



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:58 am BST

PDB ID : 2F1Z  
Title : Crystal structure of HAUSP  
Authors : Hu, M.; Gu, L.; Jeffrey, P.D.; Shi, Y.  
Deposited on : 2005-11-15  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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  
Xtriage (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) : 2.11

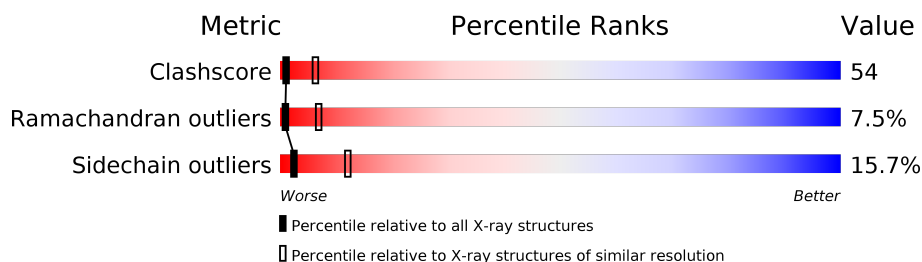
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

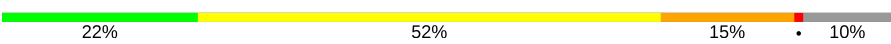
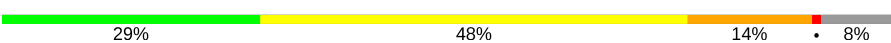
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 on 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	522	 <div>22% 52% 15% • 10%</div>
1	B	522	 <div>29% 48% 14% • 8%</div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8015 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3842	2442	652	726	22			
1	B	481	Total	C	N	O	S	0	0	0
			3933	2500	668	743	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLY	-	CLONING ARTIFACT	UNP Q93009
A	40	SER	-	CLONING ARTIFACT	UNP Q93009
A	41	HIS	-	CLONING ARTIFACT	UNP Q93009
A	42	MET	-	CLONING ARTIFACT	UNP Q93009
B	39	GLY	-	CLONING ARTIFACT	UNP Q93009
B	40	SER	-	CLONING ARTIFACT	UNP Q93009
B	41	HIS	-	CLONING ARTIFACT	UNP Q93009
B	42	MET	-	CLONING ARTIFACT	UNP Q93009

- Molecule 2 is water.

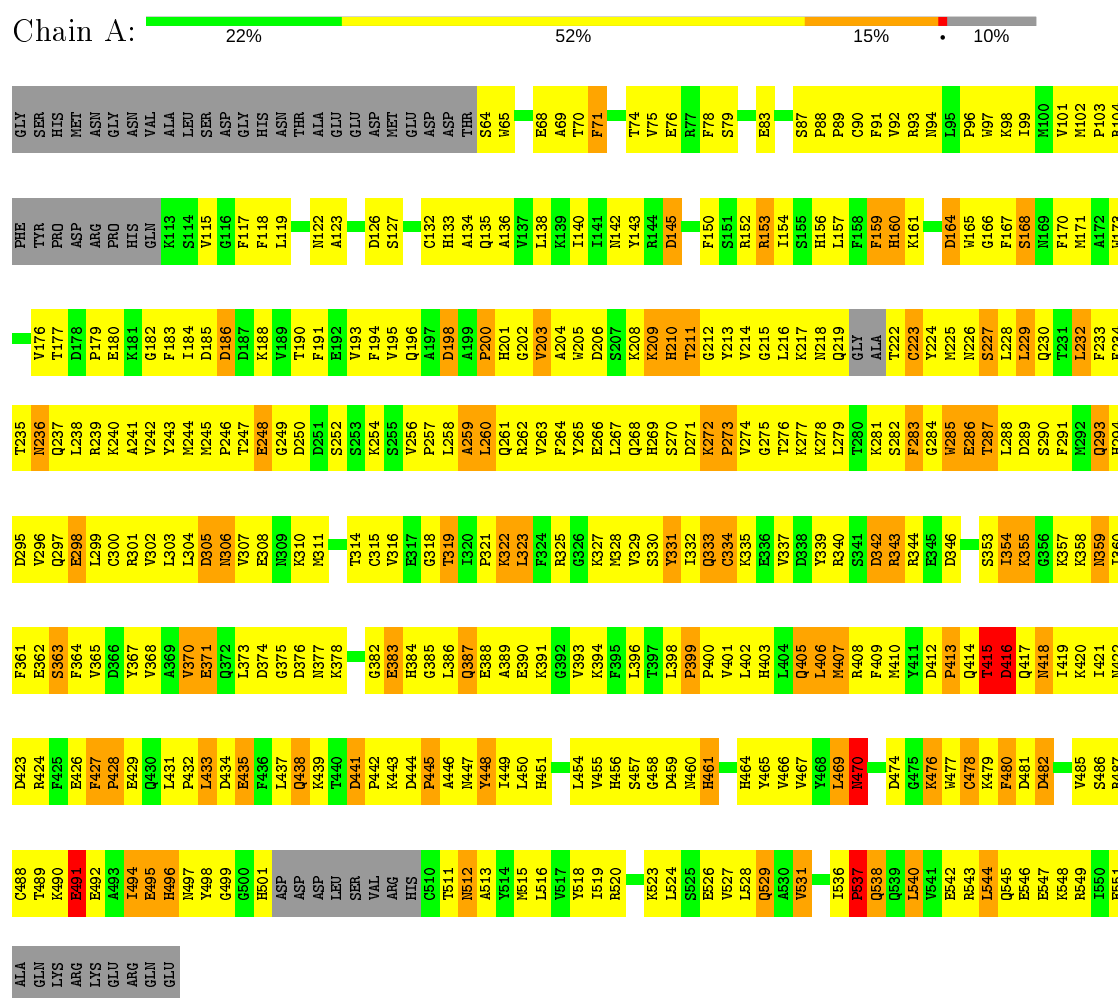
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	118	Total	O	0	0
			118	118		
2	B	122	Total	O	0	0
			122	122		

### 3 Residue-property plots

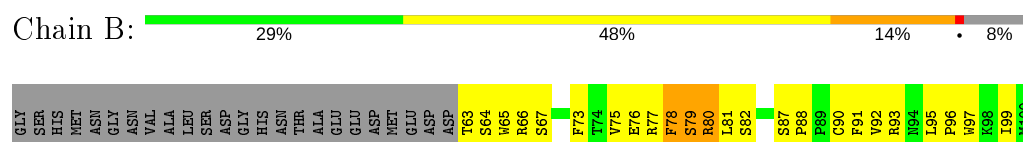
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



N512	A513	Y514	M515	L516	Y517	Y518	L524	S525	E526	V527	L528	Q529	A530	V531	T532	D533	H534	D535	L536	Q539	L540	L544	E547	E551	A552	Q553	LYS	ARG	LYS	GLU	ARG	GLN	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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Y106	F107	D108	R109	P110	H111	Q112	K113	S114	V115	G116	F117	F118	L119	N122	W130	Q135	A136	V137	L138	K139	I140	L141	N142	Y143	R144	D145	K148	S149	F150	S151	R152	R153	L154	S155	H156	L157	F158																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.62Å 219.86Å 130.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.265 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.46	0/3935	0.74	1/5312 (0.0%)
1	B	0.50	2/4032 (0.0%)	0.81	9/5449 (0.2%)
All	All	0.48	2/7967 (0.0%)	0.78	10/10761 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	ARG	CZ-NH1	5.37	1.40	1.33
1	B	104	ARG	CB-CG	5.26	1.66	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	B	414	GLN	N-CA-C	-9.00	86.71	111.00
1	B	104	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	105	PHE	N-CA-C	7.61	131.54	111.00
1	B	387	GLN	CB-CA-C	-6.44	97.52	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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	3842	0	3710	428	1
1	B	3933	0	3794	406	0
2	A	118	0	0	44	0
2	B	122	0	0	41	0
All	All	8015	0	7504	821	1

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 54.

The worst 5 of 821 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:B:109:ARG:HE	1:B:110:PRO:HD2	1.21	1.04
1:B:491:GLU:HA	1:B:495:GLU:HG3	1.39	1.03
1:A:501:HIS:HB3	1:B:413:PRO:HG3	1.38	1.01
1:B:214:VAL:HG22	1:B:215:GLY:H	1.27	1.00
1:A:294:HIS:HB3	1:A:298:GLU:HG3	1.47	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:O	1:A:287:THR:O[4_555]	1.83	0.37

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	462/522 (88%)	356 (77%)	71 (15%)	35 (8%)	1	7
1	B	477/522 (91%)	364 (76%)	78 (16%)	35 (7%)	1	7
All	All	939/1044 (90%)	720 (77%)	149 (16%)	70 (8%)	1	7

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	SER
1	A	183	PHE
1	A	203	VAL
1	A	277	LYS
1	A	334	CYS

### 5.3.2 Protein sidechains ⓘ

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	428/472 (91%)	355 (83%)	73 (17%)	2	10
1	B	437/472 (93%)	374 (86%)	63 (14%)	3	15
All	All	865/944 (92%)	729 (84%)	136 (16%)	2	12

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	CYS
1	B	106	TYR
1	B	474	ASP
1	A	486	SER
1	A	540	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	156	HIS
1	B	464	HIS
1	A	538	GLN
1	B	219	GLN

### 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 carbohydrates 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.