



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:23 PM GMT

PDB ID : 4I4N
Title : Crystal Structure of the catalytic Cys to Ala mutant of VcHsp31 from *Vibrio cholerae*
Authors : Sen, U.; Das, S.
Deposited on : 2012-11-28
Resolution : 1.84 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

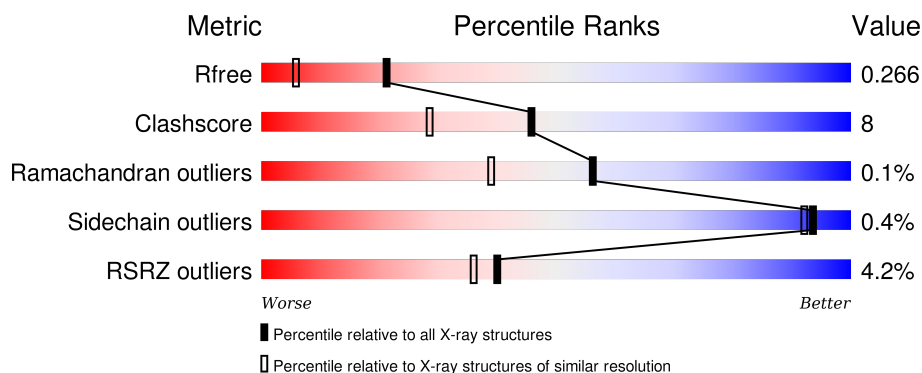
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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. 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	281	<div> <div>3%</div> <div>85%</div> <div>15%</div> </div>
1	B	281	<div> <div>2%</div> <div>86%</div> <div>14%</div> </div>
1	C	281	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
1	D	281	<div> <div>4%</div> <div>84%</div> <div>16%</div> </div>
1	E	281	<div> <div>7%</div> <div>80%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain	
			6%	24%
1	F	281	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '6%', a large green segment in the middle labeled '76%', and a yellow segment at the end labeled '24%'. The total length of the bar represents 100% of the chain's quality assessment.	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13514 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 Intracellular protease/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2163	1390	352	412	9			
1	B	281	Total	C	N	O	S	0	0	0
			2163	1390	352	412	9			
1	C	281	Total	C	N	O	S	0	0	0
			2163	1390	352	412	9			
1	D	281	Total	C	N	O	S	0	0	0
			2163	1390	352	412	9			
1	E	281	Total	C	N	O	S	0	0	0
			2163	1390	352	412	9			
1	F	281	Total	C	N	O	S	0	0	0
			2163	1390	352	412	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	-	EXPRESSION TAG	UNP A5F0Q0
A	188	ALA	CYS	ENGINEERED MUTATION	UNP A5F0Q0
A	285	GLY	-	EXPRESSION TAG	UNP A5F0Q0
B	5	ALA	-	EXPRESSION TAG	UNP A5F0Q0
B	188	ALA	CYS	ENGINEERED MUTATION	UNP A5F0Q0
B	285	GLY	-	EXPRESSION TAG	UNP A5F0Q0
C	5	ALA	-	EXPRESSION TAG	UNP A5F0Q0
C	188	ALA	CYS	ENGINEERED MUTATION	UNP A5F0Q0
C	285	GLY	-	EXPRESSION TAG	UNP A5F0Q0
D	5	ALA	-	EXPRESSION TAG	UNP A5F0Q0
D	188	ALA	CYS	ENGINEERED MUTATION	UNP A5F0Q0
D	285	GLY	-	EXPRESSION TAG	UNP A5F0Q0
E	5	ALA	-	EXPRESSION TAG	UNP A5F0Q0
E	188	ALA	CYS	ENGINEERED MUTATION	UNP A5F0Q0
E	285	GLY	-	EXPRESSION TAG	UNP A5F0Q0
F	5	ALA	-	EXPRESSION TAG	UNP A5F0Q0
F	188	ALA	CYS	ENGINEERED MUTATION	UNP A5F0Q0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	285	GLY	-	EXPRESSION TAG	UNP A5F0Q0

- Molecule 2 is water.

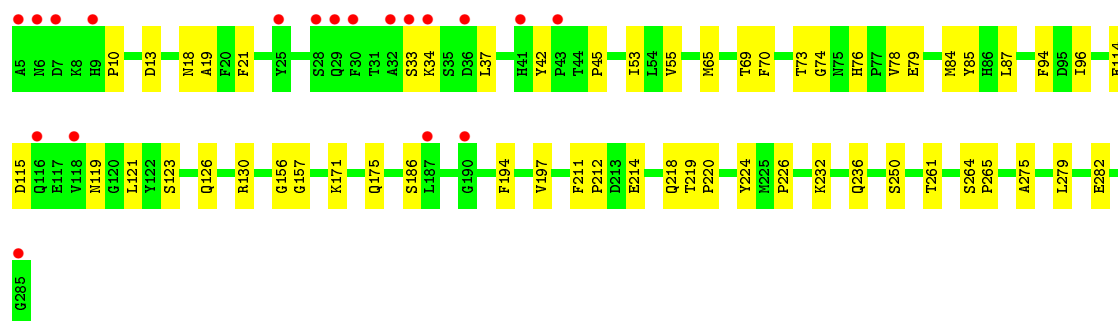
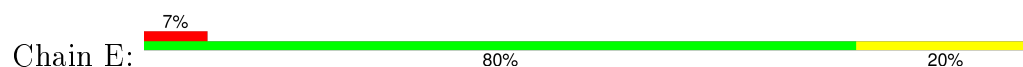
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	88	Total 88	O 88	0	0
2	B	138	Total 138	O 138	0	0
2	C	129	Total 129	O 129	0	0
2	D	77	Total 77	O 77	0	0
2	E	58	Total 58	O 58	0	0
2	F	46	Total 46	O 46	0	0

- Molecule 1: Intracellular protease/amidase

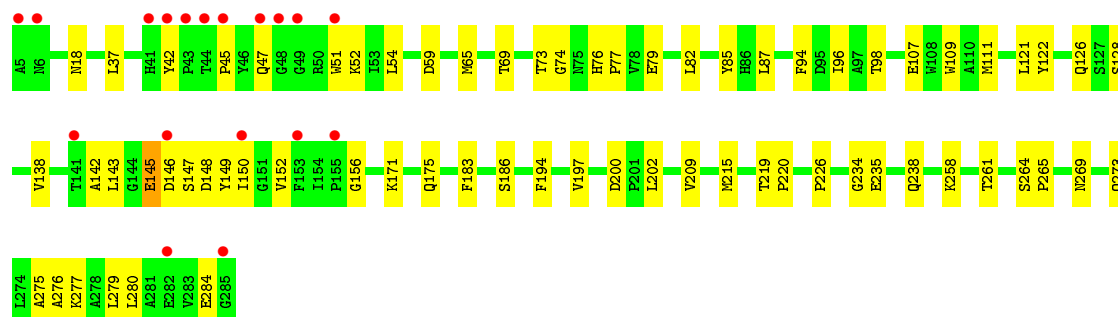
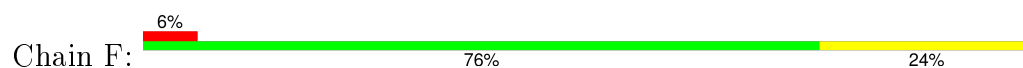




- Molecule 1: Intracellular protease/amidase



- Molecule 1: Intracellular protease/amidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.75Å 79.35Å 107.65Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	29.36 – 1.84 29.36 – 1.84	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.36-1.84) 91.1 (29.36-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.84Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.243 , 0.266 0.243 , 0.266	Depositor DCC
R_{free} test set	6528 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.0	EDS
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 130816 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13514	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/2225	0.64	0/3022
1	B	0.38	0/2225	0.64	0/3022
1	C	0.38	0/2225	0.64	1/3022 (0.0%)
1	D	0.37	0/2225	0.63	1/3022 (0.0%)
1	E	0.35	0/2225	0.62	1/3022 (0.0%)
1	F	0.35	0/2225	0.62	0/3022
All	All	0.36	0/13350	0.63	3/18132 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	GLY	N-CA-C	-5.29	99.86	113.10
1	E	157	GLY	N-CA-C	-5.29	99.89	113.10
1	D	157	GLY	N-CA-C	-5.25	99.99	113.10

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	2163	0	2077	31	0
1	B	2163	0	2077	31	0
1	C	2163	0	2077	18	0
1	D	2163	0	2077	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2163	0	2077	38	0
1	F	2163	0	2077	44	0
2	A	88	0	0	1	0
2	B	138	0	0	5	0
2	C	129	0	0	1	0
2	D	77	0	0	0	0
2	E	58	0	0	1	0
2	F	46	0	0	1	0
All	All	13514	0	12462	195	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 8.

The worst 5 of 195 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:271:LEU:HA	2:B:413:HOH:O	1.65	0.96
1:D:273:GLN:O	1:D:277:LYS:HG2	1.69	0.93
1:D:53:ILE:HD13	1:D:87:LEU:HD13	1.51	0.92
1:B:264:SER:HB2	1:B:265:PRO:HD2	1.52	0.90
1:B:58:ALA:H	1:B:75:ASN:HD21	1.25	0.84

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	279/281 (99%)	268 (96%)	11 (4%)	0	100	100
1	B	279/281 (99%)	269 (96%)	9 (3%)	1 (0%)	39	22
1	C	279/281 (99%)	268 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	279/281 (99%)	266 (95%)	13 (5%)	0	100	100
1	E	279/281 (99%)	268 (96%)	10 (4%)	1 (0%)	39	22
1	F	279/281 (99%)	265 (95%)	14 (5%)	0	100	100
All	All	1674/1686 (99%)	1604 (96%)	68 (4%)	2 (0%)	56	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	250	SER
1	B	201	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	225/225 (100%)	224 (100%)	1 (0%)	93	92
1	B	225/225 (100%)	224 (100%)	1 (0%)	93	92
1	C	225/225 (100%)	224 (100%)	1 (0%)	93	92
1	D	225/225 (100%)	224 (100%)	1 (0%)	93	92
1	E	225/225 (100%)	225 (100%)	0	100	100
1	F	225/225 (100%)	223 (99%)	2 (1%)	84	78
All	All	1350/1350 (100%)	1344 (100%)	6 (0%)	93	92

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	ASP
1	F	209	VAL
1	D	277	LYS
1	B	47	GLN
1	F	145	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	102	ASN
1	E	9	HIS
1	F	119	ASN
1	D	116	GLN
1	E	18	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](#)

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 ⓘ

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, 95th 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)	Q<0.9
1	A	281/281 (100%)	0.15	8 (2%) 56 53	11, 20, 37, 62	0
1	B	281/281 (100%)	0.06	7 (2%) 61 57	9, 16, 32, 60	0
1	C	281/281 (100%)	0.11	7 (2%) 61 57	9, 17, 34, 55	0
1	D	281/281 (100%)	0.33	11 (3%) 43 39	9, 20, 40, 61	0
1	E	281/281 (100%)	0.52	19 (6%) 20 17	14, 25, 49, 66	0
1	F	281/281 (100%)	0.61	18 (6%) 23 20	14, 26, 43, 60	0
All	All	1686/1686 (100%)	0.30	70 (4%) 40 36	9, 21, 41, 66	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	ALA	8.0
1	B	5	ALA	7.2
1	A	285	GLY	7.1
1	C	285	GLY	6.4
1	E	6	ASN	6.1

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.