



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:57 PM UTC

PDB ID : 1TPU / pdb_00001tpu
Title : S96P CHANGE IS A SECOND-SITE SUPPRESSOR FOR H95N SLUGGISH
MUTANT TRIOSEPHOSPHATE ISOMERASE
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Deposited on : 1994-11-07
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

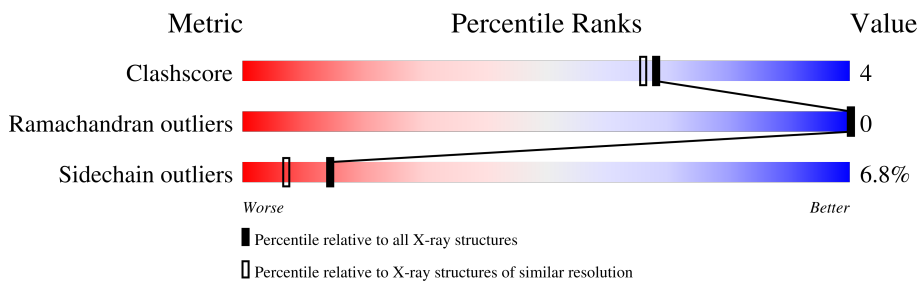
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	247	 81% 14% . .
1	B	247	 83% 13% ...

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4014 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.

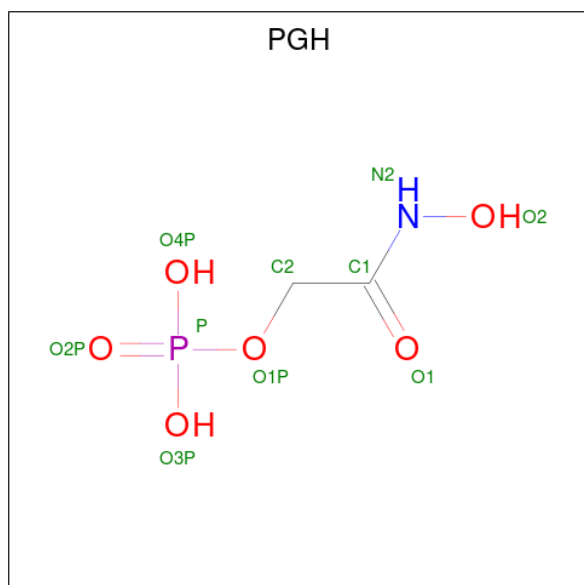
- Molecule 1 is a protein called TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1854	1174	324	350	6			
1	B	245	Total	C	N	O	S	0	0	0
			1854	1174	324	350	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ASN	HIS	engineered mutation	UNP P00940
A	194	THR	SER	conflict	UNP P00940
B	95	ASN	HIS	engineered mutation	UNP P00940
B	194	THR	SER	conflict	UNP P00940

- Molecule 2 is PHOSPHOGLYCOLOHYDROXAMIC ACID (CCD ID: PGH) (formula: $C_2H_6NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	144	Total	O	0	0
			144	144		

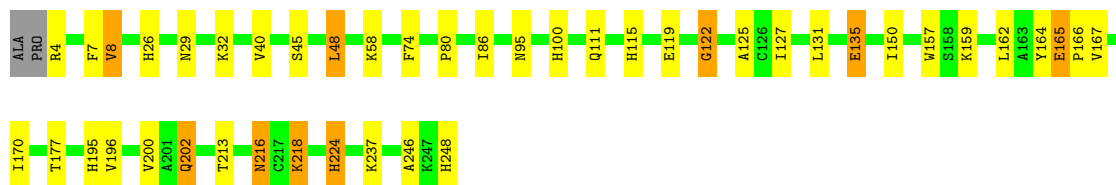
3 Residue-property plots

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.

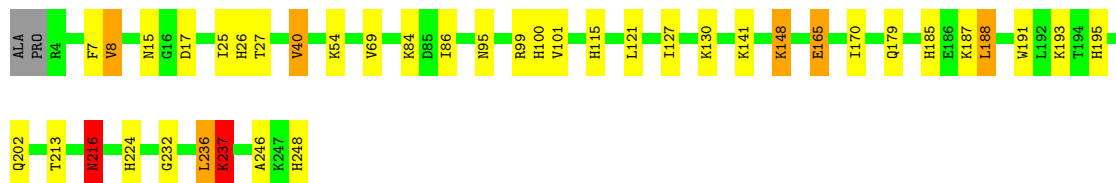
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.30Å 74.10Å 57.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4014	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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: PGH

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	1.06	7/1888 (0.4%)	1.61	21/2548 (0.8%)
1	B	1.05	11/1888 (0.6%)	1.60	19/2548 (0.7%)
All	All	1.05	18/3776 (0.5%)	1.60	40/5096 (0.8%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	VAL	CA-CB	7.51	1.63	1.54
1	B	224	HIS	CD2-NE2	-7.41	1.29	1.37
1	A	115	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	195	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	185	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	248	HIS	CD2-NE2	-6.48	1.30	1.37
1	B	195	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	100	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	8	VAL	CA-CB	6.07	1.62	1.54
1	B	26	HIS	CD2-NE2	-5.99	1.31	1.37
1	B	248	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	115	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	100	HIS	CD2-NE2	-5.93	1.31	1.37
1	B	40	VAL	CA-CB	5.60	1.62	1.54
1	A	224	HIS	CD2-NE2	-5.59	1.31	1.37
1	B	185	HIS	CG-ND1	-5.52	1.32	1.38
1	B	195	HIS	CG-ND1	-5.30	1.32	1.38
1	A	26	HIS	CD2-NE2	-5.09	1.32	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ASP	CA-CB-CG	8.19	120.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	TRP	N-CA-C	-7.18	103.39	111.07
1	B	179	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	122	GLY	N-CA-C	-6.74	103.52	112.82
1	A	224	HIS	CB-CG-CD2	-6.73	122.45	131.20
1	A	111	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	B	101	VAL	N-CA-C	-6.59	106.14	111.81
1	B	195	HIS	CA-CB-CG	-6.53	107.27	113.80
1	A	7	PHE	CA-C-N	-6.48	114.49	123.10
1	A	7	PHE	C-N-CA	-6.48	114.49	123.10
1	A	74	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	224	HIS	CB-CG-ND1	6.03	131.75	122.70
1	A	26	HIS	N-CA-C	-5.97	104.77	111.28
1	B	99	ARG	N-CA-C	5.91	117.53	111.14
1	A	224	HIS	CA-CB-CG	5.90	119.70	113.80
1	A	157	TRP	CG-CD2-CE3	5.87	139.77	133.90
1	B	187	LYS	CA-CB-CG	-5.82	102.45	114.10
1	A	115	HIS	CA-CB-CG	-5.70	108.10	113.80
1	B	7	PHE	CA-C-N	-5.62	115.18	122.99
1	B	7	PHE	C-N-CA	-5.62	115.18	122.99
1	B	246	ALA	N-CA-C	5.54	119.54	112.34
1	A	100	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	111	GLN	CG-CD-NE2	5.51	124.67	116.40
1	B	202	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	29	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	69	VAL	CA-C-N	5.42	124.93	119.19
1	B	69	VAL	C-N-CA	5.42	124.93	119.19
1	B	27	THR	CA-CB-OG1	-5.41	101.49	109.60
1	A	26	HIS	CA-CB-CG	5.38	119.18	113.80
1	A	202	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	B	216	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	115	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	B	237	LYS	O-C-N	-5.20	116.93	121.35
1	B	15	ASN	CB-CG-ND2	5.20	124.19	116.40
1	A	177	THR	CA-C-N	5.16	124.61	119.24
1	A	177	THR	C-N-CA	5.16	124.61	119.24
1	A	237	LYS	CA-C-N	5.14	124.93	119.28
1	A	237	LYS	C-N-CA	5.14	124.93	119.28
1	B	248	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	195	HIS	CB-CG-CD2	-5.02	124.67	131.20

There are no chirality outliers.

There are no planarity outliers.

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	1854	0	1862	14	0
1	B	1854	0	1862	13	0
2	A	10	0	4	0	0
2	B	10	0	4	3	0
3	A	142	0	0	1	0
3	B	144	0	0	1	0
All	All	4014	0	3732	27	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 4.

All (27) 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:127:ILE:HD11	1:B:188:LEU:HD21	1.74	0.69
1:A:45:SER:HA	1:A:48:LEU:HD22	1.73	0.68
1:A:213:THR:H	1:A:216:ASN:HD21	1.48	0.60
1:B:25:ILE:HG21	1:B:54:LYS:HB3	1.84	0.60
1:B:165:GLU:HB2	1:B:170:ILE:HD11	1.84	0.59
1:A:131:LEU:O	1:A:135:GLU:HG2	2.04	0.58
1:A:213:THR:H	1:A:216:ASN:ND2	2.03	0.55
1:A:218:LYS:HG3	1:A:246:ALA:O	2.07	0.54
1:A:167:VAL:HA	1:A:170:ILE:HD12	1.89	0.53
1:B:213:THR:H	1:B:216:ASN:HD21	1.56	0.51
1:B:213:THR:H	1:B:216:ASN:ND2	2.09	0.50
1:B:232:GLY:HA3	2:B:250:PGH:H21	1.93	0.49
1:A:80:PRO:HB2	1:A:119:GLU:HG3	1.95	0.49
1:B:216:ASN:HD22	1:B:216:ASN:C	2.21	0.48
1:B:236:LEU:O	1:B:237:LYS:HE3	2.14	0.48
1:A:4:ARG:HD3	1:A:202:GLN:O	2.16	0.46
1:B:193:LYS:HD3	3:B:623:HOH:O	2.16	0.45
1:A:196:VAL:HG11	1:A:200:VAL:HG11	1.99	0.44
1:B:232:GLY:CA	2:B:250:PGH:H21	2.47	0.44
1:A:165:GLU:HB2	1:A:170:ILE:HD11	1.99	0.44
1:B:232:GLY:N	2:B:250:PGH:H21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:HB1	1:A:150:ILE:HD13	2.00	0.44
1:A:135:GLU:HG3	3:A:736:HOH:O	2.18	0.43
1:A:122:GLY:HA2	1:A:159:LYS:HB3	2.02	0.42
1:B:84:LYS:HG3	1:B:121:LEU:HD21	2.02	0.41
1:A:164:TYR:CE2	1:A:166:PRO:HD3	2.55	0.41
1:B:148:LYS:HA	1:B:148:LYS:HE3	2.01	0.40

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	243/247 (98%)	237 (98%)	6 (2%)	0	100	100
1	B	243/247 (98%)	238 (98%)	5 (2%)	0	100	100
All	All	486/494 (98%)	475 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	191/192 (100%)	177 (93%)	14 (7%)	13	6
1	B	191/192 (100%)	179 (94%)	12 (6%)	16	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	382/384 (100%)	356 (93%)	26 (7%)	14 7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	32	LYS
1	A	40	VAL
1	A	48	LEU
1	A	58	LYS
1	A	86	ILE
1	A	95	ASN
1	A	127	ILE
1	A	135	GLU
1	A	162	LEU
1	A	165	GLU
1	A	216	ASN
1	A	218	LYS
1	A	224	HIS
1	B	8	VAL
1	B	40	VAL
1	B	86	ILE
1	B	95	ASN
1	B	130	LYS
1	B	141	LYS
1	B	148	LYS
1	B	165	GLU
1	B	188	LEU
1	B	216	ASN
1	B	236	LEU
1	B	237	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	100	HIS
1	A	111	GLN
1	A	115	HIS
1	A	179	GLN
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	223	GLN
1	B	53	GLN
1	B	100	HIS
1	B	185	HIS
1	B	216	ASN

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](#)

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	$\# Z > 2$
2	PGH	A	250	-	9,9,9	1.16	1 (11%)	10,12,12	1.17	0
2	PGH	B	250	-	9,9,9	0.94	1 (11%)	10,12,12	1.61	2 (20%)

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	PGH	A	250	-	-	3/8/8/8	-
2	PGH	B	250	-	-	6/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	250	PGH	P-O4P	-2.16	1.46	1.54
2	A	250	PGH	P-O1P	-2.09	1.53	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	PGH	C2-C1-N2	-3.20	110.91	116.41
2	B	250	PGH	O1-C1-N2	2.17	125.94	123.27

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	250	PGH	N2-C1-C2-O1P
2	A	250	PGH	C2-C1-N2-O2
2	A	250	PGH	O1-C1-N2-O2
2	B	250	PGH	N2-C1-C2-O1P
2	B	250	PGH	C2-C1-N2-O2
2	B	250	PGH	O1-C1-N2-O2
2	B	250	PGH	C2-O1P-P-O4P
2	B	250	PGH	C2-O1P-P-O2P
2	B	250	PGH	C2-O1P-P-O3P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	250	PGH	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.