



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 05:08 pm BST

PDB ID : 1XD4  
Title : Crystal structure of the DH-PH-cat module of Son of Sevenless (SOS)  
Authors : Sondermann, H.; Soisson, S.M.; Boykevisch, S.; Yang, S.S.; Bar-Sagi, D.; Kuriyan, J.  
Deposited on : 2004-09-03  
Resolution : 3.64 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

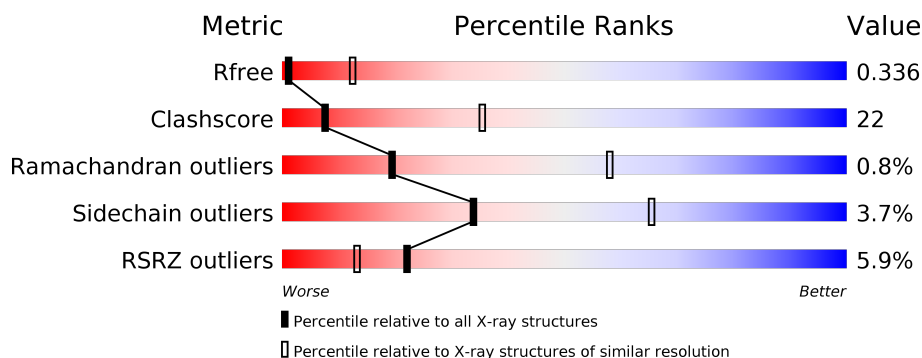
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	852	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>• •</div> </div> </div>
1	B	852	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>

## 2 Entry composition

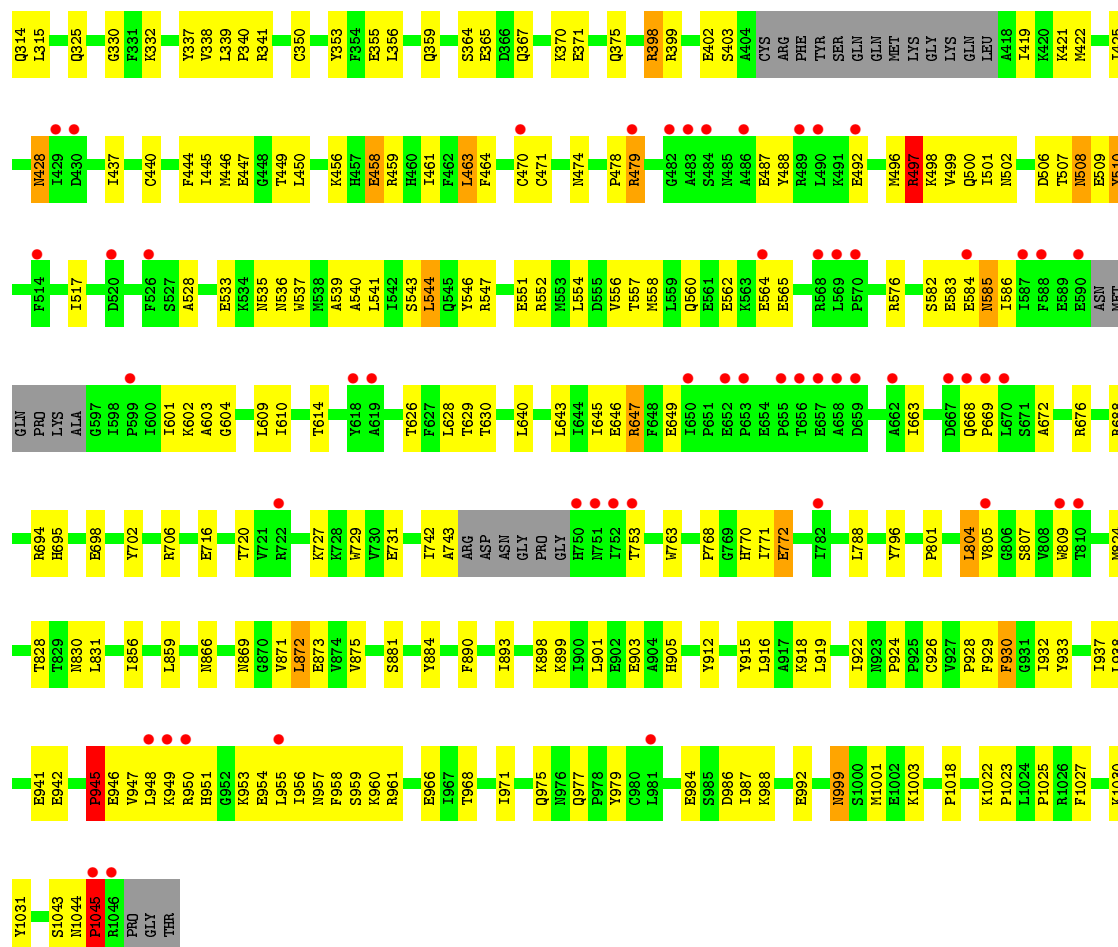
There is only 1 type of molecule in this entry. The entry contains 13542 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Son of sevenless protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	0	0
			6771	4323	1159	1258	31			
1	B	824	Total	C	N	O	S	0	0	0
			6771	4323	1159	1258	31			





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.47Å 127.36Å 279.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.99 – 3.64 47.02 – 3.64	Depositor EDS
% Data completeness (in resolution range)	92.0 (11.99-3.64) 92.1 (47.02-3.64)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.66Å)	Xtriage
Refinement program	CNS 1.1, REFMAC	Depositor
R, $R_{free}$	0.307 , 0.371 0.287 , 0.336	Depositor DCC
$R_{free}$ test set	2033 reflections (6.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	131.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 149.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	0/6918	0.69	5/9334 (0.1%)
1	B	0.47	0/6918	0.68	3/9334 (0.0%)
All	All	0.47	0/13836	0.68	8/18668 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	945	PRO	CA-N-CD	-16.27	88.72	111.50
1	A	580	PRO	CA-N-CD	-16.02	89.06	111.50
1	A	928	PRO	CA-N-CD	-14.33	91.44	111.50
1	A	570	PRO	CA-N-CD	-9.07	98.81	111.50
1	A	310	ARG	NE-CZ-NH2	6.49	123.54	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6771	0	6768	293	1
1	B	6771	0	6768	309	1
All	All	13542	0	13536	596	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 596 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:THR:HG21	1:A:962:ARG:CD	1.57	1.35
1:B:584:GLU:CA	1:B:953:LYS:HG3	1.63	1.27
1:B:584:GLU:CB	1:B:953:LYS:HE3	1.68	1.24
1:A:587:ILE:HD13	1:A:603:ALA:CB	1.69	1.22
1:B:584:GLU:HA	1:B:953:LYS:CG	1.73	1.18

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:PRO:CB	1:B:753:THR:OG1[4_555]	1.85	0.35
1:A:392:SER:CB	1:A:507:THR:CG2[4_556]	2.00	0.20

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	816/852 (96%)	774 (95%)	36 (4%)	6 (1%)	22	61
1	B	816/852 (96%)	775 (95%)	34 (4%)	7 (1%)	17	56
All	All	1632/1704 (96%)	1549 (95%)	70 (4%)	13 (1%)	19	58

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	567	MET
1	A	1045	PRO
1	B	1045	PRO
1	A	497	ARG
1	A	508	ASN



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	754/777 (97%)	723 (96%)	31 (4%)	30	63
1	B	754/777 (97%)	729 (97%)	25 (3%)	38	68
All	All	1508/1554 (97%)	1452 (96%)	56 (4%)	34	65

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	928	PRO
1	B	214	GLN
1	B	930	PHE
1	A	930	PHE
1	A	966	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	755	GLN
1	A	999	ASN
1	B	905	HIS
1	A	879	ASN
1	A	477	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	824/852 (96%)	0.12	43 (5%) 27 18	35, 135, 288, 306	0
1	B	824/852 (96%)	0.19	54 (6%) 18 11	29, 143, 289, 306	0
All	All	1648/1704 (96%)	0.15	97 (5%) 22 13	29, 139, 289, 306	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	HIS	15.1
1	A	751	ASN	9.7
1	A	1045	PRO	9.2
1	B	751	ASN	8.6
1	A	752	ILE	8.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.