

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 12:51 PM EDT

PDB ID	:	6NLH
Title	:	Structure of human triose phosphate isomerase R189A
Authors	:	Richards, K.R.; Roland, B.P.; Palladino, M.J.; VanDemark, A.P.
Deposited on		
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 2.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29986 atoms, of which 14602 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.

Mol	Chain	Residues			Atoms	5			ZeroOcc	AltConf	Trace
1	1 A	0.4.4	Total	С	Н	Ν	0	S	0	0	0
		244	3671	1161	1838	314	351	$\overline{7}$	0	0	0
1	Е	238	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0
	Ľ	230	3589	1137	1795	307	343	7	0	0	0
1	В	245	Total	С	Н	Ν	0	S	0	0	0
	D	240	3695	1167	1851	318	352	$\overline{7}$	0	0	0
1	С	239	Total	С	Н	Ν	0	S	0	0	0
	U		3612	1143	1807	311	344	7			
1	D	245	Total	С	Н	Ν	0	S	0	0	0
	D	240	3695	1167	1851	318	352	7			
1	F	239	Total	С	Н	Ν	0	S	0	0	0
	Г	239	3612	1143	1807	311	344	7	0	0	0
1	G	245	Total	С	Н	Ν	0	S	0	0	0
	I G	245	3695	1167	1851	318	352	7		U	U
1	1 H	220	Total	С	Н	Ν	0	S	0	0	0
	11	239	3603	1141	1802	308	345	7			U

• Molecule 1 is a protein called Triosephosphate isomerase.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	189	ALA	ARG	engineered mutation	UNP P60174
Е	189	ALA	ARG	engineered mutation	UNP P60174
В	189	ALA	ARG	engineered mutation	UNP P60174
С	189	ALA	ARG	engineered mutation	UNP P60174
D	189	ALA	ARG	engineered mutation	UNP P60174
F	189	ALA	ARG	engineered mutation	UNP P60174
G	189	ALA	ARG	engineered mutation	UNP P60174
Н	189	ALA	ARG	engineered mutation	UNP P60174

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).



6NLH
OT CLITT

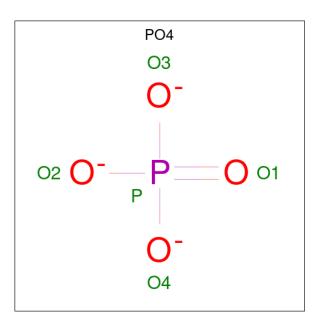
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total Na 3 3	0	0
2	Е	1	Total Na 1 1	0	0
2	В	4	Total Na 4 4	0	0
2	С	3	Total Na 3 3	0	0
2	D	3	Total Na 3 3	0	0
2	F	2	Total Na 2 2	0	0
2	G	2	Total Na 2 2	0	0
2	Н	2	Total Na 2 2	0	0

• Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Е	1	Total Br 1 1	0	0
3	С	1	Total Br 1 1	0	0
3	F	1	Total Br 1 1	0	0
3	Н	1	Total Br 1 1	0	0

• Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
4	Н	1	TotalOP541	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	118	Total O 118 118	0	0
5	Е	79	Total O 79 79	0	0
5	В	114	Total O 114 114	0	0
5	С	86	Total O 86 86	0	0
5	D	97	Total O 97 97	0	0
5	F	85	Total O 85 85	0	0
5	G	106	Total O 106 106	0	0
5	Н	85	Total O 85 85	0	0



MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	65.14Å 7 3.66 Å 9 2.84 Å	Depositor
a, b, c, α , β , γ	90.03° 90.03° 90.00°	Depositor
Resolution (Å)	19.66 - 2.20	Depositor
% Data completeness	95.9 (19.66-2.20)	Depositor
(in resolution range)		Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.54 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.174 , 0.216	Depositor
Wilson B-factor $(Å^2)$	21.8	Xtriage
Anisotropy	0.614	Xtriage
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
	0.478 for h,-k,-l	
Estimated twinning fraction	0.477 for -h,k,-l	Xtriage
	0.478 for -h,-k,l	
Total number of atoms	29986	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 24 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



			-				- · ·	<i>,</i>		
Mol	Mal Trees	Chain	Res	Link	B	ond leng	$_{ m gths}$	Bond angles		
Mol Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	PO4	Н	304	-	4,4,4	0.84	0	$6,\!6,\!6$	0.49	0
4	PO4	С	305	-	4,4,4	0.67	0	$6,\!6,\!6$	0.47	0
4	PO4	Е	303	-	4,4,4	0.87	0	$6,\!6,\!6$	0.40	0
4	PO4	F	304	-	4,4,4	0.71	0	$6,\!6,\!6$	0.61	0

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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

