, 12 % PEG 3350
28 0.2 M Sodium formate pH 7.0, 20% PEG 3350
33 2% v/v Tacsimate, pH 6.0, 0.1 M Bis-Tris PH 6.5, 20% PEG 3350
39 (0.04 M Citric acid, 0.06 M Bis-Tris propane/pH 6.4), 20% PEG 3350
40 (0.03 M Citric acid, 0.07 M Bis-Tris propane/pH 7.6), 20% PEG 3350
46 20% PEG 3350, 0.2 M Sodium bromide

Pi-Minimal Screen:

- 7** 150 mM MOPS pH 7.0, 24% PEG 4,000, 8% v/v 1, 2-Propanediol
19 150mM MOPS, pH 7.0, 22.9% PEG MME 5,000, 7% v/v PEG 300
32 150mM MOPS, pH 7.5, 25.7% w/v PEG 8,000, 60 mM Potassium Sodium tartrate
42 150 mM MES, pH 6.5, 28.6% w/v PEG 8,000, 100mM Magnesium sulfate
59 42.9% w/v PEG 1, 000, 50mM Calcium chloride
69 150mM Tris, pH 8.0, 41.1% PEG 1,000, 30mM Calcium chloride
71 150mM AMPD-Tris buffer, pH 9.0, 34.3% PEG MME 5,000, 30 mM Potassium sodium tartrate
79 150 mM MOPS, pH 7.0, 44.6% PEG 4,000, 40mM Potassium bromide
81 150 mM Tris pH 8.0, 37.1% PEG MME 5,000, 40 mM Magnesium Sulfate
84 150 mM Sodium formate pH 40, 4M Ammonium sulfate, 1% PEG 300
91 150 mM HEPES pH 7.5, 72% w/v Glycerol, 1% v/v Ethylene glycol
94 150 mM TAPS, pH 8.5, 40% PEG 8, 000, 1% v/v 2-Methyl-2, 4-pentanediol

Table S2: Intermolecular Side chain contact residues of the QR Monomer-monomer Interface.

Related to Figure 6. Residues were identified using Contact in CCP4 and verified by inspection.

Contacts are listed only for side chains. Atoms are listed for polar contacts only.

Chicken γ S

Polar:

His70(N ε 2)-Leu75(O)
 His71(ND1)-Arg145(NH1)
 Asn143(OD1)-Arg173(NH2)
 145Arg(NH1, NH2)-Glu65(O)

Non-polar:

Arg62-Asn143
 Tyr66-Arg145
 His70-Leu75
 His71-Gly146, His141
 Met73-Met73, His70
 Tyr144-Tyr144

Human β B1

Polar:

Arg122(NH2)-Tyr197(OH)
 Tyr130(OH)-Ser127(O γ)a
 Ser172(O γ)-Lys117(O)
 Arg201(N ε)-Trp126(O)
 Arg201(NH2)-Ile114(O), Trp126(O)
 Gln226(O ε 1)-Glu119(N)
 Gln226(N ε 2)-Gln119(O)
 Arg232(NH2)-Asp168(O δ 2)

Non-polar:

Glu116-Pro171
 Lys117-Trp174, Val175
 Gly118-Trp174, Pro198
 Tyr120-Pro198
 Pro121-Tyr197
 Thr125-Tyr197, Arg201
 Trp126-Arg201
 Tyr130-Asn124, Ser128
 Tyr174-Lys117, Gly118
 Val175-Lys117, Lys234
 Tyr176-Lys234
 Tyr197-Thr125, Pro121
 Pro198-Gly118, Tyr120
 Tyr200-Arg229
 Arg201-Thr125, Trp126
 Lys234-Val175, Tyr176

Human β B2

Polar:

Glu74(O ε 1)-Gly157(N)
 Tyr78(OH)-Pro156(O)
 Ser86(O γ)-Arg159(NH2)
 Ser130(O γ)-Lys75(O)
 Tyr155(OH)-Arg80(NH2)
 Arg159(N ε)-Ser83(O)
 Arg159(NH1)-Gln162(O ε 1)

Gln184(N ε 2)-Glu77(N)

Non-polar: Lys75-His132, Ala133
Gly76-His132
Pro156-Gly76, Tyr78
Tyr155-Pro79, Ser83
Tyr158-Tyr158, Arg187
Arg159-Trp84

Human β A4

Polar:

Arg71(NH2)-Gln130(O)
Glu73(O ε 1)-Gln130(O ε 1), Gln130(N ε 2), Gln189(N ε 2), Asn137(OD1) Glu73(O ε 2)-
Gln130(N ε 2)
Asn83(ND2)-Arg158(NH1, N ε)
Ser128(O γ)-Arg71(O)
Arg158(NH2)-Ile68(O)
Arg158(N ε)-Ala79(O)
Gln189(N ε 2)-Glu73(N)
Gln189(O ε 1)-Glu73(O)

Non-polar: Arg71-Gln130, Ala131
Gly72-Pro155
Glu73-Gln130
Tyr74-Pro155
Pro75-Phe154
Asp78-Ala85
Ala79-Phe154
Asn83-Arg158
Ala85-Asp78
Pro127-Arg192
Pro127-Gln195
Ala131-Gln195
Tyr157-Tyr157, Arg192