

Protein Knowledge Report — P62593

1. Target summary

- Input type: uniprot_accession
- Label: P62593
- Length: 286 aa
- UniProt accession: P62593
- Submitted: 2026-07-15T12:56:39Z
- Sequence:

MSIQHFRVALIPFFAAAFCLPVFAHPETLVKVKDAEDQLGARVGYIELDLNSGKILESFRPEERFPMMSDFKLLCGAVLSRVDAGQEQLGRRIHYSQNDLVEYSPVTEKHLTDGMTVRELCSAAITMSDNTAANLLLTIGGPKELTAFLHNMGDHVTSLDRWEPELNEAIPNDERDTTTPAAMATTLRKLLTGELLTLA

2. Family classification

- Family: Beta-lactamase2 (PF13354) — Beta-lactamase enzyme family
- E-value: 1.20e-43 Bit score: 149.9
- Model span: 7-256 of model (32-286 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: 153
- Distinct ligand scaffolds curated below: 9

PDB ID	Ligand(s)	Resolution (Å)	Why selected
8RMA	A1H1U	0.83	highest-resolution structure...
6WJM	ALA	1.00	highest-resolution structure...
8R2Y	6M9	1.03	highest-resolution structure...
8R2Z	XR9	1.10	highest-resolution structure...
7Q11	6V8	1.14	highest-resolution structure...
3W4O	NHE	1.18	highest-resolution structure...
5NJ2	AE4, ETE	1.19	highest-resolution structure...
3NY4	SMX	1.22	highest-resolution structure...

scanned the 100 highest-resolution of 153 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)

8 ligand-bound structure(s) exist for this target's Pfam family (PF13354), but none checked aligned to the query at >=50% sequence coverage — likely other members of the same broad family (e.g. related kinases), not this specific protein. Interaction fingerprints require a structure of the query protein itself.

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

4. Conservation

- Family: PF13354
- Seed alignment size: 56 sequences
- Mean pairwise identity (seed alignment): 21.8%
- Note: computed over a sample of 40/56 seed sequences

5. Structural analysis

- Structure provider: AlphaFold DB (model created 2025-08-01T00:00:00Z)
- Pocket detector: fpocket (default parameters)
- Mean per-residue confidence: 0.9485
- Conformational ensemble: 5 conformers (ANM, 5 frames)
- Static (single-frame) pocket count: 11
- Residue numbering: pipeline-sequential, with literature (author-deposited PDB 1M40) numbering shown in parentheses — 262/286 residues cross-walked
- Ensemble-informed ranked pocket clusters (customer-visible top): 3

Rank (cluster id)	Frames present	Persistence	Residues
1 (cluster 0)	5/5	1.0	39(41), 40(42), 41(43), 61(6...
2 (cluster 1)	5/5	1.0	20(?), 21(?), 22(?), 23(?), ...
3 (cluster 9)	5/5	1.0	61(63), 154(156), 155(157), ...

Pocket functional context (UniProt features + ClinVar variants):

- Pocket 1 (cluster 0): no UniProt functional features or ClinVar variants overlap with pocket residues
- Pocket 2 (cluster 1): no UniProt functional features or ClinVar variants overlap with pocket residues
- Pocket 3 (cluster 9): no UniProt functional features or ClinVar variants overlap with pocket residues

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

1 pocket cluster(s) (of 10 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
13	2/5	0.4	97(99), 100(102), 101(103), ...

3 pocket cluster(s) in the customer-visible top ranking; static (first-frame-only) fpocket found 11 pocket(s); the ensemble-informed ranker considered 21 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: 1M40) 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)
6NIQ	43.2%	(none recorded)
6WJM	36.4%	ALA
5NE3	36.2%	NXL
7D5J	36.1%	(none recorded)
3W4P	35.5%	(none recorded)

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

PDB ID	TM-score	Sequence identity	In sequence-based list...	Description
7QOR	1.000	99.6%	no	Structure of beta-lact...
1JWV	1.000	99.6%	no	Crystal structure of G...
1XXM	1.000	98.8%	no	The modular architectu...
1FQG	1.000	99.6%	no	MOLECULAR STRUCTURE OF...
6AYK	1.000	99.2%	no	Crystal structure of T...

5/5 top structural neighbor(s) — 7QOR, 1JWV, 1XXM, 1FQG, 6AYK — 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	no self-matching ligand-bound structur...	8 ligand-bound structure(s) exist for ...
Functional context (UniProt + ClinVar)	returned data	
Conservation	returned data	computed over a sample of 40/56 seed s...
Structural analysis	returned data	3 pocket cluster(s) in the customer-vi...
Similar known proteins	returned data	
Similar known proteins (structure-base...	returned data	

1 of 8 sections did not return data this run: Interaction fingerprints.