



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 06:55 PM EDT

PDB ID : 2IFU / pdb_00002ifu
Title : Crystal Structure of a Gamma-SNAP from Danio rerio
Authors : Bitto, E.; Wesenberg, G.E.; Phillips Jr., G.N.; McCoy, J.G.; Bingman, C.A.;
Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2006-09-21
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8758 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called gamma-snap.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	Se	0	2	0
			2181	1373	372	419	5	12			
1	B	275	Total	C	N	O	S	Se	0	1	0
			2176	1369	372	419	5	11			
1	C	272	Total	C	N	O	S	Se	0	0	0
			2152	1354	368	415	5	10			
1	D	270	Total	C	N	O	S	Se	0	0	0
			2135	1342	365	413	5	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	cloning artifact	UNP Q5BJK3
A	0	ILE	-	cloning artifact	UNP Q5BJK3
A	1	ALA	MET	cloning artifact	UNP Q5BJK3
A	24	MSE	MET	modified residue	UNP Q5BJK3
A	82	MSE	MET	modified residue	UNP Q5BJK3
A	83	MSE	MET	modified residue	UNP Q5BJK3
A	90	MSE	MET	modified residue	UNP Q5BJK3
A	103	MSE	MET	modified residue	UNP Q5BJK3
A	115	MSE	MET	modified residue	UNP Q5BJK3
A	124	MSE	MET	modified residue	UNP Q5BJK3
A	182	MSE	MET	modified residue	UNP Q5BJK3
A	186	MSE	MET	modified residue	UNP Q5BJK3
A	261	MSE	MET	modified residue	UNP Q5BJK3
B	-1	ALA	-	cloning artifact	UNP Q5BJK3
B	0	ILE	-	cloning artifact	UNP Q5BJK3
B	1	ALA	MET	cloning artifact	UNP Q5BJK3
B	24	MSE	MET	modified residue	UNP Q5BJK3
B	82	MSE	MET	modified residue	UNP Q5BJK3
B	83	MSE	MET	modified residue	UNP Q5BJK3
B	90	MSE	MET	modified residue	UNP Q5BJK3
B	103	MSE	MET	modified residue	UNP Q5BJK3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	115	MSE	MET	modified residue	UNP Q5BJK3
B	124	MSE	MET	modified residue	UNP Q5BJK3
B	182	MSE	MET	modified residue	UNP Q5BJK3
B	186	MSE	MET	modified residue	UNP Q5BJK3
B	261	MSE	MET	modified residue	UNP Q5BJK3
C	-1	ALA	-	cloning artifact	UNP Q5BJK3
C	0	ILE	-	cloning artifact	UNP Q5BJK3
C	1	ALA	MET	cloning artifact	UNP Q5BJK3
C	24	MSE	MET	modified residue	UNP Q5BJK3
C	82	MSE	MET	modified residue	UNP Q5BJK3
C	83	MSE	MET	modified residue	UNP Q5BJK3
C	90	MSE	MET	modified residue	UNP Q5BJK3
C	103	MSE	MET	modified residue	UNP Q5BJK3
C	115	MSE	MET	modified residue	UNP Q5BJK3
C	124	MSE	MET	modified residue	UNP Q5BJK3
C	182	MSE	MET	modified residue	UNP Q5BJK3
C	186	MSE	MET	modified residue	UNP Q5BJK3
C	261	MSE	MET	modified residue	UNP Q5BJK3
D	-1	ALA	-	cloning artifact	UNP Q5BJK3
D	0	ILE	-	cloning artifact	UNP Q5BJK3
D	1	ALA	MET	cloning artifact	UNP Q5BJK3
D	24	MSE	MET	modified residue	UNP Q5BJK3
D	82	MSE	MET	modified residue	UNP Q5BJK3
D	83	MSE	MET	modified residue	UNP Q5BJK3
D	90	MSE	MET	modified residue	UNP Q5BJK3
D	103	MSE	MET	modified residue	UNP Q5BJK3
D	115	MSE	MET	modified residue	UNP Q5BJK3
D	124	MSE	MET	modified residue	UNP Q5BJK3
D	182	MSE	MET	modified residue	UNP Q5BJK3
D	186	MSE	MET	modified residue	UNP Q5BJK3
D	261	MSE	MET	modified residue	UNP Q5BJK3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	17	Total	O	0	0
			17	17		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total	O	0	0
			6	6		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.38Å 90.81Å 264.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.05 – 2.60	Depositor
% Data completeness (in resolution range)	96.1 (40.05-2.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.239 , 0.261	Depositor
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.396	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8758	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	306	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	C	306	-	4,4,4	0.31	0	6,6,6	0.34	0
2	SO4	B	307	-	4,4,4	0.31	0	6,6,6	0.82	0
2	SO4	A	307	-	4,4,4	0.32	0	6,6,6	0.76	0
2	SO4	C	307	-	4,4,4	0.22	0	6,6,6	0.20	0
2	SO4	D	306	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	B	308	-	4,4,4	0.44	0	6,6,6	0.95	0
2	SO4	A	308	-	4,4,4	0.27	0	6,6,6	0.38	0
2	SO4	B	309	-	4,4,4	0.30	0	6,6,6	0.36	0
2	SO4	A	306	-	4,4,4	0.31	0	6,6,6	0.89	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.