

Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 07:36 pm BST

PDB ID	:	1GQ 6
Title	:	PROCLAVAMINATE AMIDINO HYDROLASE FROM STREPTOMYCES
		CLAVULIGERUS
Authors	:	Elkins, J.M.; Clifton, I.J.; Hernandez, H.; Robinson, C.V.; Schofield, C.J.;
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Deposited on		
Resolution	:	1.75 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

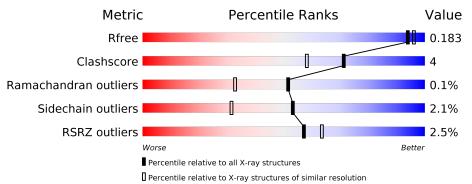
MolProbity Xtriage (Phenix) EDS		
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	$2340 \ (1.76-1.76)$
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437(1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 >=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 <=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	А	313	3% 88%	6%	• 6%
1	В	313	^{2%} 86%	9%	•••
1	С	313	87%	6%	7%



1 GQ6

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7083 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1 1		295	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		295	2151	1364	375	405	7	0	0	0
1	р	301	Total	С	Ν	Ο	S	0	0	0
		501	2201	1393	387	414	7			
1	1 C	20.2	Total	С	Ν	Ο	S	0	0	0
	292	2153	1364	377	405	7	0	0	0	

• Molecule 1 is a protein called PROCLAVAMINATE AMIDINO HYDROLASE.

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Mn 2 2	0	0
2	А	2	Total Mn 2 2	0	0
2	С	2	Total Mn 2 2	0	0

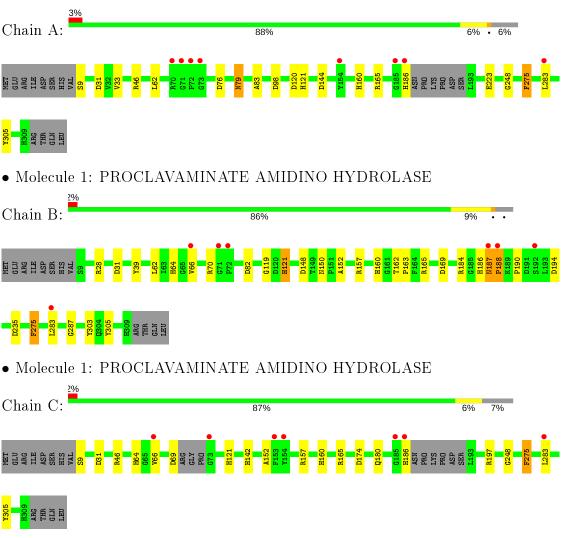
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	190	Total O 190 190	0	0
3	В	174	Total O 174 174	0	0
3	С	208	Total O 208 208	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: PROCLAVAMINATE AMIDINO HYDROLASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	139.86Å 78.93Å 93.20Å	Depositor
a, b, c, α , β , γ	90.00° 123.90° 90.00°	Depositor
Resolution (Å)	40.00 - 1.75	Depositor
	60.02 - 1.75	EDS
% Data completeness	97.1 (40.00-1.75)	Depositor
(in resolution range)	$97.1 \ (60.02 - 1.75)$	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.58 (at 1.75 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.0.32	Depositor
D D.	0.142 , 0.170	Depositor
R, R_{free}	0.156 , 0.183	DCC
R_{free} test set	4106 reflections (4.98%)	wwPDB-VP
Wilson B-factor $(Å^2)$	13.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 46.9	EDS
L-test for twinning ²	$ \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	0.96	EDS
Total number of atoms	7083	wwPDB-VP
Average B, all atoms $(Å^2)$	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MN

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		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.65	0/2204	0.81	5/3013~(0.2%)	
1	В	0.67	0/2257	0.89	7/3087~(0.2%)	
1	С	0.67	0/2204	0.87	4/3007~(0.1%)	
All	All	0.66	0/6665	0.86	16/9107~(0.2%)	

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	В	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	165	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	В	165	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	С	69	ASP	CB-CG-OD2	6.28	123.95	118.30
1	А	98	ASP	CB-CG-OD2	6.17	123.85	118.30
1	А	31	ASP	CB-CG-OD2	5.79	123.51	118.30
1	В	31	ASP	CB-CG-OD2	5.76	123.48	118.30
1	С	174	ASP	CB-CG-OD2	5.64	123.38	118.30
1	С	31	ASP	CB-CG-OD2	5.62	123.36	118.30
1	В	148	ASP	CB-CG-OD1	5.43	123.19	118.30
1	В	82	ASP	CB-CG-OD2	5.32	123.09	118.30
1	А	144	ASP	CB-CG-OD2	5.22	123.00	118.30
1	А	165	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	В	194	ASP	CB-CG-OD2	5.17	122.96	118.30

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Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	76	ASP	CB-CG-OD2	5.08	122.88	118.30
1	В	28	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	В	169	ASP	CB-CG-OD2	5.00	122.81	118.30

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There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	187	ASN	Mainchain,Peptide

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	А	2151	0	2059	17	0
1	В	2201	0	2109	21	0
1	С	2153	0	2078	22	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
3	А	190	0	0	2	0
3	В	174	0	0	7	1
3	C	208	0	0	2	1
All	All	7083	0	6246	45	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 4.

All (45) 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:188:PRO:HD2	3:B:2104:HOH:O	1.54	1.04
1:B:66:VAL:O	1:C:186:HIS:ND1	2.07	0.88
1:A:186:HIS:ND1	1:C:66:VAL:O	2.13	0.82
1:A:283:LEU:HB2	3:A:2174:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic $distance (\lambda)$	Clash	
1.D.104.ADC.O		$\frac{\text{distance (Å)}}{2.10}$	$\frac{\text{overlap}(\text{\AA})}{0.62}$	
1:B:184:ARG:O 1:A:186:HIS:CB	3:B:2100:HOH:O 1:C:66:VAL:O	2.10	0.68	
		2.49	0.61	
1:B:187:ASN:CB	3:B:2104:HOH:O	2.49	0.60	
1:A:186:HIS:CB	1:C:64:HIS:HB2	2.34	0.57	
1:B:70:ARG:NH1	1:B:303:TYR:CD2	2.73	0.57	
1:A:186:HIS:HB3	1:C:66:VAL:O	2.04	0.56	
1:A:33:VAL:CG1	1:A:83:ALA:HB2	2.36	0.55	
1:A:186:HIS:CG	1:C:66:VAL:O	2.60	0.55	
1:C:9:SER:N	3:C:2001:HOH:O	2.39	0.55	
1:B:152:ALA:HB1	1:B:157:ARG:HA	1.90	0.54	
1:B:187:ASN:HA	3:B:2103:HOH:O	2.06	0.54	
1:B:66:VAL:O	1:C:186:HIS:CG	2.61	0.54	
1:B:287:GLY:N	3:B:2163:HOH:O	2.41	0.53	
1:B:66:VAL:O	1:C:186:HIS:CB	2.57	0.52	
1:A:33:VAL:HG13	1:A:83:ALA:HB2	1.92	0.51	
1:A:186:HIS:HB3	1:C:64:HIS:HB2	1.93	0.51	
1:B:275:PHE:HZ	1:B:305:TYR:HB2	1.76	0.51	
1:C:275:PHE:HZ	1:C:305:TYR:HB2	1.77	0.48	
1:B:283:LEU:HB2	3:B:2155:HOH:O	2.15	0.47	
1:A:186:HIS:HD1	1:C:66:VAL:C	2.15	0.47	
1:A:79:ASN:ND2	3:A:2059:HOH:O	2.47	0.46	
1:C:283:LEU:HB2	3:C:2190:HOH:O	2.14	0.46	
1:A:186:HIS:CD2	1:C:64:HIS:O	2.69	0.46	
1:A:9:SER:OG	1:A:9:SER:O	2.28	0.46	
1:B:188:PRO:CD	3:B:2104:HOH:O	2.31	0.45	
1:B:66:VAL:O	1:C:186:HIS:HB3	2.14	0.45	
1:B:64:HIS:HB2	1:C:186:HIS:CB	2.47	0.44	
1:C:46:ARG:HB2	1:C:248:GLY:HA2	2.00	0.43	
1:B:150:ASN:ND2	1:B:187:ASN:O	2.52	0.43	
1:B:186:HIS:CG	1:B:190:PRO:HA	2.53	0.43	
1:B:39:TYR:O	1:B:119:GLY:HA2	2.19	0.42	
1:B:64:HIS:O	1:C:186:HIS:CD2	2.72	0.42	
1:A:186:HIS:CG	1:C:64:HIS:O	2.72	0.42	
1:A:283:LEU:HA	1:A:283:LEU:HD12	1.86	0.42	
1:B:162:THR:N	1:B:163:PRO:CD	2.82	0.41	
1:A:275:PHE:HZ	1:A:305:TYR:HB2	1.85	0.41	
1:B:121:HIS:CE1	1:B:235:ASP:HB2	2.54	0.41	
1:C:197:ARG:HH11	1:C:197:ARG:HD2	1.74	0.41	
1:C:152:ALA:HB1	1:C:157:ARG:HA	2.02	0.40	
1:A:46:ARG:HB2	1:A:248:GLY:HA2	2.03	0.40	
1:C:142:HIS:O	1:C:180:GLN:HA	2.22	0.40	

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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)
3:B:2069:HOH:O	3:C:2080:HOH:O[2_655]	2.13	0.07

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	А	291/313~(93%)	284 (98%)	7 (2%)	0	100 100
1	В	299/313~(96%)	290~(97%)	8 (3%)	1 (0%)	41 22
1	С	286/313~(91%)	279~(98%)	7 (2%)	0	100 100
All	All	876/939~(93%)	853 (97%)	22 (2%)	1 (0%)	51 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	188	PRO

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	А	215/245~(88%)	208~(97%)	7(3%)	38 15
1	В	221/245~(90%)	217~(98%)	4 (2%)	59 40
1	С	218/245~(89%)	215~(99%)	3~(1%)	67 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	654/735~(89%)	640~(98%)	14 (2%)	53 31

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	62	LEU
1	А	79	ASN
1	А	120	ASP
1	А	121	HIS
1	А	160	HIS
1	А	223	GLU
1	А	275	PHE
1	В	62	LEU
1	В	121	HIS
1	В	160	HIS
1	В	275	PHE
1	С	121	HIS
1	С	160	HIS
1	С	275	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	79	ASN
1	В	79	ASN

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 6 ligands modelled in this entry, 6 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^{th} 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 $>$	$\# RSRZ {>}2$	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	295/313~(94%)	-0.23	8 (2%) 54 60	4, 7, 16, 24	0
1	В	301/313~(96%)	-0.16	7 (2%) 60 67	3, 7, 17, 25	0
1	С	292/313~(93%)	-0.19	7 (2%) 59 65	4, 7, 15, 23	0
All	All	888/939~(94%)	-0.20	22 (2%) 57 63	3, 7, 16, 25	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	71	GLY	5.1	
1	В	72	PRO	4.7	
1	С	154	TYR	4.5	
1	В	66	VAL	4.3	
1	А	154	TYR	4.1	
1	В	188	PRO	4.0	
1	А	72	PRO	3.6	
1	А	71	GLY	3.6	
1	С	186	HIS	3.0	
1	С	185	GLY	3.0	
1	А	73	GLY	2.9	
1	С	283	LEU	2.7	
1	А	185	GLY	2.7	
1	С	66	VAL	2.7	
1	С	153	PHE	2.6	
1	А	186	HIS	2.5	
1	В	187	ASN	2.5	
1	В	283	LEU	2.4	
1	А	70	ARG	2.3	
1	С	73	GLY	2.2	
1	А	283	LEU	2.2	
1	В	192	SER	2.0	



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^{th} 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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
2	MN	А	350	1/1	1.00	0.04	9,9,9,9	0
2	MN	А	351	1/1	1.00	0.04	$11,\!11,\!11,\!11$	0
2	MN	С	351	1/1	1.00	0.04	9,9,9,9	0
2	MN	С	350	1/1	1.00	0.04	8,8,8,8	0
2	MN	В	350	1/1	1.00	0.04	8,8,8,8	0
2	MN	В	351	1/1	1.00	0.04	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.

