

# wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 05:16 PM EST

PDB ID : 1HTI

Title: CRYSTAL STRUCTURE OF RECOMBINANT HUMAN TRIOSEPHOS-

PHATE ISOMERASE AT 2.8 ANGSTROMS RESOLUTION. TRIOSEPHOSPHATE ISOMERASE RELATED HUMAN GENETIC DISORDERS AND COMPARISON WITH THE TRYPANOSOMAL

ENZYME

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Deposited on : 1994-10-12

Resolution : 2.80 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 (i) 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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)

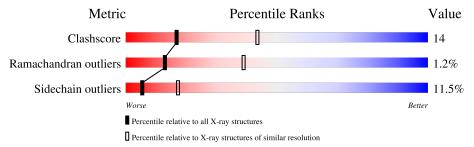
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 $(\# \text{Entries})$	$\begin{array}{c} {\bf Similar \ resolution} \\ (\#{\bf Entries, \ resolution \ range(\AA)}) \end{array}$
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	A	248	58%	34% 8%			
1	В	248	54%	40% 5% •			



## 2 Entry composition (i)

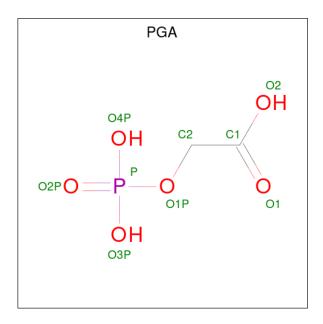
There are 2 unique types of molecules in this entry. The entry contains 3745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	248	Total	C	11	0	S	0	0	0
			1868	1181	324	356	7	_		_
1	R	248	Total	С	N	O	S	0	0	0
1	D	240	1868	1181	324	356	7		0	

• Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: C<sub>2</sub>H<sub>5</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
2	В	1	Total 9	C 2	O 6	P 1	0	0

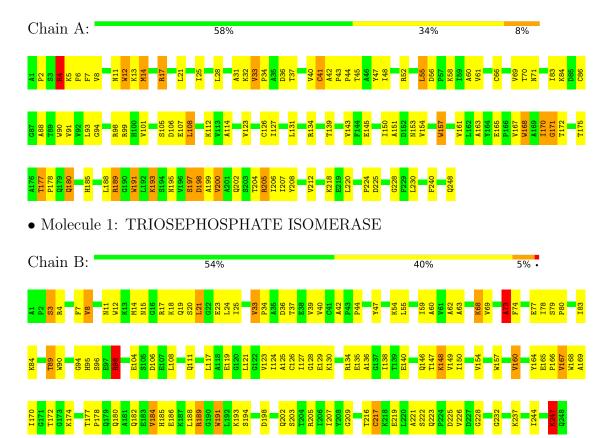


# 3 Residue-property plots (i)

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





# 4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	65.81Å 75.39Å 92.81Å	D:4	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	8.00 - 2.80	Depositor	
% Data completeness	85.5 (8.00-2.80)	Depositor	
(in resolution range)	09.9 (0.00 2.00)	Depositor	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
$R, R_{free}$	0.167 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3745	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	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: PGA

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		nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	1.01	0/1903	1.91	50/2577~(1.9%)	
1	В	1.00	1/1903 (0.1%)	1.84	41/2577 (1.6%)	
All	All	1.01	1/3806 (0.0%)	1.88	91/5154 (1.8%)	

#### All (1) bond length outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	В	194	SER	CA-CB	5.15	1.60	1.52

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	134	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	В	134	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	17	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	A	61	VAL	CA-CB-CG2	-9.40	96.80	110.90
1	В	189	ARG	NE-CZ-NH1	9.37	124.99	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1868	0	1879	50	0
1	В	1868	0	1879	59	0
2	В	9	0	2	3	0
All	All	3745	0	3760	106	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 14.

The worst 5 of 106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:6:PHE:HB3	1:A:37:THR:HG22	1.49	0.94
1:A:25:ILE:HG23	1:A:55:LEU:HD13	1.56	0.88
1:B:169:ALA:HA	1:B:174:LYS:O	1.92	0.68
1:A:11:ASN:HA	1:A:42:ALA:HB3	1.76	0.67
1:B:8:VAL:HG13	1:B:39:VAL:HG12	1.77	0.67

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	Perce	entiles
1	A	246/248 (99%)	224 (91%)	20 (8%)	2 (1%)	19	49
1	В	246/248 (99%)	221 (90%)	21 (8%)	4 (2%)	9	31
All	All	492/496 (99%)	445 (90%)	41 (8%)	6 (1%)	13	39

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	73	ALA
1	A	45	THR

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Mol	Chain	Res	Type
1	A	171	GLY
1	В	3	SER
1	В	4	ARG

#### 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	$195/195\ (100\%)$	175 (90%)	20 (10%)	7	21	
1	В	$195/195\ (100\%)$	170 (87%)	25 (13%)	4	13	
All	All	390/390 (100%)	345 (88%)	45 (12%)	5	17	

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	98	ARG
1	В	160	VAL
1	В	108	LEU
1	В	140	GLU
1	В	202	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	248	GLN
1	В	180	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 monosaccharides in this entry.

#### 5.6 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	B	ond leng	$\operatorname{gths}$	В	ond ang	cles
MIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	$\mid \# Z  > 2 \mid$
2	PGA	В	549	-	8,8,8	1.94	1 (12%)	10,11,11	3.66	5 (50%)

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	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
2	PGA	В	549	-	-	3/6/6/6	-

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	В	549	PGA	O1-C1	4.54	1.37	1.22

#### All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
2	В	549	PGA	O1P-C2-C1	-7.80	98.78	110.54
2	В	549	PGA	O2-C1-O1	-6.72	106.55	123.30
2	В	549	PGA	O2-C1-C2	3.22	128.24	113.34

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	549	PGA	O3P-P-O1P	-2.31	100.59	106.73
2	В	549	PGA	O4P-P-O2P	2.16	119.15	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	549	PGA	O2-C1-C2-O1P
2	В	549	PGA	O1-C1-C2-O1P
2	В	549	PGA	C2-O1P-P-O2P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	549	PGA	3	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 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.

