



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 10:29 PM EDT

PDB ID : 1TPE  
Title : COMPARISON OF THE STRUCTURES AND THE CRYSTAL CONTACTS OF TRYPANOSOMAL TRIOSEPHOSPHATE ISOMERASE IN FOUR DIFFERENT CRYSTAL FORMS  
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Deposited on : 1994-02-28  
Resolution : 2.10 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](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	:	4.02b-467
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)	:	2.36.2

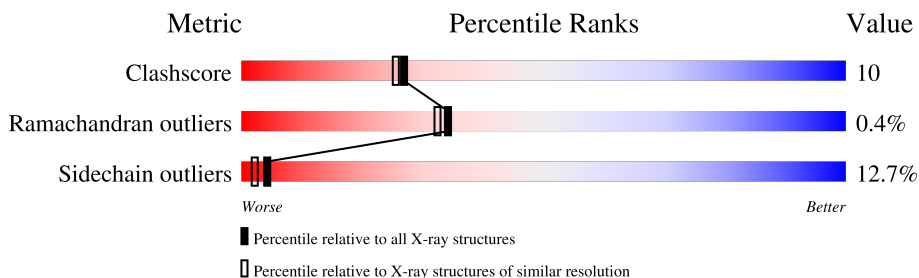
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	250	 68% 24% 6%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1989 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	249	Total	C	N	O	S	0	0	0
			1889	1200	334	350	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		



Note EDS was not executed.

Chain A:

Label	Category
Met	Grey
S2	Green
K3	Orange
P4	Orange
I7	Yellow
W12	Yellow
Q19	Yellow
E23	Orange
D26	Orange
L27	Orange
D36	Green
V37	Green
Q38	Green
C39	Green
Y40	Yellow
L48	Green
A49	Orange
M50	Orange
T51	Green
K52	Orange
E53	Orange
R54	Red
L55	Yellow
V61	Yellow
I62	Green
A63	Green
A64	Yellow
K70	Yellow
I91	Yellow
G94	Yellow
E104	Yellow
E107	Orange
D111	Yellow
V117	Yellow
C126	Yellow
I127	Yellow
G128	Yellow
F129	Yellow
T139	Yellow
A140	Green
V141	Green
V142	Yellow
V143	Yellow
L144	Yellow
T145	Green
Q146	Yellow
I147	Yellow
A151	Yellow
K152	Orange
K153	Orange
K156	Yellow
A157	Green
D158	Green
W159	Green
A160	Orange
K161	Orange
Y166	Yellow
E167	Yellow
E185	Yellow
R191	Orange
S192	Yellow
W193	Yellow
V194	Yellow
S195	Orange
S196	Yellow
D201	Yellow
V202	Yellow
R203	Orange
G204	Green
E205	Yellow
L206	Yellow
R207	Yellow
L208	Yellow
L209	Yellow
S213	Yellow
V214	Yellow
N215	Yellow
G216	Yellow
K217	Yellow
V218	Green
A219	Yellow
Y223	Orange
D227	Yellow
E241	Green
F242	Yellow
V243	Yellow
D244	Yellow
I245	Yellow
I246	Yellow
K247	Green
Q250	Yellow

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.40Å 48.20Å 67.50Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, $R_{free}$	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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	1.02	10/1923 (0.5%)	1.44	16/2606 (0.6%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	LYS	CE-NZ	-9.08	1.26	1.49
1	A	107	GLU	CD-OE1	6.91	1.33	1.25
1	A	135	GLU	CD-OE2	6.81	1.33	1.25
1	A	23	GLU	CD-OE2	6.38	1.32	1.25
1	A	185	GLU	CD-OE1	6.37	1.32	1.25
1	A	53	GLU	CD-OE1	5.92	1.32	1.25
1	A	104	GLU	CD-OE2	5.55	1.31	1.25
1	A	129	GLU	CD-OE2	5.44	1.31	1.25
1	A	133	GLU	CD-OE1	5.19	1.31	1.25
1	A	205	GLU	CD-OE2	5.06	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	134	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	A	54	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	134	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	A	26	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	A	54	ARG	CD-NE-CZ	6.96	133.35	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	36	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	A	201	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	227	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	227	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	244	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	223	TYR	CB-CG-CD2	5.43	124.26	121.00
1	A	166	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	A	201	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	36	ASP	CB-CG-OD2	5.28	123.05	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	PRO	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	1889	0	1925	39	0
2	A	100	0	0	1	0
All	All	1989	0	1925	39	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 10.

All (39) 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:50:MET:HG3	1:A:54:ARG:HD3	1.44	0.99
1:A:243:VAL:O	1:A:247:LYS:HG2	1.84	0.77
1:A:247:LYS:O	1:A:250:GLN:HG2	1.86	0.74
1:A:50:MET:HG3	1:A:54:ARG:CD	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:MET:O	1:A:54:ARG:HD2	1.98	0.64
1:A:27:LEU:HD11	1:A:240:PRO:HB3	1.80	0.63
1:A:50:MET:CG	1:A:54:ARG:HD3	2.26	0.62
1:A:191:ARG:HG2	1:A:203:ARG:HE	1.63	0.61
1:A:12:TRP:CD1	1:A:238:LEU:HD13	2.35	0.60
1:A:144:LEU:HD13	1:A:193:TRP:CD1	2.37	0.60
1:A:191:ARG:HG3	1:A:203:ARG:HG2	1.85	0.58
1:A:243:VAL:HG13	1:A:247:LYS:HE3	1.88	0.56
1:A:243:VAL:CG1	1:A:247:LYS:HE3	2.34	0.56
1:A:144:LEU:HD23	1:A:144:LEU:N	2.21	0.54
1:A:191:ARG:O	1:A:203:ARG:HG3	2.07	0.54
1:A:70:LYS:HB2	2:A:350:HOH:O	2.08	0.54
1:A:64:ALA:HB3	1:A:91:ILE:HG13	1.92	0.52
1:A:3:LYS:NZ	1:A:223:TYR:O	2.44	0.51
1:A:151:ALA:HB2	1:A:159:TRP:HZ2	1.76	0.50
1:A:195:SER:OG	1:A:203:ARG:HD2	2.12	0.49
1:A:128:GLY:HA3	1:A:167:GLU:O	2.14	0.47
1:A:111:ASP:OD1	1:A:153:LYS:HE2	2.14	0.47
1:A:142:VAL:O	1:A:146:GLN:HG3	2.14	0.46
1:A:139:THR:O	1:A:143:VAL:HG22	2.15	0.45
1:A:215:ASN:O	1:A:219:ALA:HB2	2.17	0.45
1:A:117:VAL:HG11	1:A:158:ASP:HB3	1.97	0.45
1:A:233:VAL:HG21	1:A:245:ILE:HG21	1.99	0.45
1:A:40:VAL:HG22	1:A:61:VAL:CG2	2.48	0.44
1:A:2:SER:O	1:A:3:LYS:HB2	2.16	0.44
1:A:50:MET:HE3	1:A:50:MET:HB3	1.79	0.43
1:A:19:GLN:O	1:A:23:GLU:HG3	2.18	0.43
1:A:7:ILE:HA	1:A:38:GLN:O	2.19	0.42
1:A:7:ILE:HB	1:A:209:LEU:HD21	2.01	0.42
1:A:242:PHE:CE2	1:A:246:ILE:HD11	2.55	0.42
1:A:70:LYS:HB3	1:A:70:LYS:HE2	1.90	0.41
1:A:27:LEU:HD23	1:A:27:LEU:O	2.20	0.41
1:A:161:LYS:HB3	1:A:161:LYS:HE2	1.21	0.41
1:A:94:GLY:O	1:A:126:CYS:HB2	2.21	0.41
1:A:48:LEU:O	1:A:52:LYS:HB2	2.22	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	247/250 (99%)	240 (97%)	6 (2%)	1 (0%)	34	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS

### 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	197/198 (100%)	172 (87%)	25 (13%)	4	2

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	27	LEU
1	A	50	MET
1	A	52	LYS
1	A	53	GLU
1	A	54	ARG
1	A	55	LEU
1	A	62	ILE
1	A	107	GLU
1	A	136	SER

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Mol	Chain	Res	Type
1	A	141	VAL
1	A	147	ILE
1	A	153	LYS
1	A	161	LYS
1	A	191	ARG
1	A	192	SER
1	A	195	SER
1	A	196	SER
1	A	203	ARG
1	A	205	GLU
1	A	207	ARG
1	A	213	SER
1	A	214	VAL
1	A	217	LYS
1	A	238	LEU

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	89	ASN
1	A	181	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](#)

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

### 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.