



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:17 PM UTC

PDB ID : 1R2S / pdb_00001r2s
Title : CRYSTAL STRUCTURE OF RABBIT MUSCLE TRIOSEPHOSPHATE ISOMERASE
Authors : Aparicio, R.; Ferreira, S.T.; Polikarpov, I.
Deposited on : 2003-09-29
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

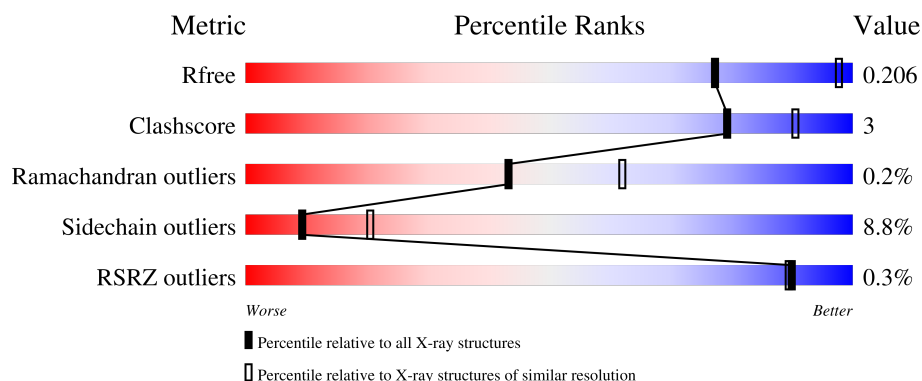
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	248	88% 10% .
1	B	248	88% 10% ..
1	C	248	86% 12% ..
1	D	248	84% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7621 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	247	Total	C	N	O	S	0	0	0
			1869	1182	324	356	7			
1	B	246	Total	C	N	O	S	0	0	0
			1862	1177	323	355	7			
1	C	247	Total	C	N	O	S	0	3	0
			1881	1189	325	360	7			
1	D	247	Total	C	N	O	S	3	1	0
			1874	1185	325	357	7			

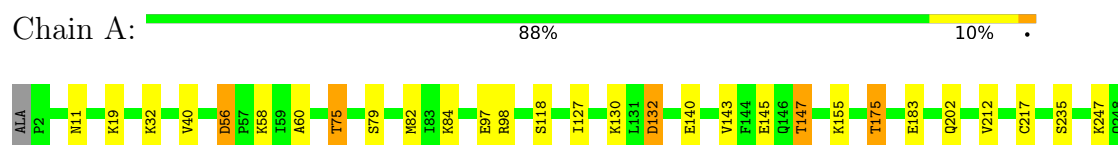
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		
2	B	34	Total	O	0	0
			34	34		
2	C	35	Total	O	0	0
			35	35		
2	D	36	Total	O	0	0
			36	36		

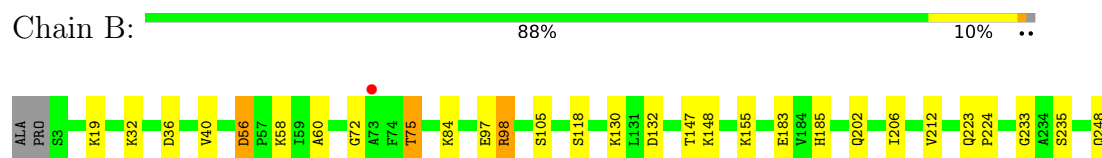
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

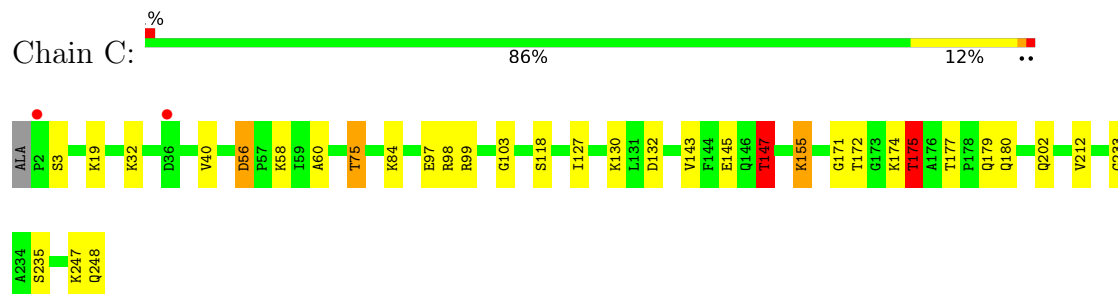
- Molecule 1: Triosephosphate isomerase



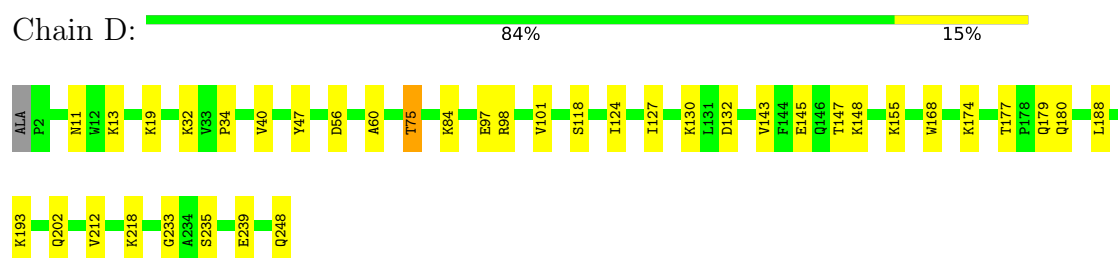
- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.23Å 80.29Å 174.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.50 – 2.85 13.50 – 2.85	Depositor EDS
% Data completeness (in resolution range)	81.6 (13.50-2.85) 80.7 (13.50-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.172 , 0.212 0.167 , 0.206	Depositor DCC
R_{free} test set	1026 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7621	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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](#)

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	0.66	0/1904	1.02	2/2577 (0.1%)
1	B	0.68	0/1896	1.00	2/2566 (0.1%)
1	C	0.85	1/1928 (0.1%)	1.06	5/2609 (0.2%)
1	D	0.86	3/1913 (0.2%)	1.06	2/2589 (0.1%)
All	All	0.77	4/7641 (0.1%)	1.04	11/10341 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	174	LYS	C-O	-7.09	1.15	1.23
1	D	124	ILE	CA-CB	6.54	1.61	1.53
1	C	175	THR	CA-C	5.92	1.60	1.52
1	D	218	LYS	CG-CD	5.65	1.69	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	THR	N-CA-C	7.11	120.30	110.35
1	C	174	LYS	N-CA-C	6.71	119.00	110.61
1	C	175	THR	N-CA-C	5.80	123.17	110.80
1	C	233	GLY	N-CA-C	5.55	119.61	112.83
1	C	172	THR	N-CA-C	-5.47	107.25	114.31
1	C	147	THR	OG1-CB-CG2	-5.36	98.57	109.30
1	D	233	GLY	N-CA-C	5.28	119.28	112.83
1	B	233	GLY	N-CA-C	5.28	120.29	113.27
1	B	72	GLY	N-CA-C	5.04	117.54	110.38
1	A	217	CYS	N-CA-C	5.01	116.74	111.28
1	D	47	TYR	N-CA-C	5.01	119.34	112.88

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	1869	0	1882	13	0
1	B	1862	0	1874	12	0
1	C	1881	0	1889	12	2
1	D	1874	0	1886	17	0
2	A	30	0	0	1	0
2	B	34	0	0	1	0
2	C	35	0	0	0	0
2	D	36	0	0	1	0
All	All	7621	0	7531	40	2

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 3.

All (40) 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:C:97:GLU:OE1	1:D:75:THR:HG23	1.82	0.80
1:A:75:THR:HG23	1:B:97:GLU:OE1	1.86	0.76
1:C:75:THR:HG23	1:D:97:GLU:OE1	1.88	0.73
1:D:179[B]:GLN:HG2	2:D:279:HOH:O	1.92	0.69
1:A:75:THR:CG2	1:B:97:GLU:OE1	2.43	0.67
1:D:40:VAL:HG22	1:D:60:ALA:HB3	1.79	0.65
1:A:97:GLU:OE1	1:B:75:THR:HG23	2.00	0.62
1:C:97:GLU:OE1	1:D:75:THR:CG2	2.50	0.58
1:C:143:VAL:O	1:C:147:THR:OG1	2.21	0.58
1:A:97:GLU:OE1	1:B:75:THR:CG2	2.57	0.53
1:D:34:PRO:HB3	1:D:248:GLN:NE2	2.23	0.53
1:C:40:VAL:HG22	1:C:60:ALA:HB3	1.90	0.52
1:A:127:ILE:HD13	1:A:147:THR:HG23	1.93	0.51
1:C:75:THR:CG2	1:D:97:GLU:OE1	2.58	0.50
1:A:40:VAL:HG22	1:A:60:ALA:HB3	1.95	0.48
1:D:143:VAL:O	1:D:147:THR:HG23	2.13	0.48
1:D:127:ILE:HD13	1:D:147:THR:CG2	2.44	0.47
1:C:177:THR:OG1	1:C:180:GLN:HG3	2.14	0.47
1:A:75:THR:O	1:B:98:ARG:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:THR:HG21	1:D:11:ASN:HD21	1.78	0.47
1:C:75:THR:HG22	1:D:13:LYS:HG2	1.97	0.47
1:A:140:GLU:HB2	2:A:263:HOH:O	2.15	0.46
1:B:40:VAL:HG22	1:B:60:ALA:HB3	1.98	0.46
1:A:143:VAL:O	1:A:147:THR:OG1	2.32	0.45
1:A:132:ASP:HB2	1:D:193:LYS:HE2	1.99	0.45
1:C:56:ASP:HB3	1:C:58:LYS:HG2	1.98	0.45
1:A:79:SER:OG	1:A:82:MET:HG3	2.18	0.44
1:B:56:ASP:HB3	1:B:58:LYS:HG2	1.99	0.44
1:B:185:HIS:CE1	1:B:206:ILE:HG22	2.53	0.44
1:D:177:THR:OG1	1:D:180:GLN:HG3	2.19	0.43
1:D:147:THR:HG21	1:D:188:LEU:HD22	2.01	0.42
1:C:99:ARG:O	1:C:103:GLY:HA2	2.18	0.42
1:D:168:TRP:CD1	1:D:168:TRP:H	2.38	0.41
1:A:11:ASN:HD21	1:B:75:THR:HG21	1.86	0.41
1:A:56:ASP:HB3	1:A:58:LYS:HG2	2.03	0.41
1:B:105:SER:HB2	1:D:145:GLU:OE2	2.21	0.41
1:C:127:ILE:HD13	1:C:147:THR:HG23	2.02	0.40
1:D:97:GLU:O	1:D:101:VAL:HB	2.20	0.40
1:B:36:ASP:N	2:B:268:HOH:O	2.31	0.40
1:B:223:GLN:HA	1:B:224:PRO:HD3	1.95	0.40

All (2) 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:C:155:LYS:NZ	1:C:171:GLY:O[4_565]	1.77	0.43
1:C:155:LYS:CE	1:C:171:GLY:O[4_565]	2.19	0.01

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	245/248 (99%)	235 (96%)	10 (4%)	0	100	100
1	B	244/248 (98%)	236 (97%)	8 (3%)	0	100	100
1	C	248/248 (100%)	235 (95%)	12 (5%)	1 (0%)	30	48
1	D	246/248 (99%)	238 (97%)	7 (3%)	1 (0%)	30	48
All	All	983/992 (99%)	944 (96%)	37 (4%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	175	THR
1	D	239	GLU

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	197/197 (100%)	179 (91%)	18 (9%)	9	19
1	B	196/197 (100%)	179 (91%)	17 (9%)	9	21
1	C	200/197 (102%)	179 (90%)	21 (10%)	6	13
1	D	198/197 (100%)	184 (93%)	14 (7%)	13	28
All	All	791/788 (100%)	721 (91%)	70 (9%)	9	20

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	32	LYS
1	A	56	ASP
1	A	75	THR
1	A	84	LYS
1	A	98	ARG
1	A	118	SER
1	A	130	LYS
1	A	132	ASP

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Mol	Chain	Res	Type
1	A	145	GLU
1	A	147	THR
1	A	155	LYS
1	A	175	THR
1	A	183	GLU
1	A	202	GLN
1	A	212	VAL
1	A	235	SER
1	A	247	LYS
1	B	19	LYS
1	B	32	LYS
1	B	56	ASP
1	B	75	THR
1	B	84	LYS
1	B	98	ARG
1	B	118	SER
1	B	130	LYS
1	B	132	ASP
1	B	147	THR
1	B	148	LYS
1	B	155	LYS
1	B	183	GLU
1	B	202	GLN
1	B	212	VAL
1	B	235	SER
1	B	248	GLN
1	C	3	SER
1	C	19	LYS
1	C	32	LYS
1	C	56	ASP
1	C	75	THR
1	C	84	LYS
1	C	98	ARG
1	C	118	SER
1	C	130	LYS
1	C	132	ASP
1	C	145	GLU
1	C	147	THR
1	C	155	LYS
1	C	175	THR
1	C	179[A]	GLN
1	C	179[B]	GLN

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Mol	Chain	Res	Type
1	C	202	GLN
1	C	212	VAL
1	C	235	SER
1	C	247	LYS
1	C	248	GLN
1	D	19	LYS
1	D	32	LYS
1	D	56	ASP
1	D	75	THR
1	D	84	LYS
1	D	98	ARG
1	D	118	SER
1	D	130	LYS
1	D	132	ASP
1	D	148	LYS
1	D	155	LYS
1	D	202	GLN
1	D	212	VAL
1	D	235	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	111	GLN
1	A	179	GLN
1	A	245	ASN
1	B	100	HIS
1	B	111	GLN
1	B	179	GLN
1	B	223	GLN
1	B	245	ASN
1	C	111	GLN
1	D	111	GLN
1	D	153	ASN
1	D	202	GLN
1	D	248	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	247/248 (99%)	-0.33	0 100 100	13, 19, 34, 43	0
1	B	246/248 (99%)	-0.36	1 (0%) 88 87	13, 19, 34, 43	0
1	C	247/248 (99%)	-0.68	2 (0%) 82 78	12, 19, 35, 43	3 (1%)
1	D	247/248 (99%)	-0.73	0 100 100	12, 19, 35, 43	2 (0%)
All	All	987/992 (99%)	-0.53	3 (0%) 90 89	12, 19, 35, 43	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	2.4
1	C	2	PRO	2.1
1	C	36	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.