

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 06:43 PM EDT

PDB ID : 6TYY

Title : Hedgehog autoprocessing mutant D46H Authors : Li, H.; Li, Z.; Wang, C.; Callahan, B.P.

Deposited on : 2019-08-09

Resolution : 1.36 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 : 2.35.1

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

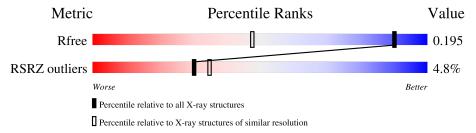
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.36 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}(\mathring{\rm A})) \end{array}$				
R_{free}	130704	1509 (1.38-1.34)				
RSRZ outliers	127900	1487 (1.38-1.34)				

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



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1309 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 Protein hedgehog.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total 1148	C 718	N 202	O 223	S 5	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Chain Residue Modelled		Actual	Comment	Reference
A	303	HIS	ASP	engineered mutation	UNP Q02936

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	161	Total O 161 161	0	0

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3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	78.38Å 78.38Å 37.35Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.66 - 1.36	Depositor
Resolution (A)	25.66 - 1.36	EDS
% Data completeness	99.5 (25.66-1.36)	Depositor
(in resolution range)	99.5 (25.66-1.36)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.37 (at 1.36Å)	Xtriage
Refinement program	PHENIX	Depositor
D D	0.171 , 0.195	Depositor
R, R_{free}	0.171 , 0.195	DCC
R_{free} test set	1994 reflections (7.08%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39 , 40.6	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1309	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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)

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4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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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)

1 non-standard protein/DNA/RNA residue is 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	Type	Chain	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI			onain Kes	S LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	CSD	A	258	1	3,7,8	0.90	0	1,8,10	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	258	1	-	0/2/6/8	-

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.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

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)

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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q < 0.9
1	A	145/146 (99%)	0.23	7 (4%) 30 35	10, 15, 32, 55	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	GLN	3.8
1	A	337	GLU	3.7
1	A	271	VAL	2.7
1	A	340	LYS	2.6
1	A	269	SER	2.5
1	A	403	VAL	2.2
1	A	290	ASN	2.0

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

Mo	l Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	CSD	A	258	8/9	0.96	0.09	11,13,25,31	0

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

There are no ligands in this entry.



5.5 Other polymers (i)

There are no such residues in this entry.

