



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 16, 2017 – 10:27 PM EST

PDB ID : 5HDF  
Title : Hydrolase SeMet-StnA  
Authors : Qian, T.  
Deposited on : 2016-01-05  
Resolution : 2.71 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442



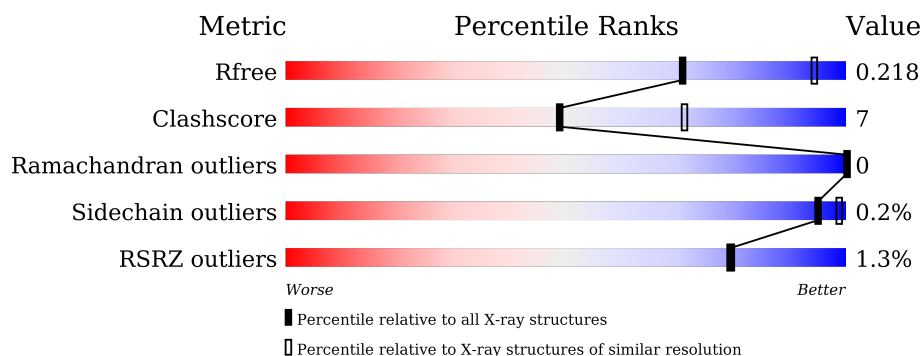
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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))
$R_{free}$	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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. 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	383	<div> <div>72%</div> <div>10%</div> <div>•</div> <div>18%</div> </div>
1	B	383	<div> <div>75%</div> <div>9%</div> <div>16%</div> </div>
1	C	383	<div> <div>2%</div> <div>73%</div> <div>10%</div> <div>17%</div> </div>
1	D	383	<div> <div>3%</div> <div>72%</div> <div>10%</div> <div>17%</div> </div>



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9646 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 Hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	320	Total	C	N	O	S	Se	0	0	0
			2431	1520	426	474	4	7			
1	A	315	Total	C	N	O	S	Se	0	0	0
			2384	1491	415	467	4	7			
1	C	316	Total	C	N	O	S	Se	0	0	0
			2392	1497	416	468	4	7			
1	D	316	Total	C	N	O	S	Se	0	0	0
			2387	1493	416	467	4	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	VAL	-	expression tag	UNP L7PIJ2
B	376	LEU	-	expression tag	UNP L7PIJ2
B	377	GLU	-	expression tag	UNP L7PIJ2
B	378	HIS	-	expression tag	UNP L7PIJ2
B	379	HIS	-	expression tag	UNP L7PIJ2
B	380	HIS	-	expression tag	UNP L7PIJ2
B	381	HIS	-	expression tag	UNP L7PIJ2
B	382	HIS	-	expression tag	UNP L7PIJ2
B	383	HIS	-	expression tag	UNP L7PIJ2
A	1	VAL	-	expression tag	UNP L7PIJ2
A	376	LEU	-	expression tag	UNP L7PIJ2
A	377	GLU	-	expression tag	UNP L7PIJ2
A	378	HIS	-	expression tag	UNP L7PIJ2
A	379	HIS	-	expression tag	UNP L7PIJ2
A	380	HIS	-	expression tag	UNP L7PIJ2
A	381	HIS	-	expression tag	UNP L7PIJ2
A	382	HIS	-	expression tag	UNP L7PIJ2
A	383	HIS	-	expression tag	UNP L7PIJ2
C	1	VAL	-	expression tag	UNP L7PIJ2
C	376	LEU	-	expression tag	UNP L7PIJ2
C	377	GLU	-	expression tag	UNP L7PIJ2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	378	HIS	-	expression tag	UNP L7PIJ2
C	379	HIS	-	expression tag	UNP L7PIJ2
C	380	HIS	-	expression tag	UNP L7PIJ2
C	381	HIS	-	expression tag	UNP L7PIJ2
C	382	HIS	-	expression tag	UNP L7PIJ2
C	383	HIS	-	expression tag	UNP L7PIJ2
D	1	VAL	-	expression tag	UNP L7PIJ2
D	376	LEU	-	expression tag	UNP L7PIJ2
D	377	GLU	-	expression tag	UNP L7PIJ2
D	378	HIS	-	expression tag	UNP L7PIJ2
D	379	HIS	-	expression tag	UNP L7PIJ2
D	380	HIS	-	expression tag	UNP L7PIJ2
D	381	HIS	-	expression tag	UNP L7PIJ2
D	382	HIS	-	expression tag	UNP L7PIJ2
D	383	HIS	-	expression tag	UNP L7PIJ2

- Molecule 2 is water.

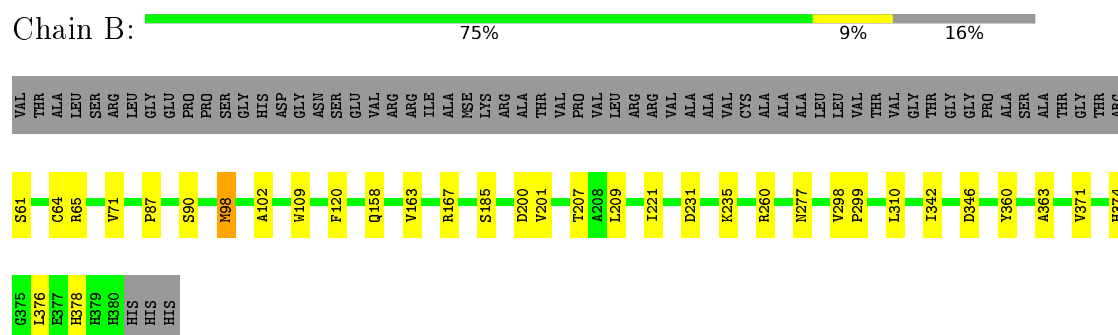
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	20	Total O 20 20	0	0
2	A	16	Total O 16 16	0	0
2	C	9	Total O 9 9	0	0
2	D	7	Total O 7 7	0	0



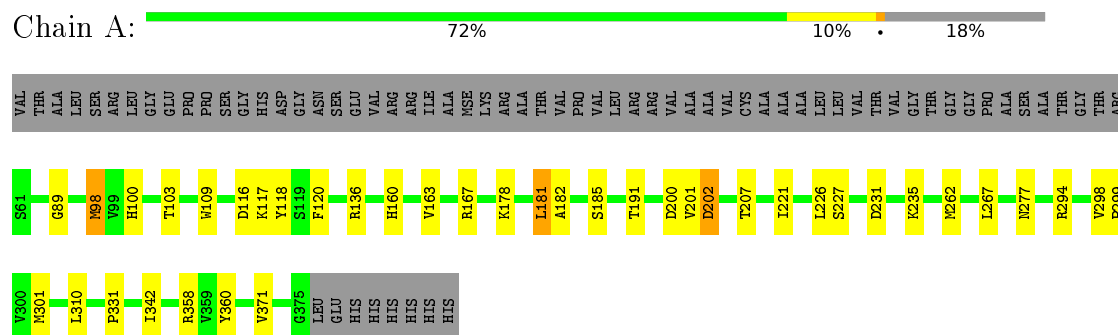
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

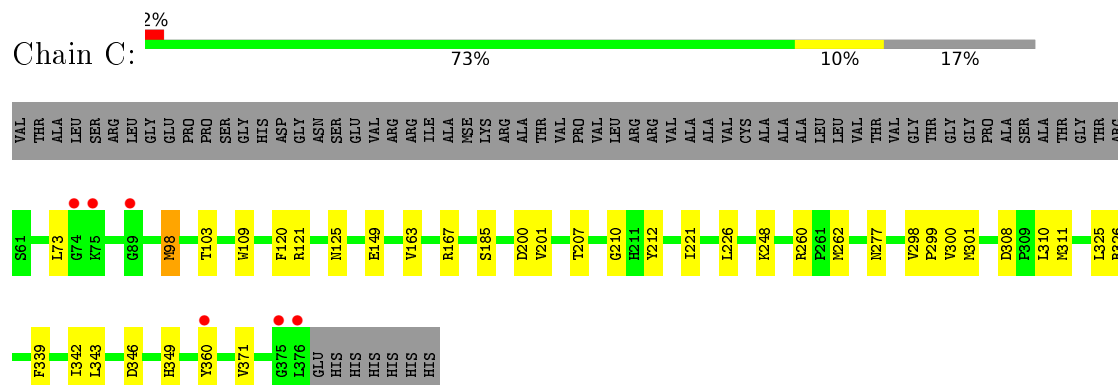
#### • Molecule 1: Hydrolase



#### • Molecule 1: Hydrolase

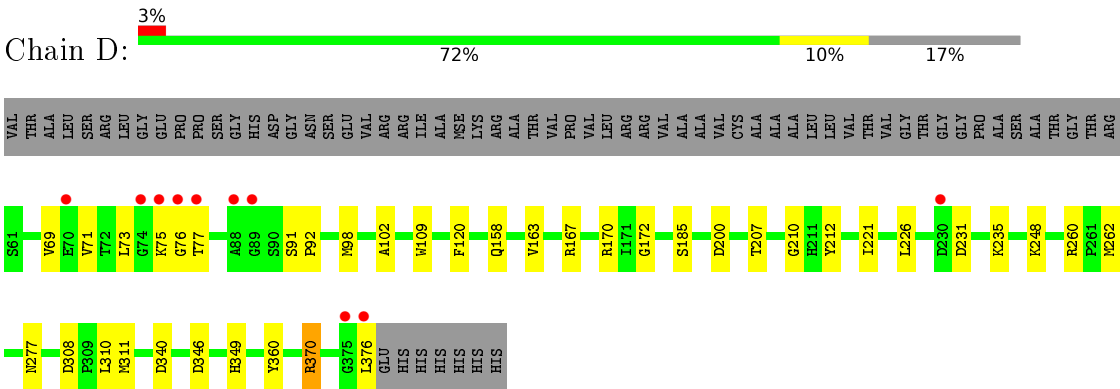


#### • Molecule 1: Hydrolase





● Molecule 1: Hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.42Å 81.97Å 118.69Å 90.00° 126.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.71 38.85 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.71) 99.5 (38.85-2.71)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.88 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.192 , 0.220 0.194 , 0.218	Depositor DCC
$R_{free}$ test set	1868 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9646	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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

### 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	0.87	2/2435 (0.1%)	0.73	3/3312 (0.1%)
1	B	0.85	1/2485 (0.0%)	0.67	1/3380 (0.0%)
1	C	0.85	2/2443 (0.1%)	0.69	2/3323 (0.1%)
1	D	0.83	3/2438 (0.1%)	0.69	2/3316 (0.1%)
All	All	0.85	8/9801 (0.1%)	0.70	8/13331 (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	B	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	SER	CA-CB	6.51	1.62	1.52
1	B	185	SER	CA-CB	6.49	1.62	1.52
1	D	76	GLY	N-CA	6.46	1.55	1.46
1	C	185	SER	CA-CB	5.91	1.61	1.52
1	C	185	SER	CB-OG	5.25	1.49	1.42

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	C	262	MSE	CA-CB-CG	-6.74	101.84	113.30
1	D	262	MSE	CG-SE-CE	6.05	112.22	98.90
1	A	181	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	B	98	MSE	CG-SE-CE	-5.23	87.39	98.90

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	61	SER	Peptide

## 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	2384	0	2278	41	0
1	B	2431	0	2316	30	0
1	C	2392	0	2289	32	0
1	D	2387	0	2276	32	0
2	A	16	0	0	0	0
2	B	20	0	0	0	0
2	C	9	0	0	0	0
2	D	7	0	0	0	0
All	All	9646	0	9159	134	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 7.

The worst 5 of 134 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:D:98:MSE:HE2	1:D:109:TRP:CE3	1.93	1.04
1:C:98:MSE:HE2	1:C:109:TRP:CE3	1.92	1.03
1:B:98:MSE:HE2	1:B:109:TRP:CE3	1.93	1.02
1:A:98:MSE:HE2	1:A:109:TRP:CE3	1.96	0.99
1:A:226:LEU:HD23	1:A:227:SER:O	1.69	0.92

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	313/383 (82%)	305 (97%)	8 (3%)	0	100	100
1	B	318/383 (83%)	309 (97%)	9 (3%)	0	100	100
1	C	314/383 (82%)	307 (98%)	7 (2%)	0	100	100
1	D	314/383 (82%)	303 (96%)	11 (4%)	0	100	100
All	All	1259/1532 (82%)	1224 (97%)	35 (3%)	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	254/297 (86%)	254 (100%)	0	100	100
1	B	259/297 (87%)	257 (99%)	2 (1%)	86	95
1	C	255/297 (86%)	255 (100%)	0	100	100
1	D	253/297 (85%)	253 (100%)	0	100	100
All	All	1021/1188 (86%)	1019 (100%)	2 (0%)	95	99

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

Mol	Chain	Res	Type
1	B	209	LEU
1	B	378	HIS



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	GLN
1	C	125	ASN
1	D	125	ASN
1	A	328	GLN
1	D	328	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 [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	308/383 (80%)	-0.45	0 100 100	18, 29, 51, 71	0
1	B	313/383 (81%)	-0.45	0 100 100	20, 32, 48, 93	6 (1%)
1	C	309/383 (80%)	-0.32	6 (1%) 70 71	22, 36, 55, 85	1 (0%)
1	D	309/383 (80%)	-0.06	10 (3%) 51 52	24, 42, 63, 98	1 (0%)
All	All	1239/1532 (80%)	-0.32	16 (1%) 79 79	18, 34, 56, 98	8 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	376	LEU	6.7
1	D	89	GLY	4.1
1	C	75	LYS	3.0
1	C	376	LEU	3.0
1	D	375	GLY	2.8

### 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](#)

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.