



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 1TPD / pdb_00001tpd
Title : STRUCTURES OF THE "OPEN" AND "CLOSED" STATE OF TRY-
PANOSOMAL TRIOSEPHOSPHATE ISOMERASE, AS OBSERVED IN A
NEW CRYSTAL FORM: IMPLICATIONS FOR THE REACTION MECH-
ANISM
Authors : Noble, M.E.M.; Zeelen, J.Ph.; Wierenga, R.K.
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

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
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

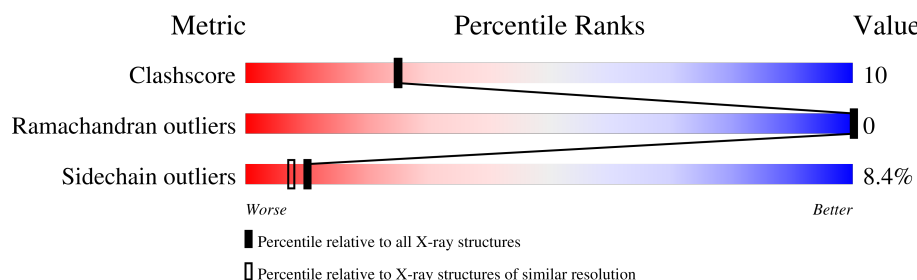
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 ≥ 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	 72% 24% .
1	B	250	 69% 26% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3966 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
			1883	1197	331	350	5			
1	B	249	Total	C	N	O	S	0	0	0
			1883	1197	331	350	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	94	Total	O	0	0
			94	94		

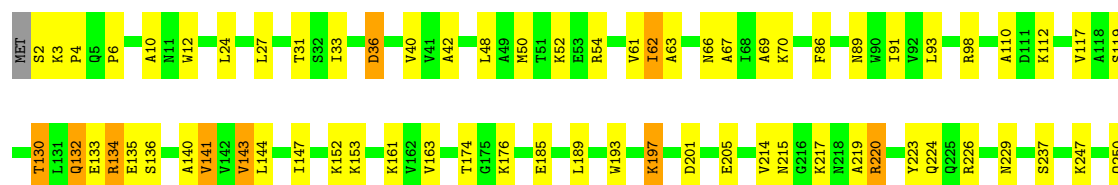
3 Residue-property plots

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.

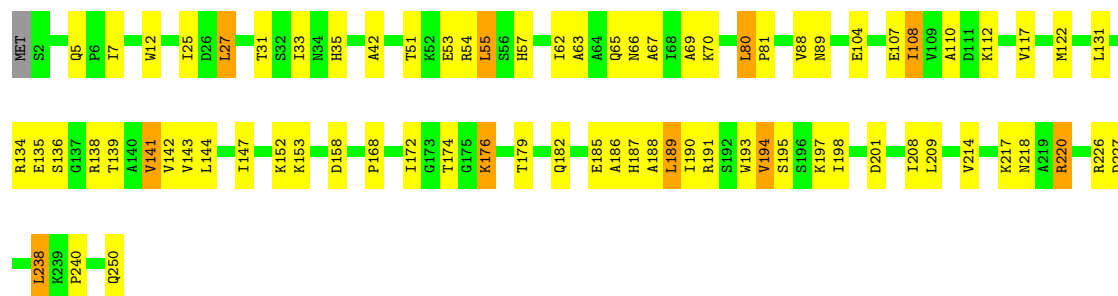
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A:  72% 24%



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B:  69% 26%



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, α , β , γ	94.80Å 48.30Å 131.00Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	1.26	1/1917 (0.1%)	1.64	16/2599 (0.6%)
1	B	1.20	1/1917 (0.1%)	1.68	15/2599 (0.6%)
All	All	1.23	2/3834 (0.1%)	1.66	31/5198 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	LYS	CE-NZ	-5.56	1.32	1.49
1	A	98	ARG	NE-CZ	5.26	1.38	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	N-CA-C	9.29	121.01	111.07
1	A	226	ARG	CD-NE-CZ	8.97	136.95	124.40
1	A	219	ALA	N-CA-C	7.68	119.65	111.28
1	A	135	GLU	N-CA-C	7.09	119.01	111.28
1	B	168	PRO	N-CA-CB	7.03	107.34	102.35
1	B	218	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	36	ASP	CA-CB-CG	6.52	119.12	112.60
1	B	69	ALA	N-CA-C	6.48	118.00	111.07
1	A	119	SER	CB-CA-C	-6.19	99.75	110.09
1	B	185	GLU	CB-CA-C	6.17	120.67	110.81
1	A	226	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	B	227	ASP	CA-C-N	6.04	129.92	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	ASP	C-N-CA	6.04	129.92	122.37
1	B	5	GLN	CB-CG-CD	-5.95	102.49	112.60
1	A	141	VAL	CB-CA-C	-5.94	104.36	111.97
1	A	117	VAL	CB-CA-C	5.93	119.57	111.97
1	A	141	VAL	N-CA-CB	5.84	117.38	110.55
1	B	80	LEU	CA-C-O	5.78	123.64	118.33
1	B	194	VAL	O-C-N	5.36	127.17	121.91
1	A	143	VAL	CB-CA-C	5.36	119.37	112.14
1	B	53	GLU	N-CA-CB	5.32	117.94	110.12
1	A	50	MET	CA-C-N	5.31	127.67	120.65
1	A	50	MET	C-N-CA	5.31	127.67	120.65
1	A	130	THR	CA-C-O	-5.30	115.89	121.88
1	B	141	VAL	CB-CA-C	-5.30	105.10	112.04
1	A	91	ILE	N-CA-C	5.28	115.31	108.35
1	A	163	VAL	N-CA-C	-5.27	100.61	108.46
1	B	220	ARG	CA-C-O	5.15	126.23	120.82
1	B	195	SER	CA-C-N	5.11	127.39	120.44
1	B	195	SER	C-N-CA	5.11	127.39	120.44
1	B	191	ARG	CA-CB-CG	-5.11	103.88	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	ALA	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	1883	0	1917	33	0
1	B	1883	0	1917	41	0
2	A	106	0	0	0	0
2	B	94	0	0	1	0
All	All	3966	0	3834	74	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 (74) 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:62:ILE:HD11	1:B:88:VAL:HG22	1.52	0.92
1:B:62:ILE:CD1	1:B:88:VAL:HG22	2.08	0.83
1:A:62:ILE:H	1:A:62:ILE:HD13	1.52	0.74
1:A:4:PRO:HD2	1:A:229:ASN:ND2	2.02	0.74
1:B:179:THR:OG1	1:B:182:GLN:HG3	1.87	0.74
1:A:215:ASN:OD1	1:A:217:LYS:HB2	1.97	0.64
1:B:144:LEU:HD11	1:B:189:LEU:HD11	1.80	0.62
1:B:104:GLU:OE2	1:B:112:LYS:NZ	2.32	0.62
1:A:247:LYS:O	1:A:250:GLN:HG3	2.02	0.60
1:A:3:LYS:NZ	1:A:223:TYR:O	2.34	0.59
1:A:10:ALA:HB1	1:A:237:SER:HB2	1.84	0.59
1:B:33:ILE:HD12	1:B:57:HIS:CE1	2.38	0.59
1:B:152:LYS:O	1:B:152:LYS:HD2	2.03	0.58
1:A:193:TRP:CZ2	1:A:197:LYS:HG2	2.38	0.58
1:B:108:ILE:HA	2:B:687:HOH:O	2.03	0.58
1:A:40:VAL:HG22	1:A:61:VAL:CG2	2.34	0.58
1:B:12:TRP:CD1	1:B:238:LEU:HD13	2.40	0.57
1:B:187:HIS:ND1	1:B:208:ILE:HG22	2.20	0.56
1:A:220:ARG:NH2	1:A:223:TYR:HD2	2.05	0.55
1:B:194:VAL:O	1:B:198:ILE:N	2.35	0.54
1:B:7:ILE:HB	1:B:209:LEU:HD21	1.89	0.53
1:A:140:ALA:HA	1:A:189:LEU:HD21	1.92	0.52
1:A:144:LEU:HA	1:A:147:ILE:HG22	1.92	0.51
1:B:186:ALA:O	1:B:190:ILE:HD12	2.10	0.51
1:B:144:LEU:HD11	1:B:189:LEU:CD1	2.39	0.51
1:A:4:PRO:HD2	1:A:229:ASN:HD21	1.74	0.50
1:A:42:ALA:HA	1:A:63:ALA:O	2.12	0.50
1:A:193:TRP:O	1:A:197:LYS:HB2	2.12	0.50
1:A:31:THR:HG22	1:A:33:ILE:HG13	1.92	0.49
1:A:220:ARG:HH21	1:A:223:TYR:HD2	1.58	0.49
1:B:187:HIS:CE1	1:B:208:ILE:HG22	2.47	0.49
1:B:110:ALA:HB1	1:B:153:LYS:HD3	1.94	0.48
1:B:33:ILE:HD12	1:B:57:HIS:NE2	2.28	0.48
1:A:12:TRP:CZ2	1:A:24:LEU:HD23	2.49	0.48
1:B:172:ILE:O	1:B:172:ILE:HG22	2.13	0.48
1:A:193:TRP:NE1	1:A:197:LYS:HE3	2.28	0.48
1:A:67:ALA:O	1:A:112:LYS:HE2	2.13	0.47
1:B:31:THR:O	1:B:57:HIS:NE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:HD12	1:B:88:VAL:HG22	1.92	0.47
1:B:117:VAL:HG11	1:B:158:ASP:HB3	1.96	0.47
1:B:201:ASP:OD1	1:B:201:ASP:N	2.45	0.47
1:A:6:PRO:HD2	1:A:36:ASP:O	2.15	0.46
1:A:134:ARG:HE	1:A:134:ARG:HB2	1.61	0.46
1:A:48:LEU:O	1:A:52:LYS:HB2	2.15	0.46
1:A:130:THR:OG1	1:A:133:GLU:HG3	2.16	0.46
1:B:51:THR:O	1:B:55:LEU:HB2	2.16	0.46
1:A:132:GLN:H	1:A:132:GLN:CD	2.25	0.45
1:B:138:ARG:O	1:B:142:VAL:HG23	2.16	0.45
1:B:25:ILE:HG21	1:B:54:ARG:HD3	1.98	0.45
1:B:122:MET:HE3	1:B:122:MET:HB3	1.87	0.45
1:B:193:TRP:O	1:B:197:LYS:HB2	2.18	0.44
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.86	0.44
1:A:62:ILE:HD13	1:A:62:ILE:N	2.28	0.43
1:A:174:THR:OG1	1:A:176:LYS:HB2	2.18	0.43
1:A:52:LYS:NZ	1:A:86:PHE:O	2.48	0.43
1:B:35:HIS:CE1	1:B:250:GLN:HB3	2.54	0.43
1:B:54:ARG:O	1:B:54:ARG:HG2	2.18	0.43
1:B:131:LEU:CD1	1:B:176:LYS:HD2	2.49	0.43
1:B:174:THR:OG1	1:B:176:LYS:HG3	2.19	0.42
1:A:201:ASP:N	1:A:201:ASP:OD1	2.51	0.42
1:A:66:ASN:OD1	1:A:67:ALA:N	2.52	0.42
1:B:139:THR:O	1:B:143:VAL:HG22	2.20	0.41
1:B:27:LEU:HD11	1:B:240:PRO:HB3	2.03	0.41
1:B:42:ALA:HA	1:B:63:ALA:O	2.20	0.41
1:B:66:ASN:O	1:B:67:ALA:HB2	2.20	0.41
1:B:66:ASN:CG	1:B:67:ALA:N	2.79	0.41
1:B:187:HIS:ND1	1:B:208:ILE:CG2	2.83	0.41
1:A:10:ALA:CB	1:A:237:SER:HB2	2.51	0.41
1:B:80:LEU:HB2	1:B:81:PRO:HD3	2.02	0.41
1:B:65:GLN:O	1:B:66:ASN:HB2	2.20	0.40
1:B:144:LEU:HA	1:B:147:ILE:HG22	2.02	0.40
1:A:220:ARG:O	1:A:224:GLN:HG3	2.22	0.40
1:B:220:ARG:NH1	1:B:250:GLN:O	2.54	0.40
1:A:110:ALA:HB1	1:A:153:LYS:HD3	2.04	0.40

There are no symmetry-related clashes.

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	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
1	B	247/250 (99%)	242 (98%)	5 (2%)	0	100	100
All	All	494/500 (99%)	484 (98%)	10 (2%)	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	196/197 (100%)	178 (91%)	18 (9%)	8	6
1	B	196/197 (100%)	181 (92%)	15 (8%)	12	9
All	All	392/394 (100%)	359 (92%)	33 (8%)	10	7

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	27	LEU
1	A	54	ARG
1	A	62	ILE
1	A	70	LYS
1	A	89	ASN
1	A	132	GLN
1	A	134	ARG

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Mol	Chain	Res	Type
1	A	136	SER
1	A	141	VAL
1	A	143	VAL
1	A	152	LYS
1	A	161	LYS
1	A	185	GLU
1	A	197	LYS
1	A	205	GLU
1	A	214	VAL
1	A	220	ARG
1	B	27	LEU
1	B	55	LEU
1	B	89	ASN
1	B	107	GLU
1	B	108	ILE
1	B	134	ARG
1	B	135	GLU
1	B	136	SER
1	B	141	VAL
1	B	176	LYS
1	B	189	LEU
1	B	214	VAL
1	B	217	LYS
1	B	226	ARG
1	B	238	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	225	GLN
1	B	34	ASN
1	B	224	GLN

5.3.3 RNA ⓘ

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](#)

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.