



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 05:22 pm GMT

PDB ID : 1R2S
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.

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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

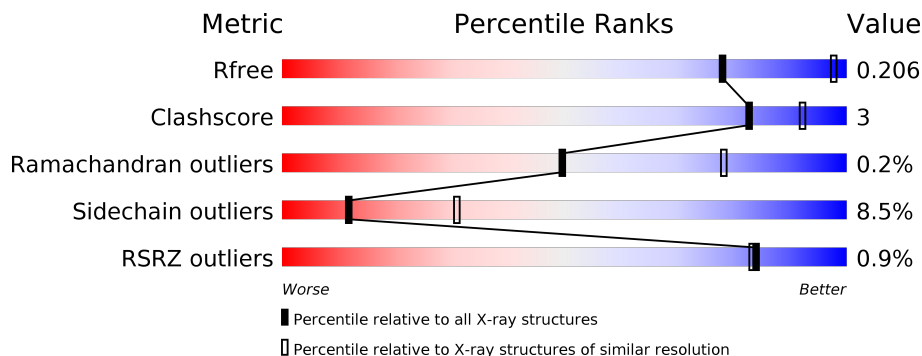
1 Overall quality at a glance

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}	111664	2715 (2.90-2.82)
Clashscore	122126	2976 (2.90-2.82)
Ramachandran outliers	120053	2913 (2.90-2.82)
Sidechain outliers	120020	2916 (2.90-2.82)
RSRZ outliers	108989	2654 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	248	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	248	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	248	<div> <div></div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>

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		

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 13.49 – 2.85	Depositor EDS
% Data completeness (in resolution range)	81.6 (13.50-2.85) 81.6 (13.49-2.85)	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)	0.27 , 39.6	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	0.95	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

5.1 Standard geometry

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	0.51	0/1904	0.76	5/2577 (0.2%)
1	B	0.54	0/1896	0.75	5/2566 (0.2%)
1	C	0.68	0/1928	0.81	7/2609 (0.3%)
1	D	0.67	0/1913	0.82	3/2589 (0.1%)
All	All	0.60	0/7641	0.79	20/10341 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	132	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	225	ASP	CB-CG-OD2	6.26	123.93	118.30
1	C	132	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	198	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	56	ASP	CB-CG-OD2	5.76	123.49	118.30
1	D	85	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	165	GLU	OE1-CD-OE2	-5.70	116.45	123.30
1	C	56	ASP	CB-CG-OD2	5.64	123.37	118.30
1	D	132	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	85	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	36	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	106	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	227	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	225	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	36	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	85	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	198	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	198	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	56	ASP	CB-CG-OD2	5.18	122.97	118.30

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	14	0
1	B	1862	0	1874	12	0
1	C	1881	0	1889	12	2
1	D	1874	0	1886	16	0
2	A	30	0	0	2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:130:LYS:NZ	2:A:275:HOH:O	2.21	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:223:GLN:HA	1:B:224:PRO:HD3	1.95	0.40
1:B:36:ASP:N	2:B:268:HOH:O	2.31	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%)	36	66
1	D	246/248 (99%)	238 (97%)	7 (3%)	1 (0%)	36	66
All	All	983/992 (99%)	944 (96%)	37 (4%)	2 (0%)	49	78

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%)	10	27
1	B	196/197 (100%)	180 (92%)	16 (8%)	12	32
1	C	200/197 (102%)	179 (90%)	21 (10%)	7	20
1	D	198/197 (100%)	185 (93%)	13 (7%)	18	43
All	All	791/788 (100%)	723 (91%)	68 (9%)	12	30

All (68) 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

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Mol	Chain	Res	Type
1	A	118	SER
1	A	130	LYS
1	A	132	ASP
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	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

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Mol	Chain	Res	Type
1	C	179[A]	GLN
1	C	179[B]	GLN
1	C	202	GLN
1	C	212	VAL
1	C	235	SER
1	C	247	LYS
1	C	248	GLN
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	179	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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 [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%)	-0.48	4 (1%) 72 70	13, 19, 34, 43	0
1	B	246/248 (99%)	-0.61	2 (0%) 86 85	13, 19, 34, 43	0
1	C	247/248 (99%)	-0.79	2 (0%) 86 85	12, 19, 35, 43	0
1	D	247/248 (99%)	-0.82	1 (0%) 92 92	13, 19, 35, 43	1 (0%)
All	All	987/992 (99%)	-0.68	9 (0%) 84 83	12, 19, 35, 43	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	PRO	4.6
1	A	2	PRO	4.5
1	D	2	PRO	3.4
1	A	36	ASP	2.6
1	C	36	ASP	2.4
1	A	3	SER	2.3
1	B	173	GLY	2.3
1	B	202	GLN	2.1
1	A	248	GLN	2.1

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 carbohydrates 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.