



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 02:20 pm BST

PDB ID : 9QFF / pdb_00009qff
Title : Structure of SOS1 in complex with compound 3
Authors : Breed, J.
Deposited on : 2025-03-11
Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

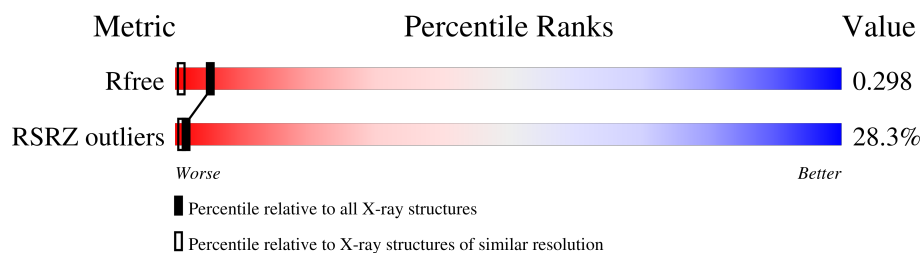
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	164625	1090 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3585 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.

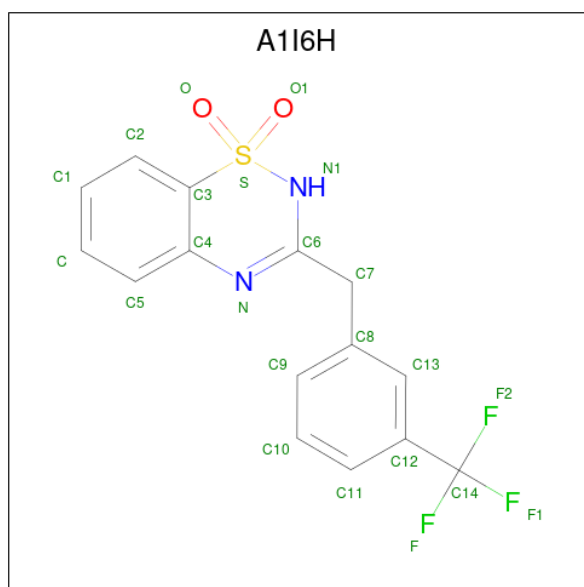
- Molecule 1 is a protein called Son of sevenless homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3492	2263	583	634	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	GLY	GLN	engineered mutation	UNP Q07889
A	561	ALA	GLU	engineered mutation	UNP Q07889
A	562	MET	GLU	engineered mutation	UNP Q07889
A	563	ALA	LYS	engineered mutation	UNP Q07889

- Molecule 2 is 3-[[3-(trifluoromethyl)phenyl]methyl]-2,4-benzothiadiazine 1,1-dioxide (CCD ID: A1I6H) (formula: C₁₅H₁₁F₃N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			23	15	3	2	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.46Å 84.69Å 176.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.19 – 1.88 88.19 – 1.88	Depositor EDS
% Data completeness (in resolution range)	64.9 (88.19-1.88) 64.9 (88.19-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.11.8 (24-FEB-2021)	Depositor
R, R_{free}	0.278 , 0.304 0.269 , 0.298	Depositor DCC
R_{free} test set	1705 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	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	0.90	EDS
Total number of atoms	3585	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% 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](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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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](#)

1 ligand is 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	A1I6H	A	1101	-	24,25,25	0.44	0	32,38,38	0.79	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1I6H	A	1101	-	-	0/9/25/25	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1I6H	C8-C7-C6	-3.43	107.47	113.93

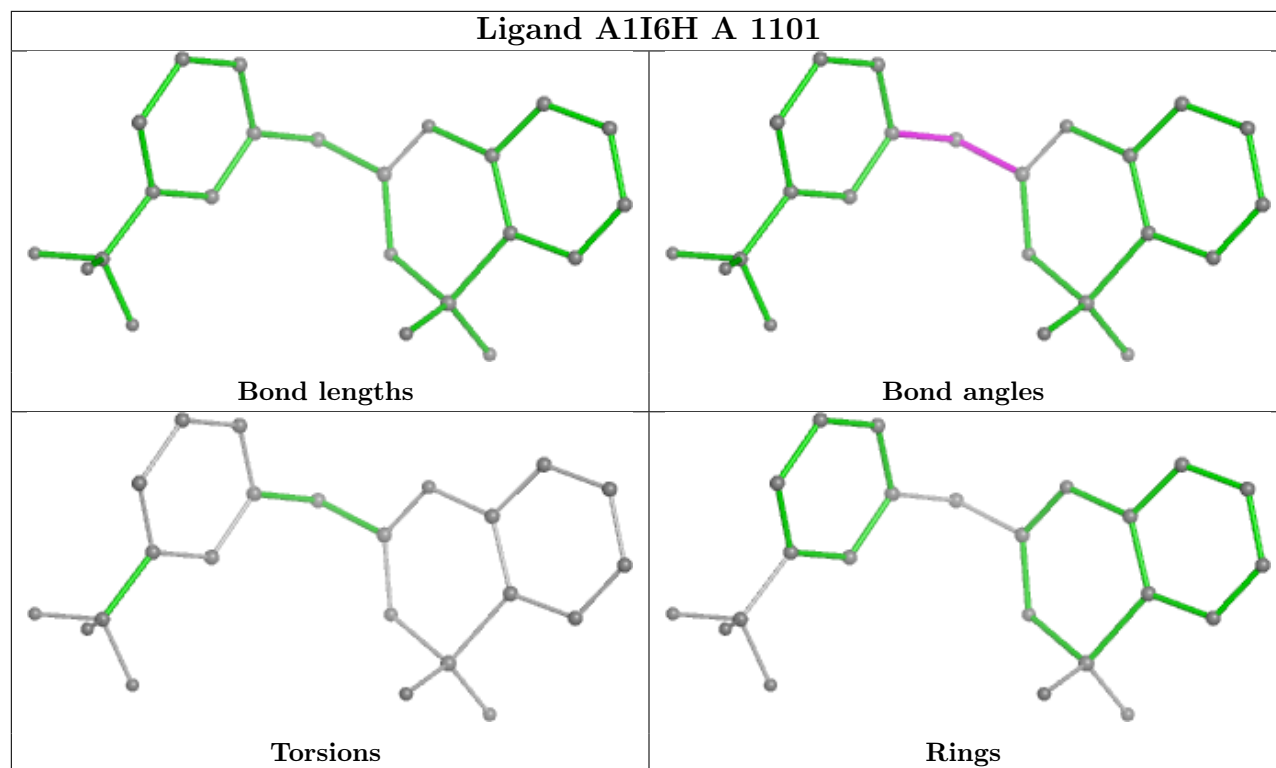
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

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	442/490 (90%)	1.50	125 (28%) 1 1	20, 39, 74, 94	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	722	ARG	6.8
1	A	674	LEU	6.2
1	A	742	ILE	5.9
1	A	675	LYS	5.9
1	A	721	VAL	5.5
1	A	681	TYR	5.3
1	A	673	GLU	5.1
1	A	574	VAL	5.1
1	A	677	PHE	5.0
1	A	678	ARG	4.9
1	A	709	TYR	4.8
1	A	568	ARG	4.7
1	A	725	ALA	4.6
1	A	717	PHE	4.6
1	A	743	ALA	4.5
1	A	812	GLU	4.5
1	A	644	ILE	4.4
1	A	679	LYS	4.4
1	A	720	THR	4.2
1	A	680	GLU	4.1
1	A	571	SER	4.0
1	A	738	GLN	4.0
1	A	676	ARG	4.0
1	A	753	THR	3.9
1	A	718	ILE	3.9
1	A	569	LEU	3.9
1	A	683	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	890	PHE	3.7
1	A	651	PRO	3.7
1	A	726	MET	3.7
1	A	1044	ASN	3.7
1	A	745	ASP	3.6
1	A	586	ILE	3.6
1	A	639	GLU	3.6
1	A	701	PHE	3.5
1	A	1020	ASN	3.5
1	A	590	GLU	3.5
1	A	711	LEU	3.5
1	A	1031	TYR	3.4
1	A	597	GLY	3.4
1	A	809	TRP	3.4
1	A	682	ILE	3.4
1	A	719	GLY	3.3
1	A	729	TRP	3.3
1	A	813	ASP	3.3
1	A	650	ILE	3.3
1	A	617	MET	3.2
1	A	911	HIS	3.2
1	A	724	LYS	3.2
1	A	710	LEU	3.2
1	A	740	LYS	3.2
1	A	930	PHE	3.2
1	A	616	HIS	3.2
1	A	684	PRO	3.1
1	A	609	LEU	3.1
1	A	579	GLU	3.0
1	A	587	ILE	3.0
1	A	953	LYS	3.0
1	A	757	SER	3.0
1	A	643	LEU	3.0
1	A	739	ARG	3.0
1	A	600	ILE	3.0
1	A	610	ILE	3.0
1	A	648	PHE	3.0
1	A	723	GLY	2.9
1	A	713	ARG	2.9
1	A	755	GLN	2.9
1	A	598	ILE	2.9
1	A	607	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	955	LEU	2.9
1	A	572	ALA	2.9
1	A	578	ALA	2.8
1	A	618	TYR	2.8
1	A	728	LYS	2.8
1	A	754	PHE	2.8
1	A	744	ARG	2.7
1	A	685	VAL	2.7
1	A	573	ASP	2.7
1	A	645	ILE	2.7
1	A	599	PRO	2.7
1	A	704	PHE	2.6
1	A	690	LEU	2.6
1	A	1024	LEU	2.6
1	A	588	PHE	2.6
1	A	863	GLN	2.6
1	A	708	ALA	2.6
1	A	623	PHE	2.6
1	A	712	GLN	2.6
1	A	1040	VAL	2.5
1	A	694	ARG	2.5
1	A	692	VAL	2.5
1	A	613	LEU	2.5
1	A	796	TYR	2.5
1	A	756	SER	2.5
1	A	990	PHE	2.5
1	A	1021	PRO	2.4
1	A	895	SER	2.4
1	A	741	LYS	2.4
1	A	577	PHE	2.4
1	A	732	SER	2.4
1	A	581	ASP	2.4
1	A	810	THR	2.4
1	A	715	GLU	2.4
1	A	951	HIS	2.4
1	A	1023	PRO	2.4
1	A	575	TYR	2.4
1	A	733	ILE	2.3
1	A	1032	SER	2.3
1	A	570	PRO	2.3
1	A	707	ASP	2.3
1	A	1026	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	956	ILE	2.2
1	A	736	ILE	2.2
1	A	835	PHE	2.2
1	A	619	ALA	2.2
1	A	949	LYS	2.2
1	A	937	ILE	2.2
1	A	727	LYS	2.1
1	A	640	LEU	2.1
1	A	706	ARG	2.1
1	A	686	GLN	2.1
1	A	687	LEU	2.1
1	A	615	TYR	2.1
1	A	825	ILE	2.0
1	A	688	ARG	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

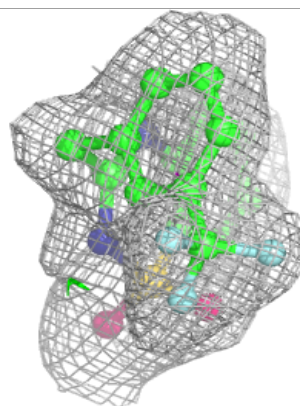
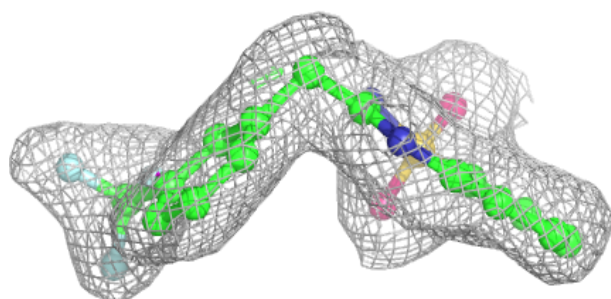
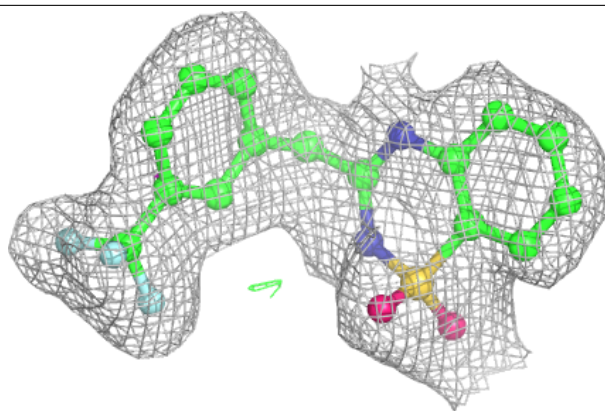
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1I6H	A	1101	23/23	0.91	0.10	33,36,40,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1I6H A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



5.5 Other polymers [i](#)

There are no such residues in this entry.