



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 07:37 PM UTC

PDB ID : 1XD4 / pdb_00001xd4
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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

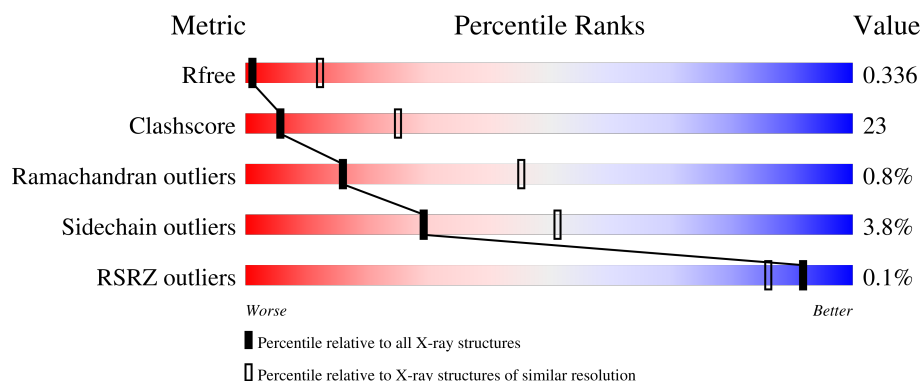
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 64% 30% . .
1	B	852	 64% 30% . .

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.

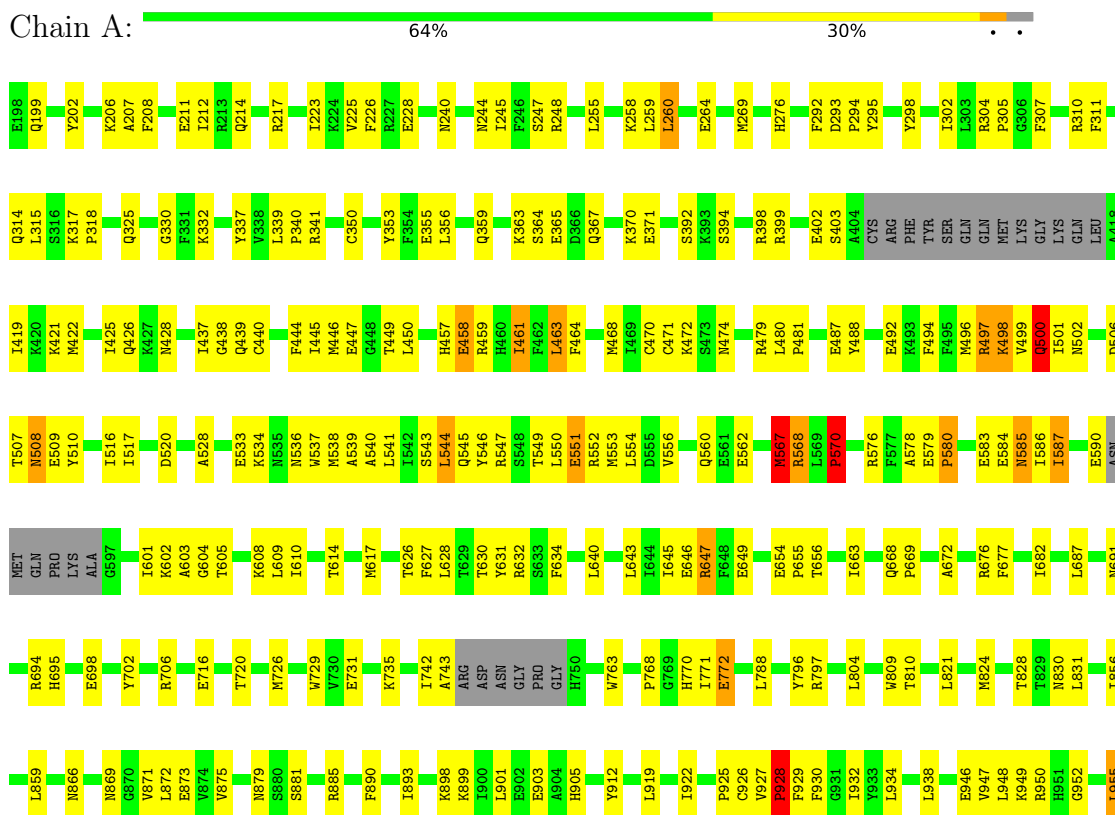
- Molecule 1 is a protein called Son of sevenless protein homolog 1.

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			

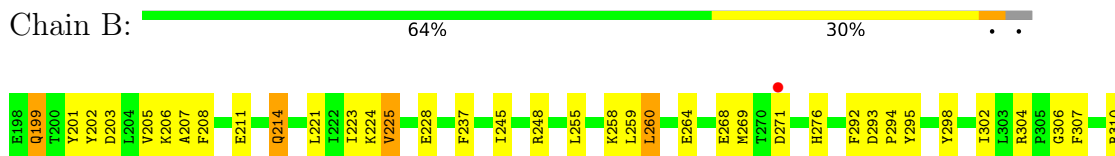
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Son of sevenless protein homolog 1



- Molecule 1: Son of sevenless protein homolog 1



S959	K960	R961	E966	E967	T968	T971	Q972	Q973	Y974	Q975	N976	Q977	Y978	Y979	E984	S985	D986	K988	R989	E992	N999	S1000	M1001	E1002	K1003	P1018	K1022	P1023	L1024	P1025	R1026	F1027	K1030	Y1031	S1043	N1044	P1045	R1046	PRO	GLY	THR										
K728	W729	V730	E731	I742	A743	ARG	ASP	ASN	GLY	PRO	GLY	H750	T753	F754	Q755	W763	P768	G769	H770	I771	E772	L788	Y796	P801	L804	V805	G806	S807	W808	W809	N824	T828	T829	N830	L831	I856	E946	L947	L948	K949	R950	H951	G952	K953	E954	L955	I956	N957	F958		
S880	S881	Y884	F890	I893	K898	K899	E901	E902	E903	A904	H905	Y912	Y915	L916	A917	L919	Y922	N923	P924	G925	C926	Y927	P928	F929	F930	G931	L932	Y933	I937	L938	E941	E942	P945	E946	L947	L948	K949	R950	H951	G952	K953	E954	L955	I956	N957	F958					
F311	K421	Q314	L315	Q325	G330	F331	K332	Y337	V338	L339	P340	R341	C350	Y353	F354	E355	L356	Q359	S364	E365	D366	Q367	K370	E371	Q375	S394	R398	R399	E402	S403	A404	CYS	ARG	PHE	TYR	SER	GLN	GLN	MET	LYS	GLY	LYS	GLN	LEU	A418	I419	K420				
K422	I425	K426	K427	N428	I437	G438	Q439	C440	F444	I445	M446	E447	G448	T449	L450	K456	H457	E458	Y459	H460	I461	F462	L463	F464	L467	M468	I469	C470	C471	N474	P478	R479	A486	E487	Y488	E492	K493	F494	F495	M496	R497	MET	K498	V499	Q500	I501	N502	D506	T507		
N508	E509	Y510	I516	I517	D520	A528	E533	E534	N535	N536	W537	M538	A539	A540	L541	I542	S543	L544	Q545	Y546	R547	E551	R552	M553	L554	D555	V556	T557	M558	L559	Q560	E561	E562	K563	E564	E565	Q566	R576	S582	E583	E584	N585	I586	E590	ASN	MET	GLN	PRO	LYS	ALA	G597
I601	K602	A603	G604	L609	I610	T614	M617	T626	F627	L628	T629	T630	Y631	R632	L640	L643	I644	I645	E646	R647	F648	E649	I663	Q668	P669	A672	R676	I682	L687	R688	R694	H695	E698	Y702	R706	E716	T720	M726	K727												
W729	V730	E731	I742	A743	ARG	ASP	ASN	GLY	PRO	GLY	H750	T753	F754	Q755	W763	P768	G769	H770	I771	E772	L788	Y796	P801	L804	V805	G806	S807	W808	W809	N824	T828	T829	N830	L831	I856	Y947	L948	K949	R950	H951	G952	K953	E954	L955	I956	N957	F958				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.47Å 127.36Å 279.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.99 – 3.64 11.99 – 3.64	Depositor EDS
% Data completeness (in resolution range)	92.0 (11.99-3.64) 89.1 (11.99-3.64)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	131.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 111.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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.

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	0.56	2/6918 (0.0%)	1.02	32/9334 (0.3%)
1	B	0.55	0/6918	1.04	41/9334 (0.4%)
All	All	0.56	2/13836 (0.0%)	1.03	73/18668 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	975	GLN	N-CA	5.38	1.52	1.46
1	A	974	TYR	CA-C	5.21	1.59	1.52

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	945	PRO	CA-N-CD	-16.63	88.72	112.00
1	A	580	PRO	CA-N-CD	-16.38	89.06	112.00
1	A	928	PRO	CA-N-CD	-14.69	91.44	112.00
1	B	972	GLN	OE1-CD-NE2	-10.46	112.14	122.60
1	B	977	GLN	OE1-CD-NE2	-10.27	112.33	122.60

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	313	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6771	0	6768	326	1
All	All	13542	0	13536	630	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 23.

The worst 5 of 630 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%)	18	48
1	B	816/852 (96%)	775 (95%)	34 (4%)	7 (1%)	14	43
All	All	1632/1704 (96%)	1549 (95%)	70 (4%)	13 (1%)	16	45

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%)	722 (96%)	32 (4%)	26	49
1	B	754/777 (97%)	729 (97%)	25 (3%)	33	54
All	All	1508/1554 (97%)	1451 (96%)	57 (4%)	29	51

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	966	GLU
1	B	1003	LYS
1	B	259	LEU
1	B	999	ASN
1	B	830	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	276	HIS
1	B	585	ASN
1	B	352	HIS
1	B	457	HIS
1	B	695	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q < 0.9
1	A	824/852 (96%)	-0.35	1 (0%)	92 86	35, 135, 288, 306	0
1	B	824/852 (96%)	-0.29	1 (0%)	92 86	29, 143, 289, 306	0
All	All	1648/1704 (96%)	-0.32	2 (0%)	92 86	29, 139, 289, 306	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	ASP	3.0
1	A	958	PHE	2.4

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 oligosaccharides 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.