



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:54 am BST

PDB ID : 5GND  
Title : Structure of Deg protease HhoA from Synechocystis sp. PCC 6803  
Authors : Dong, W.; Wang, J.; Liu, L.  
Deposited on : 2016-07-20  
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](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	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)	:	2.11

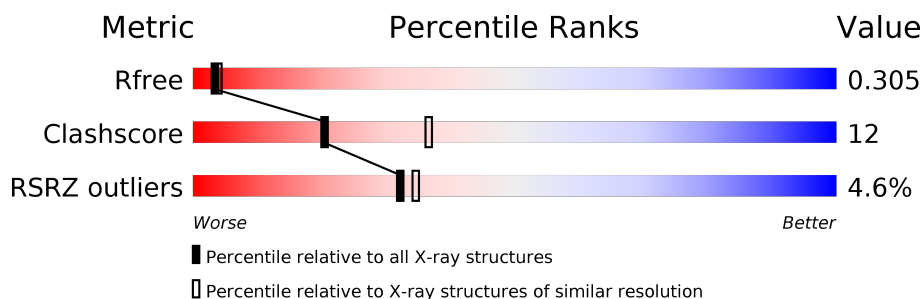
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\leq 5\%$ . 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	A	348	
2	U	5	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2143 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 Putative serine protease HhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	2	0
			2047	1280	369	395	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	expression tag	UNP P72780
A	395	LEU	-	expression tag	UNP P72780
A	396	GLU	-	expression tag	UNP P72780
A	397	HIS	-	expression tag	UNP P72780
A	398	HIS	-	expression tag	UNP P72780
A	399	HIS	-	expression tag	UNP P72780
A	400	HIS	-	expression tag	UNP P72780
A	401	HIS	-	expression tag	UNP P72780
A	402	HIS	-	expression tag	UNP P72780

- Molecule 2 is a protein called UNK-UNK-UNK-UNK-TRP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	5	Total	C	N	O	0	0	0
			30	19	6	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

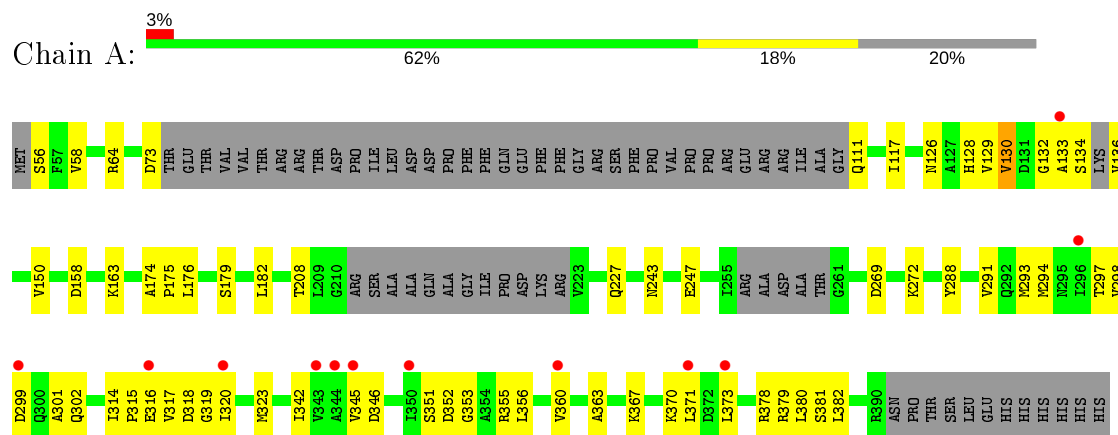
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	U	1	Total O 1 1	0	0

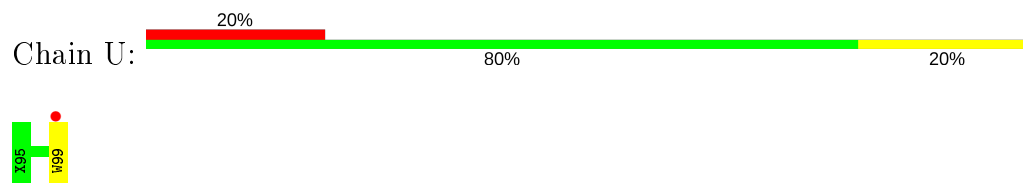
### 3 Residue-property plots [i](#)

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 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: Putative serine protease HhoA



#### • Molecule 2: UNK-UNK-UNK-UNK-TRP



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.22Å 135.22Å 113.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.92 – 2.50 40.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.92-2.50) 97.0 (40.80-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.247 , 0.305 0.249 , 0.305	Depositor DCC
$R_{free}$ test set	676 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: NA, ZN

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	0.32	0/2073	0.66	6/2823 (0.2%)
2	U	0.28	0/15	0.31	0/20
All	All	0.32	0/2088	0.66	6/2843 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	SER	N-CA-CB	12.61	129.41	110.50
1	A	136	VAL	O-C-N	9.61	138.07	122.70
1	A	133	ALA	N-CA-C	9.31	136.14	111.00
1	A	136	VAL	CA-C-N	-7.22	101.31	117.20
1	A	130	VAL	O-C-N	5.39	131.32	122.70
1	A	130	VAL	CA-C-N	-5.03	106.15	117.20

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	2047	0	2087	52	0
2	U	30	0	12	5	0
3	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	63	0	0	10	1
5	U	1	0	0	0	0
All	All	2143	0	2099	52	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 12.

All (52) 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:A:342:ILE:O	5:A:601:HOH:O	2.04	0.74
1:A:320:ILE:O	5:A:602:HOH:O	2.11	0.69
1:A:111:GLN:N	5:A:609:HOH:O	2.31	0.64
1:A:297:THR:HG22	1:A:299:ASP:H	1.63	0.64
1:A:130:VAL:C	1:A:132:GLY:H	2.05	0.60
1:A:243:ASN:HD21	1:A:247:GLU:HG3	1.67	0.60
1:A:363:ALA:HB1	1:A:367:LYS:HG2	1.84	0.59
1:A:297:THR:O	1:A:301:ALA:N	2.35	0.58
1:A:130:VAL:HG11	1:A:150:VAL:HG21	1.86	0.58
1:A:208:THR:HG23	1:A:227:GLN:HB2	1.86	0.57
1:A:130:VAL:O	1:A:132:GLY:N	2.31	0.57
1:A:288:TYR:HD1	2:U:99:TRP:HB3	1.69	0.57
1:A:117:ILE:O	5:A:603:HOH:O	2.18	0.56
1:A:130:VAL:C	1:A:132:GLY:N	2.62	0.53
1:A:130:VAL:CG1	1:A:150:VAL:HG21	2.38	0.53
1:A:126:ASN:HB2	1:A:129:VAL:HG23	1.91	0.53
1:A:117:ILE:HD11	1:A:176:LEU:HD11	1.91	0.51
1:A:378:ARG:HD2	1:A:380:LEU:HD22	1.91	0.51
1:A:342:ILE:N	5:A:602:HOH:O	2.42	0.51
1:A:288:TYR:HB2	2:U:99:TRP:HE3	1.75	0.51
1:A:163:LYS:NZ	5:A:615:HOH:O	2.44	0.50
1:A:360:VAL:HG21	2:U:99:TRP:HH2	1.76	0.50
1:A:73:ASP:OD2	1:A:111:GLN:NE2	2.45	0.49
1:A:319:GLY:HA2	1:A:351:SER:HA	1.94	0.48
1:A:371:LEU:N	1:A:382:LEU:O	2.46	0.48
1:A:288:TYR:HB2	2:U:99:TRP:CE3	2.48	0.48
1:A:379:ARG:HG2	5:A:627:HOH:O	2.12	0.48
1:A:297:THR:HG22	1:A:299:ASP:N	2.27	0.48
1:A:298:VAL:O	1:A:302:GLN:HG2	2.13	0.48
1:A:346[A]:ASP:HA	1:A:370:LYS:HD3	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:O	5:A:604:HOH:O	2.20	0.47
1:A:294:MET:HB2	1:A:323:MET:HG3	1.97	0.47
1:A:293:MET:HB2	1:A:320:ILE:HG22	1.97	0.47
1:A:371:LEU:O	1:A:381:SER:HA	2.15	0.47
1:A:345:VAL:HG23	1:A:346[B]:ASP:H	1.80	0.46
1:A:352:ASP:HB3	1:A:355:ARG:HB3	1.99	0.45
1:A:293:MET:SD	1:A:356:LEU:HD23	2.57	0.45
1:A:302:GLN:HB3	1:A:316:GLU:OE1	2.17	0.45
1:A:291:VAL:O	2:U:99:TRP:CD1	2.70	0.44
1:A:298:VAL:N	1:A:318:ASP:OD2	2.38	0.43
1:A:293:MET:HE3	1:A:353:GLY:O	2.19	0.43
1:A:269:ASP:HA	1:A:272:LYS:HD2	2.00	0.43
1:A:342:ILE:HA	1:A:373:LEU:HB3	2.00	0.42
1:A:342:ILE:O	5:A:602:HOH:O	2.20	0.42
1:A:320:ILE:HG13	5:A:602:HOH:O	2.19	0.42
1:A:243:ASN:ND2	1:A:247:GLU:HG3	2.34	0.42
1:A:314:ILE:HA	1:A:315:PRO:HD3	1.95	0.42
1:A:56:SER:OG	1:A:58:VAL:HG13	2.20	0.41
1:A:128:HIS:ND1	1:A:158:ASP:OD2	2.46	0.41
1:A:174:ALA:HA	1:A:175:PRO:HD2	1.97	0.41
1:A:179:SER:HA	1:A:182:LEU:HG	2.02	0.41
1:A:315:PRO:O	1:A:317:VAL:HG13	2.22	0.40

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)
5:A:653:HOH:O	5:A:653:HOH:O[18_445]	1.58	0.62

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	280/348 (80%)	0.26	12 (4%) 35 38	11, 34, 64, 83	0
2	U	1/5 (20%)	4.32	1 (100%) 0 0	81, 81, 81, 81	0
All	All	281/353 (79%)	0.28	13 (4%) 32 34	11, 34, 64, 83	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	99	TRP	4.3
1	A	360	VAL	3.7
1	A	320	ILE	3.5
1	A	344	ALA	3.4
1	A	345	VAL	3.3
1	A	299	ASP	2.7
1	A	316	GLU	2.7
1	A	343	VAL	2.3
1	A	373	LEU	2.3
1	A	350	ILE	2.2
1	A	371	LEU	2.1
1	A	133	ALA	2.1
1	A	296	ILE	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 carbohydrates 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<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	A	502	1/1	0.92	0.20	21,21,21,21	1
3	ZN	A	501	1/1	0.96	0.14	33,33,33,33	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.