Protein Knowledge Report — P62942

1. Target summary

- Input type: uniprot_accession
- Label: P62942
- Length: 108 aa
- UniProt accession: P62942
- Submitted: 2026-07-15T13:01:31Z
- Sequence:

MGVQVETISPGDGRTFPKRGQTCVVHYTGMLEDGKKFDSSRDRNKPFKFMLGKQEVIRGWEEGVAQMSVGQRAKLTISPDYAYGATGHPGIIPPHATLV
FDVELLKLE

2. Family classification

- Family: FKBP_C (PF00254) — FKBP-type peptidyl-prolyl cis-trans isomerase
- E-value: 4.30e-37 Bit score: 127.0
- Model span: 2-94 of model (14-105 of query)
- Passes family's curated gathering threshold: yes

Source: HMMER hmmscan vs Pfam-A (local)

3. Known ligand precedent

- Total structures in this family: 439
- Distinct ligand scaffolds curated below: 8

PDB ID	Ligand(s)	Resolution (Å)	Why selected
7AOT	RTQ	0.85	highest-resolution structure...
7APW	RSB	0.89	highest-resolution structure...
8R5K	Y6Z	0.89	highest-resolution structure...
7APS	RR5	0.94	highest-resolution structure...
6TX6	NCA	0.98	highest-resolution structure...
8CHN	UUI	0.99	highest-resolution structure...
4DRQ	0OS	1.00	highest-resolution structure...
5OBK	9QN	1.00	highest-resolution structure...

scanned the 100 highest-resolution of 439 total structures in this family (RCSB result capped for query cost) — the curated examples below are drawn from that subset, not from the full family

Source: RCSB PDB REST API, curated top-N by distinct ligand scaffold + resolution

Interaction fingerprints (Evidence Integration Layer, Phase 1)

Representative complex: PDB 6YF3 (OOZ, 1.00 Å)

Residue (PDB)	Residue (pipeline)	Interaction	Partner
37	38	hydrogen bond	ASP37 (hydrogen bond) with l...
54	55	hydrogen bond	GLU54 (hydrogen bond) with l...
56	57	hydrogen bond	ILE56 (hydrogen bond) with l...
26	27	hydrophobic contact	TYR26 (hydrophobic) with lig...
36	37	hydrophobic contact	PHE36 (hydrophobic) with lig...
46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
56	57	hydrophobic contact	ILE56 (hydrophobic) with lig...
59	60	hydrophobic contact	TRP59 (hydrophobic) with lig...
90	91	hydrophobic contact	ILE90 (hydrophobic) with lig...

46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
59	60	hydrophobic contact	TRP59 (hydrophobic) with lig...

Representative complex: PDB 6YF2 (OP5, 1.03 Å)

Residue (PDB)	Residue (pipeline)	Interaction	Partner
37	38	hydrogen bond	ASP37 (hydrogen bond) with l...
54	55	hydrogen bond	GLU54 (hydrogen bond) with l...
56	57	hydrogen bond	ILE56 (hydrogen bond) with l...
26	27	hydrophobic contact	TYR26 (hydrophobic) with lig...
46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
56	57	hydrophobic contact	ILE56 (hydrophobic) with lig...
59	60	hydrophobic contact	TRP59 (hydrophobic) with lig...
59	60	hydrophobic contact	TRP59 (hydrophobic) with lig...
82	83	hydrophobic contact	TYR82 (hydrophobic) with lig...
91	92	hydrophobic contact	ILE91 (hydrophobic) with lig...

Representative complex: PDB 6YF1 (OP8, 1.12 Å)

Residue (PDB)	Residue (pipeline)	Interaction	Partner
37	38	hydrogen bond	ASP37 (hydrogen bond) with l...
26	27	hydrogen bond	TYR26 (hydrogen bond) with l...
82	83	hydrogen bond	TYR82 (hydrogen bond) with l...
56	57	hydrogen bond	ILE56 (hydrogen bond) with l...
26	27	hydrophobic contact	TYR26 (hydrophobic) with lig...
36	37	hydrophobic contact	PHE36 (hydrophobic) with lig...
46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
55	56	hydrophobic contact	VAL55 (hydrophobic) with lig...
56	57	hydrophobic contact	ILE56 (hydrophobic) with lig...
59	60	hydrophobic contact	TRP59 (hydrophobic) with lig...
91	92	hydrophobic contact	ILE91 (hydrophobic) with lig...
46	47	hydrophobic contact	PHE46 (hydrophobic) with lig...
59	60	hydrophobic contact	TRP59 (hydrophobic) with lig...
82	83	hydrophobic contact	TYR82 (hydrophobic) with lig...
85	86	water bridge	THR85 (water bridge) with li...

Source: PLIP (Protein-Ligand Interaction Profiler), run on representative structures from known ligand precedent

4. Conservation

- Family: PF00254
- Seed alignment size: 126 sequences
- Mean pairwise identity (seed alignment): 31.4%
- Note: computed over a sample of 40/126 seed sequences

Source: Pfam seed alignment (via InterPro API), mean pairwise identity across aligned members at matched-region columns

5. Structural analysis

- Structure provider: AlphaFold DB (model created 2025-08-01T00:00:00Z)
- Pocket detector: fpocket (default parameters)
- Mean per-residue confidence: 0.9627
- Conformational ensemble: 5 conformers (ANM, 5 frames)
- Static (single-frame) pocket count: 5
- Residue numbering: pipeline-sequential, with literature (author-deposited PDB 2PPN) numbering shown in

parentheses — 107/108 residues cross-walked
- Ensemble-informed ranked pocket clusters (customer-visible top): 3

Rank (cluster id)	Frames present	Persistence	Residues
1 (cluster 7)	4/5	0.8	1(?), 2(1), 3(2), 4(3), 32(3...
2 (cluster 3)	3/5	0.6	31(30), 35(34), 86(85), 88(8...
3 (cluster 1)	4/5	0.8	19(18), 51(50), 52(51), 53(5...

Pocket residues overlapping known interaction sites (from Interaction fingerprints, section 3):

- Pocket 1 (cluster 7): no overlap with known interaction sites (9 pocket residues checked)
- Pocket 2 (cluster 3): residues 86(85), 91(90), 92(91) (3 of 10 pocket residues match a known interaction site)
- Pocket 3 (cluster 1): no overlap with known interaction sites (8 pocket residues checked)

Pocket functional context (UniProt features + ClinVar variants):

- Pocket 1 (cluster 7): no UniProt functional features or ClinVar variants overlap with pocket residues
- Pocket 2 (cluster 3): no UniProt functional features or ClinVar variants overlap with pocket residues
- Pocket 3 (cluster 1):
  - Residue 53: Modified residue — N6-acetyllysine; alternate
  - Residue 53: Modified residue — N6-succinyllysine; alternate

Source: UniProt REST API (features) + ClinVar via NCBI E-utilities (variants, filtered by clinical significance)

6 pocket cluster(s) (of 8 total, filtered to those present in >=2 frames) appear only in later ensemble frames, absent from the static structure-provider output:

Cluster id	Frames present	Persistence	Residues
7	4/5	0.8	1(?), 2(1), 3(2), 4(3), 32(3...
4	3/5	0.6	26(25), 40(39), 41(40), 42(4...
5	3/5	0.6	54(53), 56(55), 57(56), 58(5...
6	2/5	0.4	7(6), 10(9), 11(10), 13(12),...
8	2/5	0.4	31(30), 32(31), 33(32), 93(9...
10	2/5	0.4	8(7), 30(29), 31(30), 32(31)...

3 pocket cluster(s) in the customer-visible top ranking; static (first-frame-only) fpocket found 5 pocket(s); the ensemble-informed ranker considered 12 cluster(s) across 5 conformers — compare static_pocket_count against pocket_ranking.clusters to see whether the ensemble surfaces anything the static structure alone misses; no binding-site ground truth supplied, so no recovery/overlap metrics are reported; residue numbers above are pipeline-sequential, NOT necessarily literature convention — see numbering_crosswalk (ref: 2PPN) for author-deposited numbering

Source: StructureProvider + PocketDetector abstraction (see api/knowledge_protein/structural.py)

6. Confidence flags

No confidence flags triggered — none of the rules-based checks below found a condition worth discounting. This is not itself a confidence score; it means the specific checks run did not fire, not that every aspect of this report is high-confidence.

Source: rules-based checks in api/knowledge_protein/confidence_flags.py — fixed thresholds on numbers already computed elsewhere in this report, no learned calibration, no combined/weighted score.

7. Similar known proteins

Sequence-based (Pfam family co-membership, top 5 by identity):

PDB ID	Sequence identity to query	Ligand(s)
8X6P	100.0%	(none recorded)
2PPN	98.1%	(none recorded)
6YF3	97.2%	CD, OOZ
6YF2	97.2%	CD, OP5

6YF1	97.2%	OP8

Structure-based (Foldseek vs. full PDB structural index, Evidence Integration Layer Phase 2):

PDB ID	TM-score	Sequence identity	In sequence-based list…	Description
4N19	1.000	98.1%	yes	Structural basis of co…
8PPZ	1.000	99.0%	no	Co-crystal structure o…
4IPX	1.000	98.1%	no	Analyzing the visible …
6M4W	1.000	100.0%	no	Crystal structure of M…
8VK3	0.999	97.1%	no	Structure of mouse RyR…

4/5 top structural neighbor(s) — 8PPZ, 4IPX, 6M4W, 8VK3 — are not in the small cached sequence-based sample above (similar_protein.py surveys only the ~60 highest-resolution structures per family, itself capped for query cost, while Foldseek searches the full PDB structural index) — this does not mean they're unrelated, only that they weren't in that capped sample; treat both lists as complementary, partial views, not a contradiction

Source: sequence-based: Pfam family co-membership among cached PDB reference structures (sequence-based); Foldseek vs local PDB structural database (structure-based)

8. Limitations & data provenance

Auto-populated from each section's own status — not hand-maintained.

Section	Status	Detail
Family classification	returned data	
Known ligand precedent	returned data	scanned the 100 highest-resolution of …
Interaction fingerprints	returned data	
Functional context (UniProt + ClinVar)	returned data	
Conservation	returned data	computed over a sample of 40/126 seed …
Structural analysis	returned data	3 pocket cluster(s) in the customer-vi…
Similar known proteins	returned data	
Similar known proteins (structure-base…	returned data	

All sections returned data this run.