



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 11:03 AM UTC

PDB ID : 1FUG / pdb\_00001fug  
Title : S-ADENOSYLMETHIONINE SYNTHETASE  
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Deposited on : 1996-02-25  
Resolution : 3.20 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

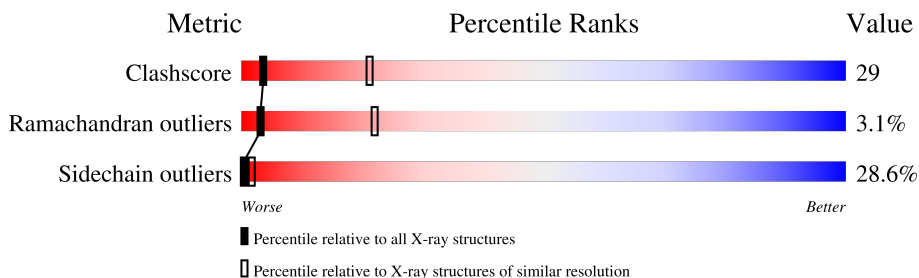
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	 29% 39% 24% 8%
1	B	383	 26% 41% 25% 8%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7170 atoms, of which 1286 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 S-ADENOSYLMETHIONINE SYNTHETASE.

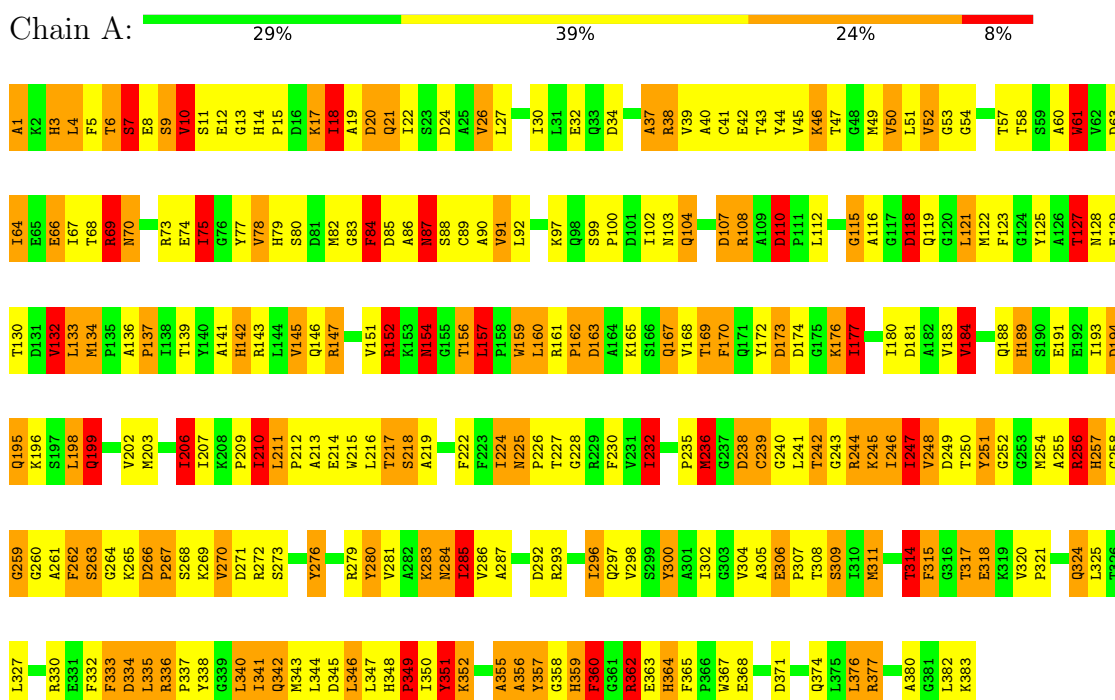
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	383	Total 3585	C 1856	H 643	N 503	O 570	S 13	0	0	0
1	B	383	Total 3585	C 1856	H 643	N 503	O 570	S 13	0	0	0

### 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. 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. 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.

Note EDS was not executed.

- Molecule 1: S-ADENOSYLMETHIONINE SYNTHETASE



R256	H257	G258	G259	G260	A261	F262	S263	G264	P267	S268	D271	R272	S273	A274	A275	Y276	A277	A278	R279	Y280	V281	A282	K283	N284	I285	V286	A287	A288	G289	L290	C294	E295	I296	Q297	V298	S299	Y300	A301	I302	G303	V304	T308	S309	I310	M311	V312	E313	T314	F315	G316	T317	E318	K319	V320	P321
S322	L325	T326	L328	V329	R330	E331	F332	F333	D334	L335	K336	P337	Y338	G339	L340	I341	Q342	M343	L344	D345	L346	L347	H348	P349	I350	Y351	K352	F353	T354	A355	A356	Y357	G358	H359	F360	G361	R362	E363	H364	F365	P366	W367	E368	D371	K372	A373	Q374	D378	A379	A380	G381	L382	K383		

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.00Å 121.00Å 171.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.4 (8.00-3.20)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.210 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 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	1.23	15/3001 (0.5%)	2.31	167/4068 (4.1%)
1	B	1.22	14/3001 (0.5%)	2.35	168/4068 (4.1%)
All	All	1.23	29/6002 (0.5%)	2.33	335/8136 (4.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	19
1	B	0	18
All	All	0	37

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	ALA	CA-C	-8.79	1.42	1.53
1	B	359	HIS	CD2-NE2	-7.71	1.29	1.37
1	A	102	ILE	CA-CB	7.37	1.63	1.54
1	A	257	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	359	HIS	CD2-NE2	-6.99	1.30	1.37

The worst 5 of 335 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ASP	CA-CB-CG	14.84	127.44	112.60
1	B	146	GLN	N-CA-C	-13.14	96.69	113.12
1	B	84	PHE	CA-CB-CG	12.90	126.70	113.80
1	B	286	VAL	N-CA-C	-12.43	99.89	111.45
1	B	261	ALA	O-C-N	10.84	135.36	122.46

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ASP	Peptide
1	A	125	TYR	Sidechain
1	A	44	TYR	Sidechain
1	A	69	ARG	Sidechain
1	A	84	PHE	Sidechain

## 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	2942	643	2908	171	0
1	B	2942	643	2908	187	0
All	All	5884	1286	5816	344	0

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 29.

The worst 5 of 344 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:B:45:VAL:HG12	1:B:50:VAL:HG13	1.54	0.87
1:A:30:ILE:HG12	1:A:58:THR:HG21	1.59	0.85
1:B:251:TYR:HB2	1:B:255:ALA:HB2	1.60	0.84
1:B:203:MET:SD	1:B:222:PHE:HE2	2.01	0.83
1:B:134:MET:SD	1:B:279:ARG:NH2	2.51	0.83

There are no symmetry-related clashes.

## 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	381/383 (100%)	303 (80%)	69 (18%)	9 (2%)	4	28
1	B	381/383 (100%)	295 (77%)	71 (19%)	15 (4%)	2	18
All	All	762/766 (100%)	598 (78%)	140 (18%)	24 (3%)	3	22

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	B	136	ALA
1	A	228	GLY
1	B	47	THR
1	B	227	THR

### 5.3.2 Protein sidechains [i](#)

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	311/311 (100%)	223 (72%)	88 (28%)	0	2
1	B	311/311 (100%)	221 (71%)	90 (29%)	0	1
All	All	622/622 (100%)	444 (71%)	178 (29%)	0	2

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	119	GLN
1	B	225	ASN
1	B	131	ASP
1	B	185	LEU
1	B	268	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	B	70	ASN
1	B	348	HIS
1	B	128	ASN
1	B	257	HIS

### 5.3.3 RNA [i](#)

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.