

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

Dec 4, 2023 – 10:54 am GMT

PDB ID : 2VUH

Title : Crystal structure of the D55E mutant of the HupR receiver domain

Authors: Davies, K.M.; Lowe, E.D.; Venien-Bryan, C.; Johnson, L.N.

Deposited on : 2008-05-26

Resolution : 2.50 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 Xtriage (Phenix) : 1.13

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.36

 ${\tt PERCENTILES\ INFOmissing INFO}$ 



## 1 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1088 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 HYDROGENASE TRANSCRIPTIONAL REGULATORY PROTEIN HUPR1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	В	135	Total 1062	C 669	N 184	O 202	S 7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	55	GLU	ASP	engineered mutation	UNP P26408

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	26	Total O 26 26	0	0

SEQUENCE-PLOTS INFOmissingINFO



# 2 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 32 1 2	Depositor	
Cell constants	81.78Å 81.78Å 61.05Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	24.52 - 2.50	Depositor	
Resolution (A)	24.52 - 2.50	EDS	
% Data completeness	99.8 (24.52-2.50)	Depositor	
(in resolution range)	99.5 (24.52-2.50)	EDS	
$R_{merge}$	0.06	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	5.53  (at  2.50Å)	Xtriage	
Refinement program	REFMAC 5.2.0019	Depositor	
D.D.	0.221 , 0.247	Depositor	
$R, R_{free}$	0.222 , $0.252$	DCC	
$R_{free}$ test set	395 reflections $(4.83\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage	
Anisotropy	0.194	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 36.9	EDS	
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage	
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage	
$F_o, F_c$ correlation	0.94	EDS	
Total number of atoms	1088	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  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.

# 3 Model quality (i)

### 3.1 Standard geometry (i)

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

### 3.2 Too-close contacts (i)

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

#### 3.3 Torsion angles (i)

#### 3.3.1 Protein backbone (i)

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

#### 3.3.2 Protein sidechains (i)

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

#### 3.3.3 RNA (i)

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

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

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

### 3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 3.6 Ligand geometry (i)

There are no ligands in this entry.

### 3.7 Other polymers (i)

There are no such residues in this entry.



# 3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 4 Fit of model and data (i)

### 4.1 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	В	135/139 (97%)	0.28	11 (8%) 12 12	34, 51, 76, 89	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	80	ILE	3.7
1	В	86	THR	3.2
1	В	53	ILE	3.2
1	В	93	ALA	2.9
1	В	52	ILE	2.8
1	В	5	ALA	2.6
1	В	6	PRO	2.3
1	В	138	ARG	2.1
1	В	89	ALA	2.1
1	В	85	TYR	2.1
1	В	51	VAL	2.0

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

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

## 4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 4.4 Ligands (i)

There are no ligands in this entry.



# 4.5 Other polymers (i)

There are no such residues in this entry.

