



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 10:03 AM BST

PDB ID : 1YJS
Title : K226Q Mutant Of Serine Hydroxymethyltransferase From B. Stearothermophilus, Complex With Glycine
Authors : Bhavani, S.; Trivedi, V.; Jala, V.R.; Subramanya, H.S.; Kaul, P.; Purnima, K.; Prakash, V.; Appaji, R.N.; Savithri, H.S.
Deposited on : 2005-01-15
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

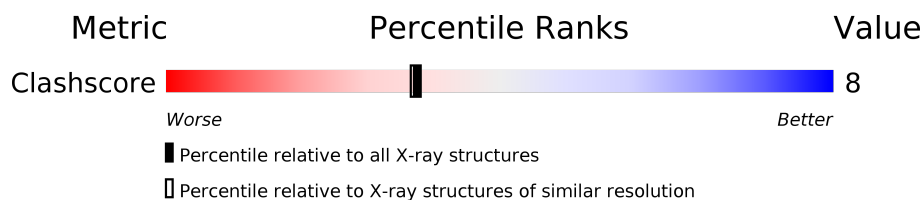
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)

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 ≥ 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	419	 82% 13% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3275 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3116	1969	551	585	11			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



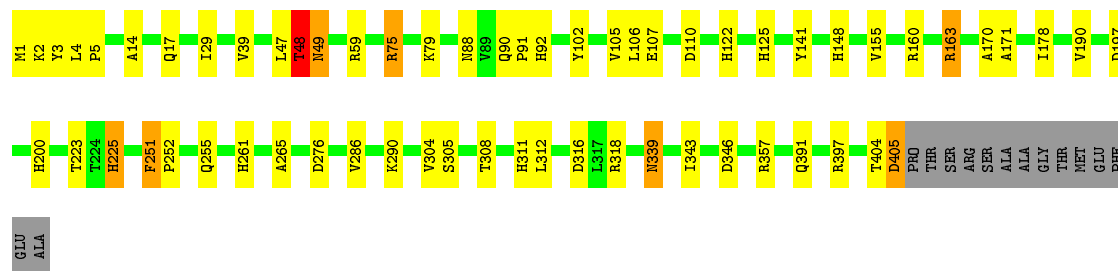
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		

Note EDS failed to run properly.

- Chain A: 82% 13% . .



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	61.37Å 106.29Å 56.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.227	Depositor
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.601	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3275	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% 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: PLP

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	0.60	2/3179 (0.1%)	1.28	31/4310 (0.7%)

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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	THR	C-O	10.48	1.43	1.23
1	A	48	THR	C-N	5.35	1.46	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ARG	NE-CZ-NH2	-17.05	111.78	120.30
1	A	397	ARG	NE-CZ-NH1	10.91	125.75	120.30
1	A	397	ARG	CD-NE-CZ	9.61	137.05	123.60
1	A	163	ARG	NE-CZ-NH1	-9.58	115.51	120.30
1	A	312	LEU	CA-CB-CG	8.30	134.39	115.30
1	A	251	PHE	CA-C-O	-7.85	103.61	120.10
1	A	48	THR	N-CA-C	-7.54	90.66	111.00
1	A	48	THR	N-CA-CB	7.41	124.37	110.30
1	A	171	ALA	N-CA-CB	-7.05	100.23	110.10
1	A	75	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	252	PRO	CA-N-CD	-6.55	102.33	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	102	TYR	CB-CG-CD2	-6.19	117.28	121.00
1	A	252	PRO	N-CA-CB	6.09	110.61	103.30
1	A	357	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	48	THR	O-C-N	-5.98	113.14	122.70
1	A	48	THR	C-N-CA	5.94	136.54	121.70
1	A	48	THR	CA-C-O	-5.90	107.71	120.10
1	A	225	HIS	N-CA-C	5.85	126.80	111.00
1	A	160	ARG	CD-NE-CZ	5.66	131.52	123.60
1	A	49	ASN	N-CA-CB	5.64	120.74	110.60
1	A	397	ARG	CG-CD-NE	-5.61	100.01	111.80
1	A	102	TYR	CB-CG-CD1	5.56	124.34	121.00
1	A	405	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	316	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	225	HIS	CA-C-N	5.30	128.85	117.20
1	A	276	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	316	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	A	339	ASN	CB-CA-C	-5.19	100.03	110.40
1	A	225	HIS	O-C-N	-5.11	114.52	122.70
1	A	59	ARG	CD-NE-CZ	5.01	130.61	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	PHE	Mainchain,Peptide
1	A	48	THR	Mainchain

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	3116	0	3090	47	4
2	A	15	0	6	1	0
3	A	5	0	2	2	0
4	A	139	0	0	1	4
All	All	3275	0	3098	48	4

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 8.

All (48) 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:17:GLN:HG2	4:A:682:HOH:O	1.74	0.87
1:A:148:HIS:HD2	1:A:305:SER:H	1.26	0.81
1:A:290:LYS:HE2	1:A:308:THR:HG23	1.62	0.81
1:A:92:HIS:H	1:A:255:GLN:HE22	1.28	0.81
1:A:47:LEU:O	1:A:48:THR:C	2.21	0.75
1:A:48:THR:HA	1:A:261:HIS:CD2	2.22	0.75
1:A:261:HIS:H	1:A:261:HIS:CD2	2.10	0.69
1:A:105:VAL:HG23	1:A:106:LEU:HG	1.75	0.68
1:A:286:VAL:HG13	1:A:290:LYS:NZ	2.12	0.63
1:A:122:HIS:H	1:A:125:HIS:CD2	2.20	0.60
1:A:148:HIS:CD2	1:A:305:SER:H	2.14	0.59
1:A:163:ARG:NH1	1:A:190:VAL:HB	2.18	0.58
1:A:290:LYS:CE	1:A:308:THR:HG23	2.35	0.56
1:A:311:HIS:H	1:A:311:HIS:HD1	1.52	0.55
1:A:88:ASN:ND2	1:A:91:PRO:HD3	2.22	0.55
1:A:290:LYS:N	1:A:290:LYS:HE3	2.23	0.54
1:A:163:ARG:HH12	1:A:190:VAL:HB	1.73	0.52
1:A:286:VAL:HG13	1:A:290:LYS:HZ2	1.74	0.52
1:A:200:HIS:HE1	3:A:601:GLY:O	1.96	0.49
1:A:1:MET:SD	1:A:4:LEU:HD23	2.53	0.48
1:A:75:ARG:O	1:A:79:LYS:HD3	2.13	0.48
1:A:2:LYS:HD3	1:A:3:TYR:CZ	2.48	0.48
1:A:88:ASN:HD22	1:A:91:PRO:HD3	1.77	0.48
2:A:501:PLP:O3	3:A:601:GLY:N	2.46	0.47
1:A:90:GLN:N	1:A:91:PRO:CD	2.78	0.47
1:A:107:GLU:HG2	1:A:110:ASP:OD1	2.15	0.46
1:A:261:HIS:H	1:A:261:HIS:HD2	1.58	0.46
1:A:200:HIS:HD2	1:A:311:HIS:NE2	2.13	0.46
1:A:125:HIS:HE1	1:A:197:ASP:OD2	1.99	0.45
1:A:261:HIS:CD2	1:A:261:HIS:N	2.83	0.45
1:A:343:ILE:O	1:A:346:ASP:HB2	2.17	0.45
1:A:170:ALA:HB3	1:A:197:ASP:O	2.17	0.45
1:A:14:ALA:HA	1:A:17:GLN:OE1	2.17	0.44
1:A:163:ARG:HH12	1:A:190:VAL:CB	2.31	0.44
1:A:92:HIS:H	1:A:255:GLN:NE2	2.04	0.44
1:A:286:VAL:HG13	1:A:290:LYS:HZ3	1.81	0.43
1:A:88:ASN:C	1:A:88:ASN:HD22	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:N	1:A:255:GLN:HE22	2.06	0.43
1:A:4:LEU:HB3	1:A:5:PRO:HD3	1.99	0.42
1:A:148:HIS:CD2	1:A:304:VAL:HG13	2.55	0.42
1:A:170:ALA:HA	1:A:178:ILE:HD13	2.02	0.42
1:A:404:THR:O	1:A:405:ASP:HB3	2.20	0.41
1:A:141:TYR:CG	1:A:155:VAL:HG22	2.55	0.41
1:A:91:PRO:HA	1:A:255:GLN:HE22	1.85	0.41
1:A:223:THR:HB	1:A:225:HIS:CE1	2.55	0.41
1:A:29:ILE:HG23	1:A:339:ASN:OD1	2.21	0.41
1:A:39:VAL:HG13	1:A:265:ALA:HB1	2.02	0.40
1:A:391:GLN:H	1:A:391:GLN:HG2	1.60	0.40

All (4) 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:A:48:THR:O	4:A:619:HOH:O[2_555]	1.36	0.84
1:A:48:THR:C	4:A:619:HOH:O[2_555]	1.77	0.43
1:A:49:ASN:N	4:A:619:HOH:O[2_555]	1.82	0.38
1:A:49:ASN:CA	4:A:619:HOH:O[2_555]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	GLY	A	601	2	1,4,4	0.05	0	0,4,4	0.00	-
2	PLP	A	501	3	15,15,16	1.69	2 (13%)	20,22,23	2.19	8 (40%)

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
3	GLY	A	601	2	-	0/0/2/2	-
2	PLP	A	501	3	-	0/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C3-C2	3.53	1.44	1.40
2	A	501	PLP	C4A-C4	-2.76	1.45	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C2A-C2-C3	5.88	128.15	120.89
2	A	501	PLP	C5A-C5-C6	-3.34	113.88	119.37
2	A	501	PLP	C6-N1-C2	3.19	125.08	119.17
2	A	501	PLP	C3-C2-N1	-2.94	116.97	120.77
2	A	501	PLP	O3P-P-O1P	2.65	121.06	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C3-C4-C5	2.30	121.23	118.74
2	A	501	PLP	C4A-C4-C5	-2.27	118.60	120.94
2	A	501	PLP	C5-C6-N1	-2.20	120.16	123.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	GLY	2	0
2	A	501	PLP	1	0

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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.