



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 08:47 AM UTC

PDB ID : 1MSS / pdb_00001mss
Title : LARGE SCALE STRUCTURAL REARRANGEMENTS OF THE FRONT LOOPS IN MONOMERISED TRIOSEPHOSPHATE ISOMERASE, AS DEDUCED FROM THE COMPARISON OF THE STRUCTURAL PROPERTIES OF MONOTIM AND ITS POINT MUTATION VARIANT MONOSS
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Deposited on : 1994-07-27
Resolution : 2.40 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 ⓘ 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

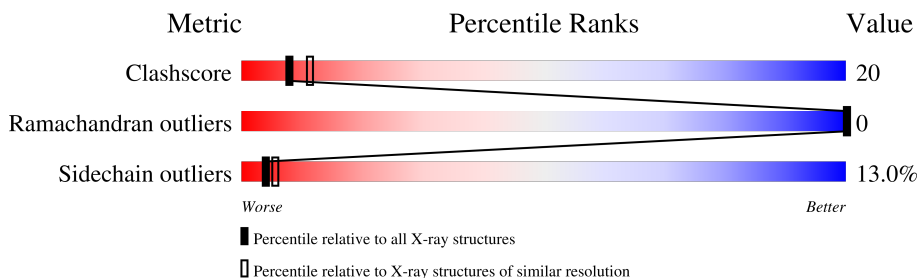
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	243	69% 24% 7%
1	B	243	61% 36% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3698 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	242	Total	C	N	O	S	0	0	0
			1821	1149	324	344	4			
1	B	242	Total	C	N	O	S	0	0	0
			1821	1149	324	344	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	SER	PHE	engineered mutation	UNP P04789
A	46	SER	VAL	engineered mutation	UNP P04789
A	68	GLY	ILE	engineered mutation	UNP P04789
A	69	ASN	ALA	engineered mutation	UNP P04789
A	70	ALA	LYS	engineered mutation	UNP P04789
A	71	ASP	SER	engineered mutation	UNP P04789
A	72	ALA	GLY	engineered mutation	UNP P04789
A	?	-	ALA	deletion	UNP P04789
A	?	-	PHE	deletion	UNP P04789
A	?	-	THR	deletion	UNP P04789
A	?	-	GLU	deletion	UNP P04789
A	?	-	VAL	deletion	UNP P04789
A	?	-	SER	deletion	UNP P04789
A	81	ALA	PRO	engineered mutation	UNP P04789
A	82	SER	ILE	engineered mutation	UNP P04789
B	45	SER	PHE	engineered mutation	UNP P04789
B	46	SER	VAL	engineered mutation	UNP P04789
B	68	GLY	ILE	engineered mutation	UNP P04789
B	69	ASN	ALA	engineered mutation	UNP P04789
B	70	ALA	LYS	engineered mutation	UNP P04789
B	71	ASP	SER	engineered mutation	UNP P04789
B	72	ALA	GLY	engineered mutation	UNP P04789
B	?	-	ALA	deletion	UNP P04789
B	?	-	PHE	deletion	UNP P04789
B	?	-	THR	deletion	UNP P04789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P04789
B	?	-	VAL	deletion	UNP P04789
B	?	-	SER	deletion	UNP P04789
B	81	ALA	PRO	engineered mutation	UNP P04789
B	82	SER	ILE	engineered mutation	UNP P04789

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	29	Total O 29 29	0	0

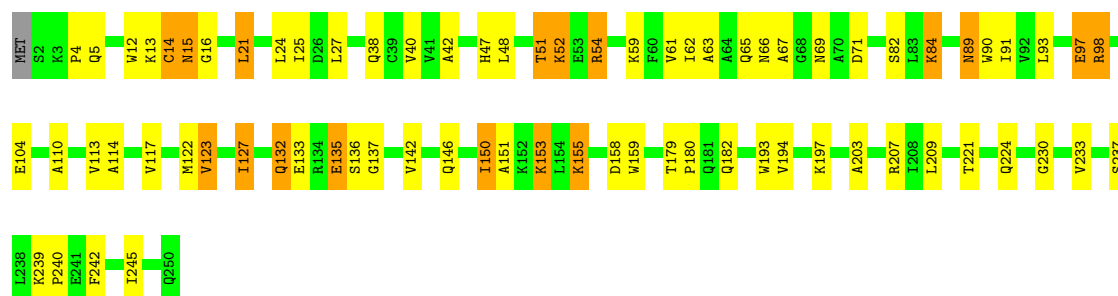
3 Residue-property plots

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.

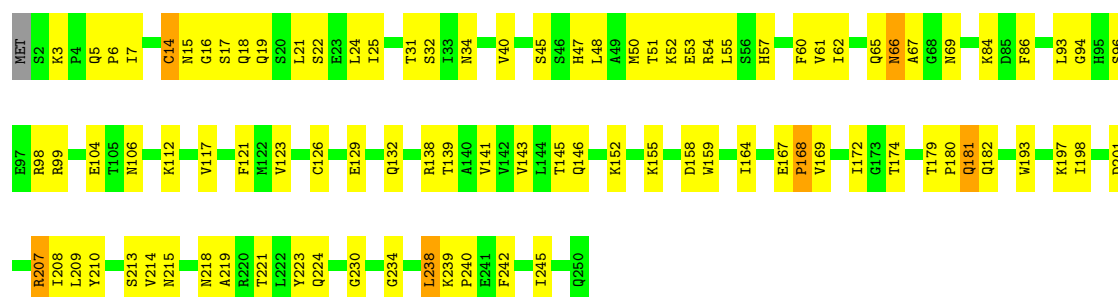
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain A: 



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.57Å 46.58Å 66.65Å 94.47° 69.82° 75.83°	Depositor
Resolution (Å)	24.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (24.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3698	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	1.01	2/1852 (0.1%)	0.94	3/2511 (0.1%)
1	B	0.95	0/1852	0.94	4/2511 (0.2%)
All	All	0.98	2/3704 (0.1%)	0.94	7/5022 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	CYS	C-O	9.11	1.35	1.24
1	A	15	ASN	C-N	-5.21	1.25	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	PRO	N-CA-CB	6.29	106.82	102.35
1	B	14	CYS	N-CA-C	6.12	119.59	111.75
1	A	15	ASN	CA-C-N	5.86	125.63	121.65
1	A	15	ASN	C-N-CA	5.86	125.63	121.65
1	B	66	ASN	N-CA-C	5.62	117.08	108.42

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	1821	0	1840	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1821	0	1840	79	0
2	A	27	0	0	1	0
2	B	29	0	0	0	0
All	All	3698	0	3680	144	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 20.

The worst 5 of 144 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:110:ALA:HB1	1:A:153:LYS:HD2	1.54	0.89
1:B:179:THR:H	1:B:182:GLN:NE2	1.77	0.83
1:B:179:THR:H	1:B:182:GLN:HE21	1.26	0.82
1:B:66:ASN:HD21	1:B:98:ARG:HD2	1.44	0.81
1:A:84:LYS:HE2	1:A:89:ASN:HB3	1.64	0.78

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	B	16/243 (7%)	16 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	136/190 (72%)	118 (87%)	18 (13%)	4	5
1	B	56/190 (30%)	49 (88%)	7 (12%)	4	6
All	All	192/380 (50%)	167 (87%)	25 (13%)	4	5

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	155	LYS
1	B	238	LEU
1	A	153	LYS
1	B	181	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	B	181	GLN
1	B	182	GLN
1	A	65	GLN
1	A	34	ASN

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 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.