



# wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 02:17 AM GMT

PDB ID : 3FEQ  
Title : Crystal structure of uncharacterized protein eah89906  
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S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-11-30  
Resolution : 2.63 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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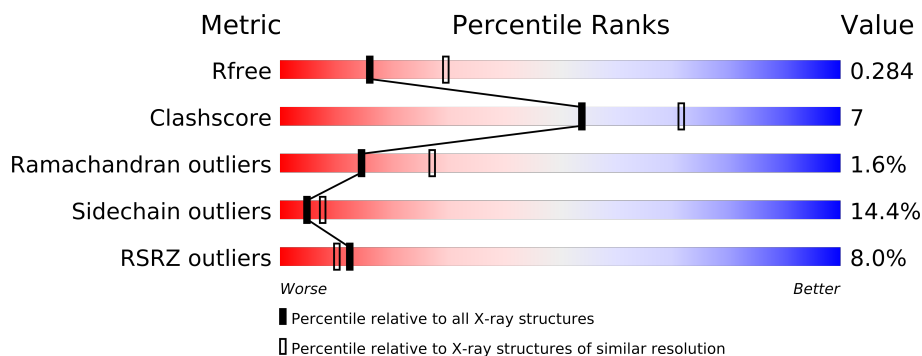
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.63 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))
$R_{free}$	66092	2393 (2.68-2.60)
Clashscore	79885	2915 (2.68-2.60)
Ramachandran outliers	78287	2865 (2.68-2.60)
Sidechain outliers	78261	2865 (2.68-2.60)
RSRZ outliers	66119	2393 (2.68-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	423	
1	B	423	
1	C	423	
1	D	423	
1	E	423	
1	F	423	
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	
1	M	423	
1	N	423	

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Mol	Chain	Length	Quality of chain
1	O	423	
1	P	423	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	C	425	-	X
2	ZN	C	426	-	X
2	ZN	D	426	-	X
2	ZN	E	426	-	X
2	ZN	F	426	-	X
2	ZN	G	425	-	X
2	ZN	H	425	-	X
2	ZN	J	425	-	X
2	ZN	J	426	-	X
2	ZN	L	425	-	X
2	ZN	L	426	-	X
2	ZN	M	426	-	X
2	ZN	N	425	-	X
2	ZN	N	426	-	X
2	ZN	O	425	-	X
2	ZN	O	426	-	X
2	ZN	P	426	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 48417 atoms, of which 0 are hydrogen and 0 are deuterium.

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 AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	4	0
			3028	1886	547	580	15			
1	B	405	Total	C	N	O	S	0	6	0
			3040	1894	552	579	15			
1	C	406	Total	C	N	O	S	0	2	0
			3025	1883	550	577	15			
1	D	405	Total	C	N	O	S	0	4	0
			3035	1890	553	577	15			
1	E	405	Total	C	N	O	S	0	4	0
			3026	1883	550	578	15			
1	F	405	Total	C	N	O	S	0	2	0
			3016	1878	546	577	15			
1	G	405	Total	C	N	O	S	0	2	0
			3021	1881	549	576	15			
1	H	405	Total	C	N	O	S	0	2	0
			3016	1878	546	577	15			
1	I	405	Total	C	N	O	S	0	1	0
			3013	1876	546	576	15			
1	J	402	Total	C	N	O	S	0	1	0
			2994	1866	543	571	14			
1	K	403	Total	C	N	O	S	0	1	0
			3000	1869	544	572	15			
1	L	404	Total	C	N	O	S	0	1	0
			3005	1870	545	575	15			
1	M	406	Total	C	N	O	S	0	1	0
			3017	1878	547	577	15			
1	N	404	Total	C	N	O	S	0	1	0
			3003	1869	545	575	14			
1	O	401	Total	C	N	O	S	0	1	0
			2983	1857	542	570	14			
1	P	405	Total	C	N	O	S	0	2	0
			3018	1879	547	577	15			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	N	2	Total 2	Zn 2	0	0
2	O	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0
2	M	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0
3	B	27	Total 27	O 27	0	0
3	C	13	Total 13	O 13	0	0

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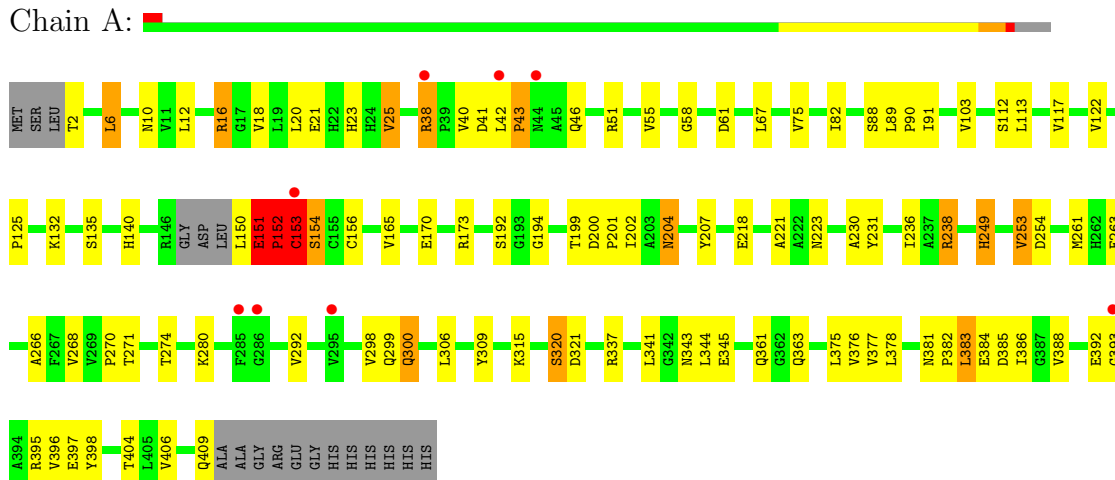
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	20	Total 20	O 20	0	0
3	E	18	Total 18	O 18	0	0
3	F	17	Total 17	O 17	0	0
3	G	16	Total 16	O 16	0	0
3	H	6	Total 6	O 6	0	0
3	O	2	Total 2	O 2	0	0
3	P	2	Total 2	O 2	0	0

### 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 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.

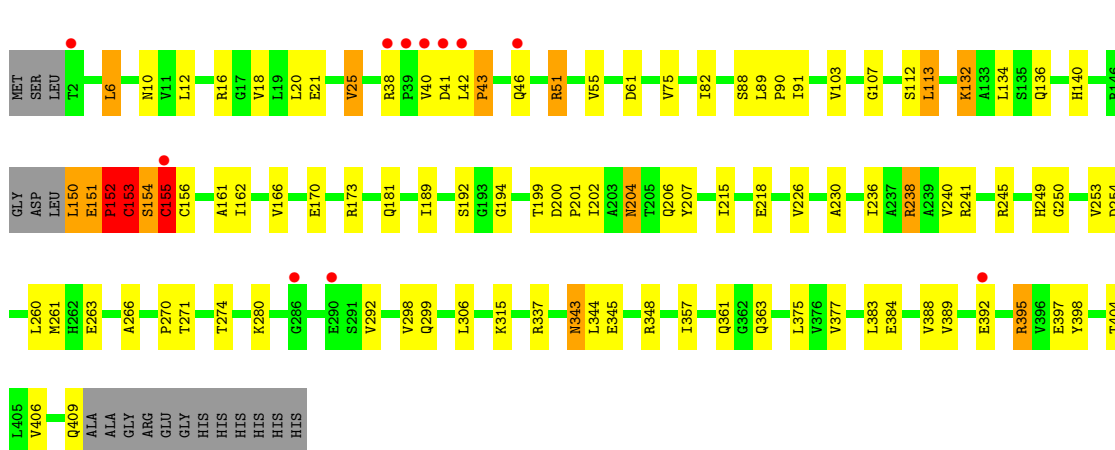
#### • Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain A:



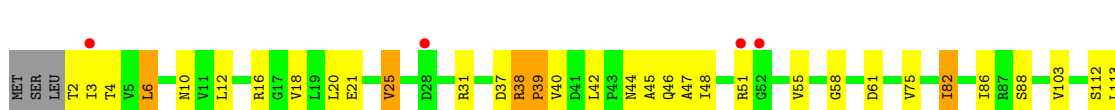
#### • Molecule 1: PUTATIVE AMIDOHYDROLASE

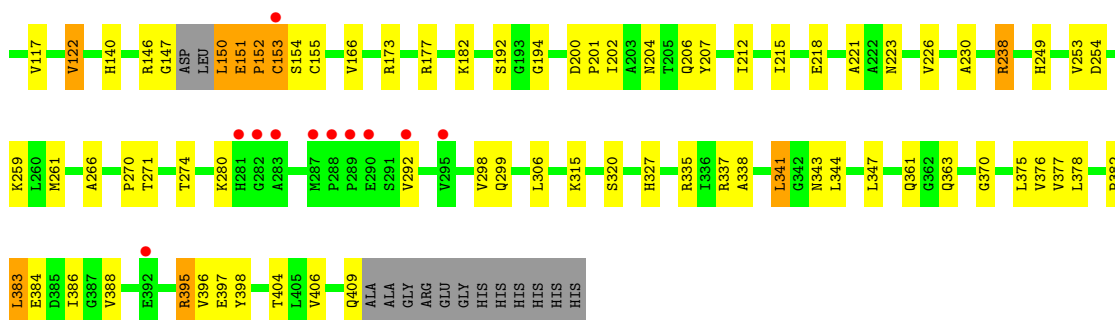
Chain B:



#### • Molecule 1: PUTATIVE AMIDOHYDROLASE

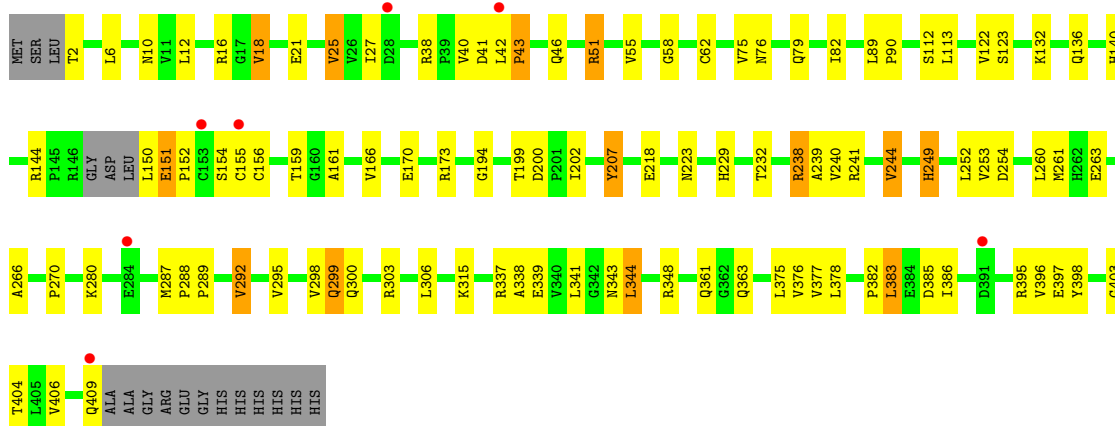
Chain C:





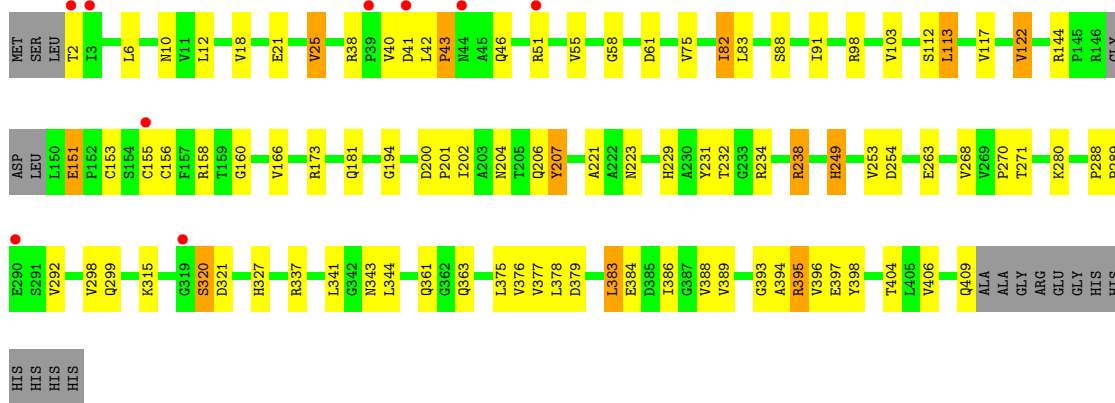
● Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain D: 



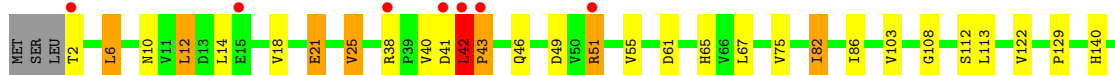
● Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain E: 



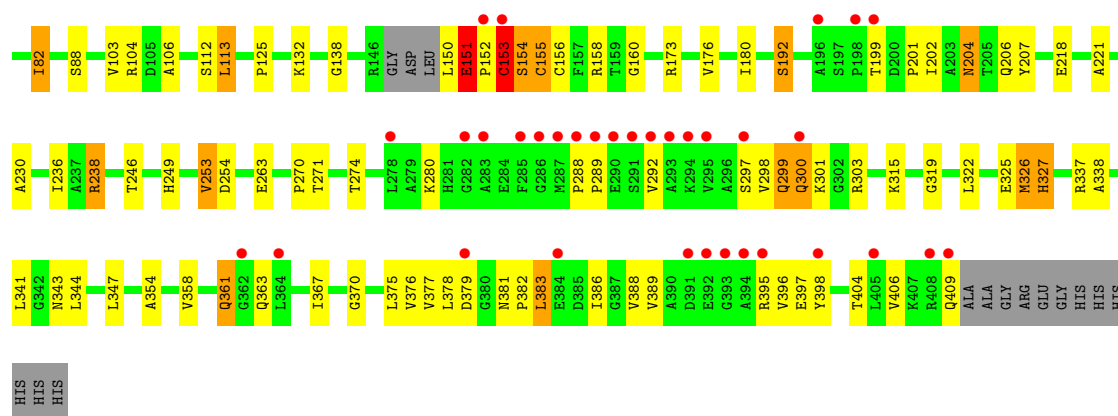
● Molecule 1: PUTATIVE AMIDOHYDROLASE

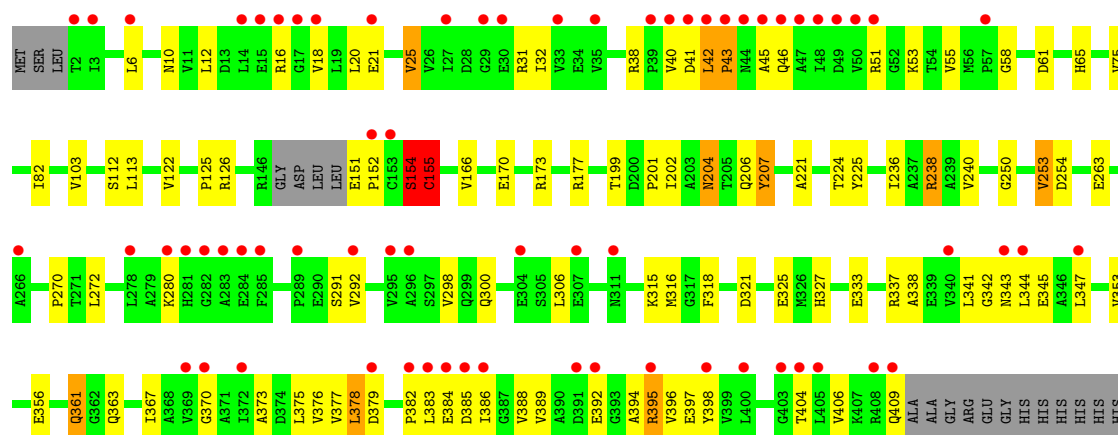
Chain F: 





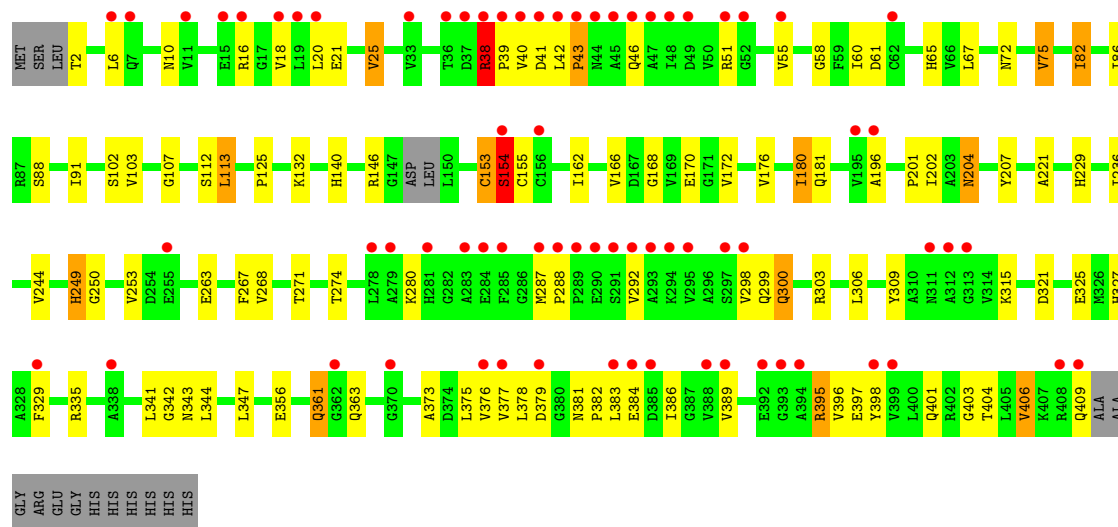






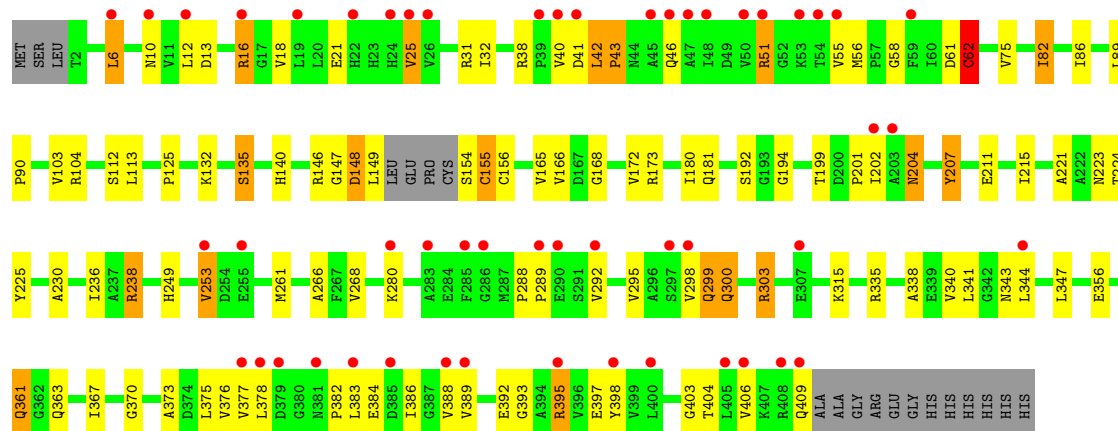
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain M:



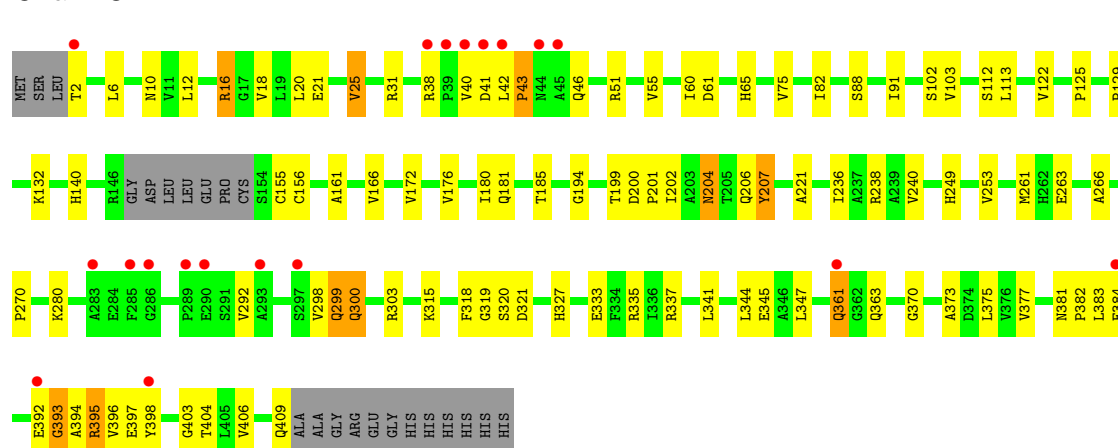
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain N:



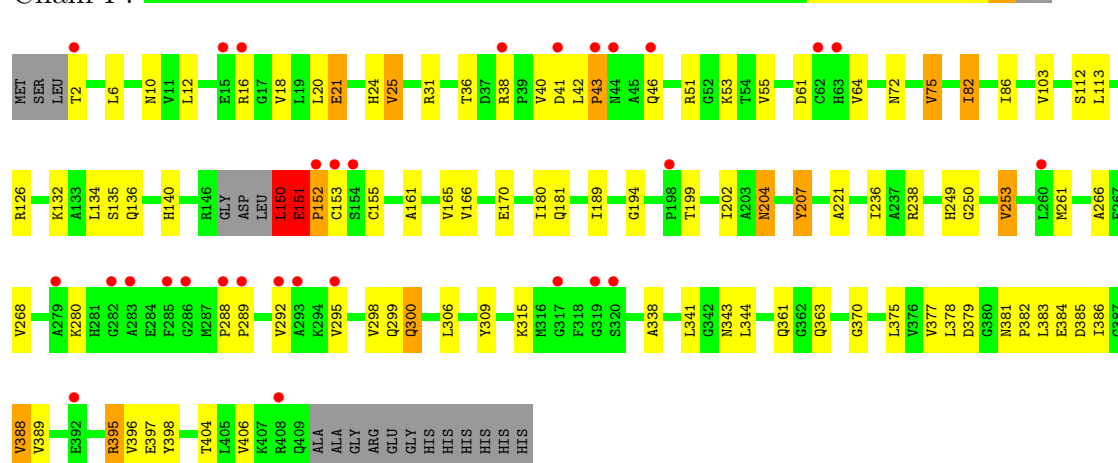
• Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain O:



- Molecule 1: PUTATIVE AMIDOHYDROLASE

Chain P:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.21Å 108.05Å 171.13Å 81.75° 80.36° 74.40°	Depositor
Resolution (Å)	20.00 – 2.63 35.90 – 2.63	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.63) 96.4 (35.90-2.63)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.238 , 0.281 0.242 , 0.284	Depositor DCC
$R_{free}$ test set	6591 reflections (3.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.3	EDS
Estimated twinning fraction	0.011 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 219029 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/3083	0.58	2/4180 (0.0%)
1	B	0.44	0/3102	0.58	1/4205 (0.0%)
1	C	0.43	0/3074	0.55	0/4167
1	D	0.46	1/3090 (0.0%)	0.57	0/4188
1	E	0.43	0/3081	0.58	1/4177 (0.0%)
1	F	0.41	0/3065	0.59	1/4156 (0.0%)
1	G	0.41	0/3070	0.56	0/4162
1	H	0.44	0/3065	0.56	0/4156
1	I	0.46	0/3059	0.56	0/4148
1	J	0.44	0/3038	0.53	0/4117
1	K	0.44	0/3045	0.55	0/4128
1	L	0.43	0/3051	0.54	0/4137
1	M	0.43	0/3063	0.56	0/4153
1	N	0.44	1/3048 (0.0%)	0.54	0/4132
1	O	0.41	0/3028	0.54	0/4105
1	P	0.42	0/3067	0.57	0/4159
All	All	0.43	2/49029 (0.0%)	0.56	5/66470 (0.0%)

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	4
1	B	0	2
1	C	0	3
1	D	0	2
1	E	0	3
1	F	0	2
1	G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	4
1	I	0	2
1	J	0	3
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	1
1	O	0	3
1	P	0	5
All	All	0	46

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	62	CYS	CB-SG	-6.20	1.71	1.82
1	D	62	CYS	CB-SG	-5.68	1.72	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	F	42	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	238	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	173	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	16	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	GLU	Peptide
1	A	152	PRO	Peptide
1	A	2	THR	Peptide
1	A	38	ARG	Peptide
1	B	38	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3028	0	3044	47	0
1	B	3040	0	3063	45	0
1	C	3025	0	3041	43	1
1	D	3035	0	3059	43	0
1	E	3026	0	3040	39	0
1	F	3016	0	3030	45	0
1	G	3021	0	3038	38	0
1	H	3016	0	3030	51	0
1	I	3013	0	3025	58	1
1	J	2994	0	3009	39	0
1	K	3000	0	3015	43	0
1	L	3005	0	3014	40	0
1	M	3017	0	3028	51	0
1	N	3003	0	3014	55	0
1	O	2983	0	2996	36	0
1	P	3018	0	3031	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	24	0	0	0	0
3	B	27	0	0	1	0
3	C	13	0	0	1	0
3	D	20	0	0	1	0
3	E	18	0	0	3	0
3	F	17	0	0	1	0
3	G	16	0	0	1	0
3	H	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2	0	0	0	0
3	P	2	0	0	0	0
All	All	48417	0	48477	663	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 663 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:263:GLU:OE2	1:M:38:ARG:HD2	1.55	1.07
1:I:221:ALA:O	1:K:204:ASN:HB2	1.60	1.01
1:A:16:ARG:HH12	1:A:20:LEU:HD21	1.27	0.97
1:C:221:ALA:O	1:F:204:ASN:HB2	1.72	0.88
1:C:3:ILE:HG23	1:C:45:ALA:HA	1.59	0.85

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	Distance(Å)	Clash(Å)
1:C:45:ALA:O	1:I:301:LYS:NZ[1_546]	1.98	0.22

## 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	405/423 (96%)	385 (95%)	13 (3%)	7 (2%)	14	25
1	B	407/423 (96%)	384 (94%)	16 (4%)	7 (2%)	14	25
1	C	404/423 (96%)	380 (94%)	18 (4%)	6 (2%)	15	29
1	D	405/423 (96%)	383 (95%)	17 (4%)	5 (1%)	19	37
1	E	405/423 (96%)	378 (93%)	23 (6%)	4 (1%)	22	43
1	F	403/423 (95%)	379 (94%)	19 (5%)	5 (1%)	19	37
1	G	403/423 (95%)	380 (94%)	18 (4%)	5 (1%)	19	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	403/423 (95%)	374 (93%)	21 (5%)	8 (2%)	11	20
1	I	402/423 (95%)	374 (93%)	20 (5%)	8 (2%)	11	20
1	J	395/423 (93%)	368 (93%)	22 (6%)	5 (1%)	18	34
1	K	398/423 (94%)	369 (93%)	22 (6%)	7 (2%)	13	24
1	L	401/423 (95%)	371 (92%)	21 (5%)	9 (2%)	10	18
1	M	403/423 (95%)	378 (94%)	17 (4%)	8 (2%)	11	20
1	N	401/423 (95%)	367 (92%)	28 (7%)	6 (2%)	15	29
1	O	398/423 (94%)	373 (94%)	18 (4%)	7 (2%)	13	24
1	P	403/423 (95%)	380 (94%)	17 (4%)	6 (2%)	15	29
All	All	6436/6768 (95%)	6023 (94%)	310 (5%)	103 (2%)	14	27

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	152	PRO
1	A	153	CYS
1	B	151	GLU
1	B	152	PRO

### 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	317/326 (97%)	268 (84%)	49 (16%)	4	6
1	B	319/326 (98%)	272 (85%)	47 (15%)	4	7
1	C	315/326 (97%)	267 (85%)	48 (15%)	4	6
1	D	317/326 (97%)	270 (85%)	47 (15%)	4	7
1	E	316/326 (97%)	272 (86%)	44 (14%)	5	8
1	F	315/326 (97%)	266 (84%)	49 (16%)	4	6
1	G	315/326 (97%)	272 (86%)	43 (14%)	5	9
1	H	315/326 (97%)	271 (86%)	44 (14%)	5	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	314/326 (96%)	270 (86%)	44 (14%)	5	8
1	J	312/326 (96%)	272 (87%)	40 (13%)	6	11
1	K	313/326 (96%)	265 (85%)	48 (15%)	4	6
1	L	313/326 (96%)	268 (86%)	45 (14%)	5	7
1	M	314/326 (96%)	269 (86%)	45 (14%)	5	8
1	N	312/326 (96%)	265 (85%)	47 (15%)	4	6
1	O	310/326 (95%)	266 (86%)	44 (14%)	5	8
1	P	315/326 (97%)	274 (87%)	41 (13%)	6	10
All	All	5032/5216 (96%)	4307 (86%)	725 (14%)	5	7

5 of 725 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	6	LEU
1	I	344	LEU
1	O	341	LEU
1	H	82	ILE
1	H	404	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	300	GLN
1	J	65	HIS
1	O	299	GLN
1	H	361	GLN
1	I	299	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 32 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	405/423 (95%)	-0.06	8 (1%) 62 60	16, 50, 100, 117	0
1	B	405/423 (95%)	-0.03	11 (2%) 52 49	11, 48, 102, 119	0
1	C	406/423 (95%)	0.05	15 (3%) 39 36	14, 49, 104, 118	0
1	D	405/423 (95%)	0.02	7 (1%) 67 66	14, 44, 98, 116	0
1	E	405/423 (95%)	0.05	9 (2%) 59 56	14, 47, 102, 119	0
1	F	405/423 (95%)	0.05	15 (3%) 39 36	15, 49, 99, 119	0
1	G	405/423 (95%)	0.11	19 (4%) 30 27	18, 50, 103, 136	0
1	H	405/423 (95%)	0.02	7 (1%) 67 66	12, 46, 100, 119	0
1	I	405/423 (95%)	0.63	63 (15%) 3 2	28, 58, 106, 123	0
1	J	402/423 (95%)	0.60	57 (14%) 3 2	27, 60, 103, 121	0
1	K	403/423 (95%)	0.64	58 (14%) 3 2	25, 59, 103, 119	0
1	L	404/423 (95%)	0.68	68 (16%) 2 1	22, 61, 106, 133	0
1	M	406/423 (95%)	0.78	71 (17%) 2 1	23, 60, 107, 130	0
1	N	404/423 (95%)	0.50	52 (12%) 4 3	21, 58, 106, 121	0
1	O	401/423 (94%)	0.02	19 (4%) 30 27	22, 53, 103, 121	0
1	P	405/423 (95%)	0.19	30 (7%) 14 12	13, 51, 100, 121	0
All	All	6471/6768 (95%)	0.27	509 (7%) 12 10	11, 53, 103, 136	0

The worst 5 of 509 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	GLU	8.1
1	J	18	VAL	7.9
1	M	398	TYR	7.1
1	P	44	ASN	7.0
1	M	393	GLY	6.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	J	426	1/1	0.33	5.77	68,68,68,68	1
2	ZN	C	425	1/1	0.29	5.17	42,42,42,42	1
2	ZN	L	425	1/1	0.28	4.92	55,55,55,55	1
2	ZN	E	426	1/1	0.41	4.57	45,45,45,45	1
2	ZN	O	425	1/1	0.29	4.30	50,50,50,50	1
2	ZN	O	426	1/1	0.32	3.86	58,58,58,58	1
2	ZN	N	426	1/1	0.31	3.77	55,55,55,55	1
2	ZN	J	425	1/1	0.25	3.65	60,60,60,60	1
2	ZN	M	426	1/1	0.37	3.49	63,63,63,63	1
2	ZN	L	426	1/1	0.31	3.46	63,63,63,63	1
2	ZN	D	426	1/1	0.31	3.10	33,33,33,33	1
2	ZN	G	425	1/1	0.26	2.93	40,40,40,40	1
2	ZN	C	426	1/1	0.26	2.84	38,38,38,38	1
2	ZN	F	426	1/1	0.29	2.80	51,51,51,51	1
2	ZN	P	426	1/1	0.38	2.72	59,59,59,59	1
2	ZN	N	425	1/1	0.27	2.39	41,41,41,41	1
2	ZN	H	425	1/1	0.27	2.10	40,40,40,40	1
2	ZN	A	425	1/1	0.23	1.79	51,51,51,51	1
2	ZN	A	426	1/1	0.21	1.77	52,52,52,52	1
2	ZN	E	425	1/1	0.28	1.76	43,43,43,43	1
2	ZN	H	426	1/1	0.28	1.76	39,39,39,39	1
2	ZN	B	426	1/1	0.25	1.70	44,44,44,44	1
2	ZN	B	425	1/1	0.25	1.38	44,44,44,44	1
2	ZN	F	425	1/1	0.24	1.33	52,52,52,52	1
2	ZN	P	425	1/1	0.30	1.27	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	I	426	1/1	0.19	1.27	58,58,58,58	1
2	ZN	K	425	1/1	0.24	0.97	55,55,55,55	1
2	ZN	G	426	1/1	0.21	0.92	37,37,37,37	1
2	ZN	I	425	1/1	0.18	0.91	42,42,42,42	1
2	ZN	D	425	1/1	0.20	-0.05	34,34,34,34	1
2	ZN	K	426	1/1	0.15	-0.89	68,68,68,68	1
2	ZN	M	425	1/1	0.19	-1.84	50,50,50,50	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.