



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 04:09 PM JST

PDB ID : 8HFW  
Title : The crystal structure of alpha/beta fold hydrolase  
Authors : Lu, H.; Xu, Y.  
Deposited on : 2022-11-12  
Resolution : 1.66 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.36

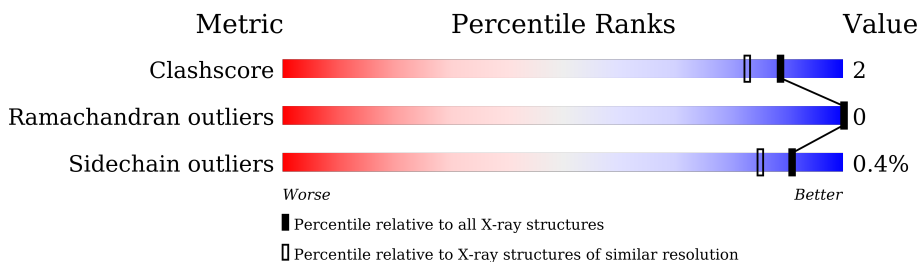
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.66 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	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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  $\geq 3$ , 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	304	 91% 6%
1	B	304	 87% 5% 8%
1	C	304	 88% 8%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 6318 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 Alpha/beta fold hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2077	1322	366	379	10	0	2	1
1	B	280	1975	1257	341	367	10	0	2	1
1	C	281	1937	1228	342	358	9	0	1	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	VAL	ILE	conflict	UNP A0A4V2WUI0
A	8	ALA	PRO	conflict	UNP A0A4V2WUI0
A	9	ALA	GLN	conflict	UNP A0A4V2WUI0
A	10	PRO	GLN	conflict	UNP A0A4V2WUI0
A	11	SER	ALA	conflict	UNP A0A4V2WUI0
A	38	GLU	ALA	conflict	UNP A0A4V2WUI0
A	92	GLU	GLN	conflict	UNP A0A4V2WUI0
A	102	HIS	ARG	conflict	UNP A0A4V2WUI0
A	160	ALA	GLY	conflict	UNP A0A4V2WUI0
A	161	PRO	ALA	conflict	UNP A0A4V2WUI0
A	186	ALA	ASP	conflict	UNP A0A4V2WUI0
A	187	LEU	THR	conflict	UNP A0A4V2WUI0
A	188	ALA	MET	conflict	UNP A0A4V2WUI0
A	197	ALA	PRO	conflict	UNP A0A4V2WUI0
A	204	MET	VAL	conflict	UNP A0A4V2WUI0
A	208	MET	LEU	conflict	UNP A0A4V2WUI0
A	219	THR	SER	conflict	UNP A0A4V2WUI0
A	226	ALA	VAL	conflict	UNP A0A4V2WUI0
A	240	ALA	GLN	conflict	UNP A0A4V2WUI0
A	260	VAL	ALA	conflict	UNP A0A4V2WUI0
A	280	GLN	GLU	conflict	UNP A0A4V2WUI0
A	281	PRO	ALA	conflict	UNP A0A4V2WUI0
A	282	GLY	ALA	conflict	UNP A0A4V2WUI0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	289	VAL	ALA	conflict	UNP A0A4V2WUI0
A	295	ILE	-	expression tag	UNP A0A4V2WUI0
A	296	ALA	-	expression tag	UNP A0A4V2WUI0
A	297	LEU	-	expression tag	UNP A0A4V2WUI0
A	298	GLU	-	expression tag	UNP A0A4V2WUI0
A	299	HIS	-	expression tag	UNP A0A4V2WUI0
A	300	HIS	-	expression tag	UNP A0A4V2WUI0
A	301	HIS	-	expression tag	UNP A0A4V2WUI0
A	302	HIS	-	expression tag	UNP A0A4V2WUI0
A	303	HIS	-	expression tag	UNP A0A4V2WUI0
A	304	HIS	-	expression tag	UNP A0A4V2WUI0
B	5	VAL	ILE	conflict	UNP A0A4V2WUI0
B	8	ALA	PRO	conflict	UNP A0A4V2WUI0
B	9	ALA	GLN	conflict	UNP A0A4V2WUI0
B	10	PRO	GLN	conflict	UNP A0A4V2WUI0
B	11	SER	ALA	conflict	UNP A0A4V2WUI0
B	38	GLU	ALA	conflict	UNP A0A4V2WUI0
B	92	GLU	GLN	conflict	UNP A0A4V2WUI0
B	102	HIS	ARG	conflict	UNP A0A4V2WUI0
B	160	ALA	GLY	conflict	UNP A0A4V2WUI0
B	161	PRO	ALA	conflict	UNP A0A4V2WUI0
B	186	ALA	ASP	conflict	UNP A0A4V2WUI0
B	187	LEU	THR	conflict	UNP A0A4V2WUI0
B	188	ALA	MET	conflict	UNP A0A4V2WUI0
B	197	ALA	PRO	conflict	UNP A0A4V2WUI0
B	204	MET	VAL	conflict	UNP A0A4V2WUI0
B	208	MET	LEU	conflict	UNP A0A4V2WUI0
B	219	THR	SER	conflict	UNP A0A4V2WUI0
B	226	ALA	VAL	conflict	UNP A0A4V2WUI0
B	240	ALA	GLN	conflict	UNP A0A4V2WUI0
B	260	VAL	ALA	conflict	UNP A0A4V2WUI0
B	280	GLN	GLU	conflict	UNP A0A4V2WUI0
B	281	PRO	ALA	conflict	UNP A0A4V2WUI0
B	282	GLY	ALA	conflict	UNP A0A4V2WUI0
B	289	VAL	ALA	conflict	UNP A0A4V2WUI0
B	295	ILE	-	expression tag	UNP A0A4V2WUI0
B	296	ALA	-	expression tag	UNP A0A4V2WUI0
B	297	LEU	-	expression tag	UNP A0A4V2WUI0
B	298	GLU	-	expression tag	UNP A0A4V2WUI0
B	299	HIS	-	expression tag	UNP A0A4V2WUI0
B	300	HIS	-	expression tag	UNP A0A4V2WUI0
B	301	HIS	-	expression tag	UNP A0A4V2WUI0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP A0A4V2WUI0
B	303	HIS	-	expression tag	UNP A0A4V2WUI0
B	304	HIS	-	expression tag	UNP A0A4V2WUI0
C	5	VAL	ILE	conflict	UNP A0A4V2WUI0
C	8	ALA	PRO	conflict	UNP A0A4V2WUI0
C	9	ALA	GLN	conflict	UNP A0A4V2WUI0
C	10	PRO	GLN	conflict	UNP A0A4V2WUI0
C	11	SER	ALA	conflict	UNP A0A4V2WUI0
C	38	GLU	ALA	conflict	UNP A0A4V2WUI0
C	92	GLU	GLN	conflict	UNP A0A4V2WUI0
C	102	HIS	ARG	conflict	UNP A0A4V2WUI0
C	160	ALA	GLY	conflict	UNP A0A4V2WUI0
C	161	PRO	ALA	conflict	UNP A0A4V2WUI0
C	186	ALA	ASP	conflict	UNP A0A4V2WUI0
C	187	LEU	THR	conflict	UNP A0A4V2WUI0
C	188	ALA	MET	conflict	UNP A0A4V2WUI0
C	197	ALA	PRO	conflict	UNP A0A4V2WUI0
C	204	MET	VAL	conflict	UNP A0A4V2WUI0
C	208	MET	LEU	conflict	UNP A0A4V2WUI0
C	219	THR	SER	conflict	UNP A0A4V2WUI0
C	226	ALA	VAL	conflict	UNP A0A4V2WUI0
C	240	ALA	GLN	conflict	UNP A0A4V2WUI0
C	260	VAL	ALA	conflict	UNP A0A4V2WUI0
C	280	GLN	GLU	conflict	UNP A0A4V2WUI0
C	281	PRO	ALA	conflict	UNP A0A4V2WUI0
C	282	GLY	ALA	conflict	UNP A0A4V2WUI0
C	289	VAL	ALA	conflict	UNP A0A4V2WUI0
C	295	ILE	-	expression tag	UNP A0A4V2WUI0
C	296	ALA	-	expression tag	UNP A0A4V2WUI0
C	297	LEU	-	expression tag	UNP A0A4V2WUI0
C	298	GLU	-	expression tag	UNP A0A4V2WUI0
C	299	HIS	-	expression tag	UNP A0A4V2WUI0
C	300	HIS	-	expression tag	UNP A0A4V2WUI0
C	301	HIS	-	expression tag	UNP A0A4V2WUI0
C	302	HIS	-	expression tag	UNP A0A4V2WUI0
C	303	HIS	-	expression tag	UNP A0A4V2WUI0
C	304	HIS	-	expression tag	UNP A0A4V2WUI0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	167	Total O 167 167	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	B	80	Total	O	0	0
			80	80		
2	C	82	Total	O	0	0
			82	82		

### 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. 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.

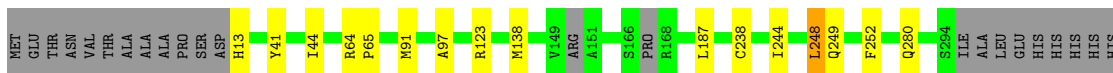
- Molecule 1: Alpha/beta fold hydrolase

Chain A:  91% 6%




- Molecule 1: Alpha/beta fold hydrolase

Chain B:  87% 5% 8%



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- Molecule 1: Alpha/beta fold hydrolase

Chain C:  88% 8%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.96Å 68.41Å 75.34Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	57.64 – 1.66	Depositor
% Data completeness (in resolution range)	98.4 (57.64-1.66)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.194 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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	0.52	0/2140	0.78	2/2925 (0.1%)
1	B	0.45	0/2029	0.73	1/2761 (0.0%)
1	C	0.44	0/1986	0.70	0/2699
All	All	0.47	0/6155	0.74	3/8385 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ARG	NE-CZ-NH1	11.85	126.22	120.30
1	A	233	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	248	LEU	O-C-N	-5.35	114.15	122.70

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	2077	0	1979	4	0
1	B	1975	0	1789	9	0
1	C	1937	0	1708	9	0
2	A	167	0	0	0	0
2	B	80	0	0	0	0
2	C	82	0	0	2	0
All	All	6318	0	5476	22	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 2.

All (22) 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:C:16:PHE:CG	1:C:16:PHE:CE1	2.41	1.01
1:B:238:CYS:H	1:B:249:GLN:HE22	1.37	0.71
1:B:244:ILE:HG23	1:B:248:LEU:HD23	1.74	0.67
1:B:138:MET:O	1:B:252:PHE:HD1	1.90	0.54
1:B:138:MET:O	1:B:252:PHE:CD1	2.62	0.52
1:B:91:MET:SD	1:B:123:ARG:HD2	2.50	0.52
1:C:209:THR:HG21	2:C:417:HOH:O	2.09	0.52
1:C:234:HIS:CD2	1:C:291:ILE:HG23	2.48	0.49
1:B:13:HIS:HB3	1:B:41:TYR:CE2	2.54	0.43
1:C:234:HIS:ND1	1:C:234:HIS:N	2.67	0.43
1:C:134:LEU:O	1:C:135:ALA:C	2.57	0.42
1:B:248:LEU:O	1:B:249:GLN:C	2.57	0.42
1:C:64:ARG:HA	1:C:65:PRO:C	2.39	0.42
1:C:293:LYS:O	1:C:294:SER:C	2.58	0.42
1:B:44:ILE:HD12	1:B:97:ALA:HB2	2.02	0.41
1:C:209:THR:CG2	2:C:417:HOH:O	2.67	0.41
1:A:104:LYS:HB2	1:A:129:ALA:HB2	2.03	0.41
1:A:39:ARG:HD3	1:A:289:VAL:HG21	2.03	0.41
1:A:160:ALA:N	1:A:161:PRO:HD2	2.34	0.41
1:B:64:ARG:HA	1:B:65:PRO:C	2.41	0.41
1:C:225:ALA:C	1:C:227:ARG:CG	2.90	0.40

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	A	285/304 (94%)	280 (98%)	5 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	275/304 (90%)	269 (98%)	6 (2%)	0	100	100
1	C	278/304 (91%)	273 (98%)	5 (2%)	0	100	100
All	All	838/912 (92%)	822 (98%)	16 (2%)	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	193/226 (85%)	193 (100%)	0	100	100
1	B	170/226 (75%)	168 (99%)	2 (1%)	71	53
1	C	153/226 (68%)	153 (100%)	0	100	100
All	All	516/678 (76%)	514 (100%)	2 (0%)	91	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	187	LEU
1	B	280	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	B	24	HIS
1	B	110	HIS
1	B	249	GLN
1	B	268	HIS

### 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](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.