



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 02:18 AM UTC

PDB ID : 5X3V / pdb_00005x3v
Title : Structure of human SHMT2 protein mutant
Authors : Li, J.; Sheng, J.
Deposited on : 2017-02-09
Resolution : 2.85 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

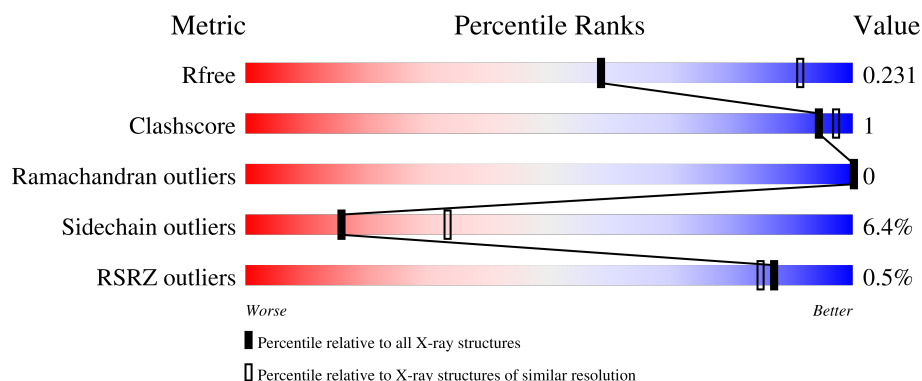
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	496	 82% 7% 10%
1	B	496	 82% 7% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6984 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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3457	2179	622	641	15			
1	B	442	Total	C	N	O	S	0	2	0
			3433	2164	616	638	15			

There are 28 discrepancies between the modelled and reference sequences:

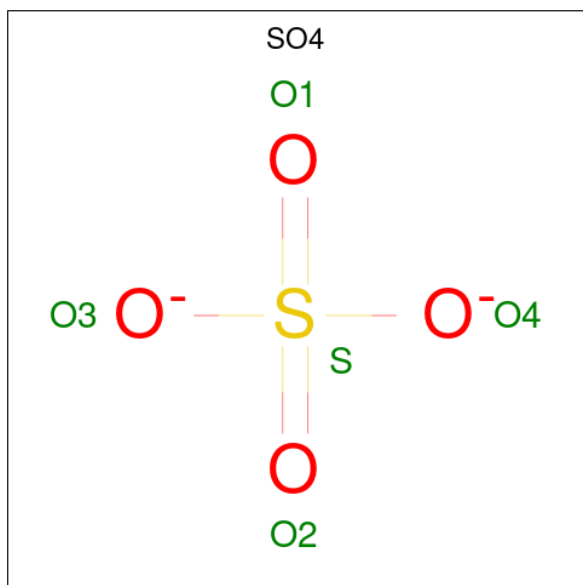
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ARG	LYS	engineered mutation	UNP P34897
A	484	LYS	-	expression tag	UNP P34897
A	485	LEU	-	expression tag	UNP P34897
A	486	ALA	-	expression tag	UNP P34897
A	487	ALA	-	expression tag	UNP P34897
A	488	ALA	-	expression tag	UNP P34897
A	489	LEU	-	expression tag	UNP P34897
A	490	GLU	-	expression tag	UNP P34897
A	491	HIS	-	expression tag	UNP P34897
A	492	HIS	-	expression tag	UNP P34897
A	493	HIS	-	expression tag	UNP P34897
A	494	HIS	-	expression tag	UNP P34897
A	495	HIS	-	expression tag	UNP P34897
A	496	HIS	-	expression tag	UNP P34897
B	74	ARG	LYS	engineered mutation	UNP P34897
B	484	LYS	-	expression tag	UNP P34897
B	485	LEU	-	expression tag	UNP P34897
B	486	ALA	-	expression tag	UNP P34897
B	487	ALA	-	expression tag	UNP P34897
B	488	ALA	-	expression tag	UNP P34897
B	489	LEU	-	expression tag	UNP P34897
B	490	GLU	-	expression tag	UNP P34897
B	491	HIS	-	expression tag	UNP P34897
B	492	HIS	-	expression tag	UNP P34897
B	493	HIS	-	expression tag	UNP P34897

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	494	HIS	-	expression tag	UNP P34897
B	495	HIS	-	expression tag	UNP P34897
B	496	HIS	-	expression tag	UNP P34897

- 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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	28	Total	O	0	0
			28	28		

- Molecule 1: Serine hydroxymethyltransferase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.66Å 158.66Å 209.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.85) 75.7 (50.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.23 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.177 , 0.231 0.181 , 0.231	Depositor DCC
R_{free} test set	1414 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6984	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.57	0/3525	0.86	1/4769 (0.0%)
1	B	0.59	0/3505	0.87	0/4742
All	All	0.58	0/7030	0.86	1/9511 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	53	ILE	N-CA-C	5.00	115.89	108.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	ASP	Peptide
1	B	357	ASP	Peptide

5.2 Too-close contacts ⓘ

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	3457	0	3430	11	0
1	B	3433	0	3396	8	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	36	0	0	0	1
3	B	28	0	0	0	0
All	All	6984	0	6826	18	1

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 1.

The worst 5 of 18 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:441:THR:HG21	1:B:447:PHE:HA	1.86	0.57
1:B:437:VAL:O	1:B:441:THR:HG22	2.11	0.51
1:B:340:MET:HE3	1:B:361:VAL:HG22	1.93	0.49
1:A:205:SER:HB2	1:A:233:HIS:CE1	2.48	0.49
1:B:127:LEU:O	1:B:131:THR:HG23	2.17	0.44

All (1) 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)
3:A:632:HOH:O	3:A:632:HOH:O[7_554]	1.95	0.25

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	439/496 (88%)	415 (94%)	24 (6%)	0	100	100
1	B	436/496 (88%)	417 (96%)	19 (4%)	0	100	100
All	All	875/992 (88%)	832 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	361/405 (89%)	340 (94%)	21 (6%)	18	38
1	B	358/405 (88%)	333 (93%)	25 (7%)	14	29
All	All	719/810 (89%)	673 (94%)	46 (6%)	16	33

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	SER
1	B	188	LEU
1	B	123	SER
1	B	145	LEU
1	B	204	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	25	GLN
1	B	233	HIS
1	B	387	ASN
1	A	135	GLN
1	A	112	GLN

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](#)

6 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	A	501	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	A	503	-	4,4,4	0.42	0	6,6,6	0.20	0
2	SO4	B	501	-	4,4,4	0.39	0	6,6,6	0.25	0
2	SO4	B	503	-	4,4,4	0.41	0	6,6,6	0.19	0
2	SO4	B	502	-	4,4,4	0.44	0	6,6,6	0.23	0
2	SO4	A	502	-	4,4,4	0.44	0	6,6,6	0.15	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.

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	445/496 (89%)	-0.68	0 100 100	22, 33, 54, 75	0
1	B	442/496 (89%)	-0.41	4 (0%) 81 76	15, 43, 68, 78	2 (0%)
All	All	887/992 (89%)	-0.54	4 (0%) 87 85	15, 36, 62, 78	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394	ASP	2.7
1	B	286	ILE	2.5
1	B	151	LEU	2.4
1	B	396	SER	2.3

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](#)

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(Å ²)	Q<0.9
2	SO4	A	502	5/5	0.89	0.16	103,103,104,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	502	5/5	0.91	0.10	60,61,64,66	0
2	SO4	B	503	5/5	0.93	0.10	69,70,71,71	0
2	SO4	B	501	5/5	0.96	0.10	60,63,64,64	0
2	SO4	A	501	5/5	0.96	0.08	14,14,14,14	5
2	SO4	A	503	5/5	0.96	0.10	47,47,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.