

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 27, 2023 – 09:22 PM EDT

PDB ID	:	3HQC
Title	:	Crystal structure of Phosphotyrosine-binding domain from the Human Tensin-
		like C1 domain-containing phosphatase (TENC1)
Authors	:	Sampathkumar, P.; Romero, R.; Wasserman, S.; Do, J.; Dickey, M.; Bain, K.;
		Gheyi, T.; Klemke, R.; Atwell, S.; Sauder, J.M.; Burley, S.K.; New York SGX
		Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-06-05
Resolution	:	1.80 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:

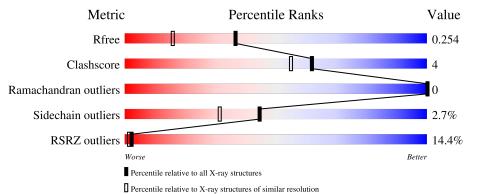
Xtriage (Phenix) EDS Percentile statistics Refmac CCP4	: : : :	<ul> <li>1.8.5 (274361), CSD as541be (2020)</li> <li>1.13</li> <li>2.35</li> <li>20191225.v01 (using entries in the PDB archive December 25th 2019)</li> <li>5.8.0158</li> <li>7.0.044 (Gargrove)</li> </ul>
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5950(1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	٨	157	13%						
1	А	157	80%	8% •	11%				



#### 3HQC

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1229 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 Tensin-like C1 domain-containing phosphatase.

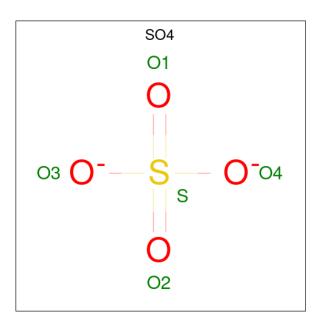
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	140	Total 1115	С 712	N 184	0 214	$\frac{S}{4}$	${ m Se} 1$	0	16	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1261	MSE	-	expression tag	UNP Q63HR2
А	1262	SER	-	expression tag	UNP Q63HR2
A	1263	LEU	-	expression tag	UNP Q63HR2
А	1404	MSE	LEU	engineered mutation	UNP Q63HR2
A	1410	GLU	-	expression tag	UNP Q63HR2
A	1411	GLY	-	expression tag	UNP Q63HR2
А	1412	HIS	-	expression tag	UNP Q63HR2
A	1413	HIS	-	expression tag	UNP Q63HR2
А	1414	HIS	-	expression tag	UNP Q63HR2
А	1415	HIS	-	expression tag	UNP Q63HR2
А	1416	HIS	-	expression tag	UNP Q63HR2
А	1417	HIS	-	expression tag	UNP Q63HR2

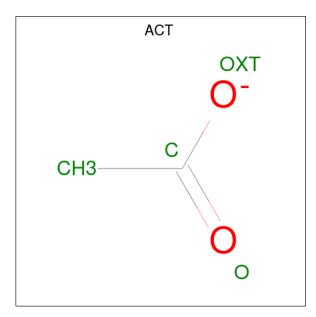
• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

 $\bullet\,$  Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C\_2H\_3O\_2).



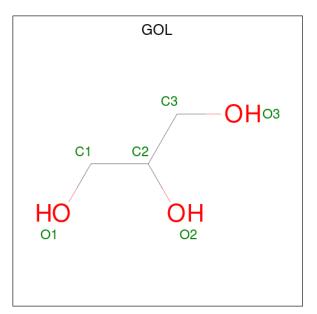
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	А	1	Total 4	${ m C} { m 2}$	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 4	${ m C} 2$	O 2	0	0



Mol	Chain	Residues	Aton	ıs	ZeroOcc	AltConf
4	А	1	Total C 6 3	CO 33	0	0

• Molecule 5 is water.

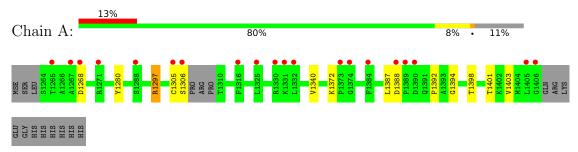
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	79	Total O 85 85	0	6



# 3 Residue-property plots (i)

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: Tensin-like C1 domain-containing phosphatase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
$\begin{array}{c} \text{Cell constants} \\ \text{a, b, c, } \alpha, \beta, \gamma \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	$26.16 - 1.80 \ 26.16 - 1.80$	Depositor EDS
% Data completeness	$100.0 \ (26.16-1.80)$	Depositor
(in resolution range)	$99.9\ (26.16-1.80)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.12	Depositor
$< I/\sigma(I) > 1$	$10.55 (at 1.80 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.212 , $0.242$	Depositor
$R, R_{free}$	0.227 , $0.254$	DCC
$R_{free}$ test set	1182 reflections $(5.13\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	24.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40 , $56.6$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.54, < L^2>=0.38$	Xtriage
Estimated twinning fraction	0.007 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1229	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SO4, GOL

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.65	0/1190	0.74	2/1627~(0.1%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	1297	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	А	1297	ARG	NE-CZ-NH2	5.24	122.92	120.30

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	А	1115	0	1117	10	0
2	А	15	0	0	1	0
3	А	8	0	6	0	0
4	А	6	0	8	2	0
5	А	85	0	0	3	0
All	All	1229	0	1131	10	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 4.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:PRO:HB2	4:A:1420:GOL:H2	1.41	1.02
1:A:1392:PRO:HB2	4:A:1420:GOL:C2	2.23	0.67
1:A:1394:GLY:O	1:A:1398[B]:THR:HG23	2.03	0.58
1:A:1401[A]:THR:HG23	5:A:60:HOH:O	2.03	0.58
1:A:1340[A]:VAL:HG21	1:A:1403:VAL:O	2.07	0.54
1:A:1372[B]:LYS:NZ	2:A:3:SO4:O1	2.44	0.48
1:A:1387:LEU:HD23	5:A:19:HOH:O	2.17	0.44
1:A:1305[A]:CYS:SG	1:A:1306:SER:N	2.91	0.43
1:A:1297:ARG:NH1	5:A:34:HOH:O	2.53	0.42

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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		
1	А	153/157~(98%)	151 (99%)	2(1%)	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	А	129/131~(98%)	125~(97%)	4(3%)	40 25	



All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1268	ASP
1	А	1280	TYR
1	А	1388[A]	ASP
1	А	1388[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	1357	ASN

#### 5.3.3 RNA (i)

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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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 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).

Mol	ol Type Chain Res Lin		Link	B	ond leng	gths	Bond angles			
NIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	SO4	А	3	-	4,4,4	0.23	0	$6,\!6,\!6$	0.34	0
3	ACT	А	1419	-	3,3,3	0.68	0	$3,\!3,\!3$	1.28	0
3	ACT	А	1418	-	3,3,3	0.80	0	$3,\!3,\!3$	1.57	1 (33%)



Mal	Mol Type Chai		Chain Res		B	Bond lengths			Bond angles		
IVIOI	туре	Unam	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	SO4	А	1	-	4,4,4	0.36	0	$6,\!6,\!6$	0.19	0	
2	SO4	А	2	-	$4,\!4,\!4$	0.18	0	$6,\!6,\!6$	0.23	0	
4	GOL	А	1420	-	$5,\!5,\!5$	0.73	0	$5,\!5,\!5$	0.38	0	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	А	1420	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	1418	ACT	OXT-C-O	-2.09	114.35	122.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	1420	GOL	C1-C2-C3-O3
4	А	1420	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	3	SO4	1	0
4	А	1420	GOL	2	0

## 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,  $95^{th}$  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	А	139/157~(88%)	0.74	20 (14%)	2	1	22, 29, 47, 57	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1405	LEU	7.6
1	А	1305[A]	CYS	5.3
1	А	1331	LYS	4.5
1	А	1271	ARG	4.2
1	А	1330	ARG	3.8
1	А	1268	ASP	3.8
1	А	1389	PRO	3.4
1	А	1306	SER	3.4
1	А	1267	ALA	3.2
1	А	1373	PRO	2.8
1	А	1332	LEU	2.7
1	А	1316	PHE	2.6
1	А	1325	LEU	2.6
1	А	1406	GLY	2.5
1	А	1288	SER	2.5
1	А	1374	GLY	2.4
1	А	1388[A]	ASP	2.4
1	А	1265	THR	2.3
1	А	1384	PHE	2.3
1	А	1390	ASP	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 monosaccharides in this entry.

### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	ACT	А	1418	4/4	0.71	0.20	43,44,44,45	0
4	GOL	А	1420	6/6	0.73	0.30	34,37,40,43	6
2	SO4	А	2	5/5	0.74	0.20	77,78,79,79	0
2	SO4	А	3	5/5	0.91	0.15	$55,\!57,\!58,\!58$	0
3	ACT	А	1419	4/4	0.93	0.11	52,52,52,52	0
2	SO4	А	1	5/5	0.99	0.09	32,33,34,34	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

