



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2016 – 04:33 AM EDT

PDB ID : 4ZXP
Title : Crystal structure of Peptidyl- tRNA Hydrolase from *Vibrio cholerae*
Authors : Shahid, S.; Pal, R.K.; Kabra, A.; Yadav, R.; Kumar, A.; Arora, A.
Deposited on : 2015-05-20
Resolution : 1.63 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
<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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-20027790

i

X-RAY DIFFRACTION

A.

 R_{free} 1

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6047 atoms, of which 2737 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.

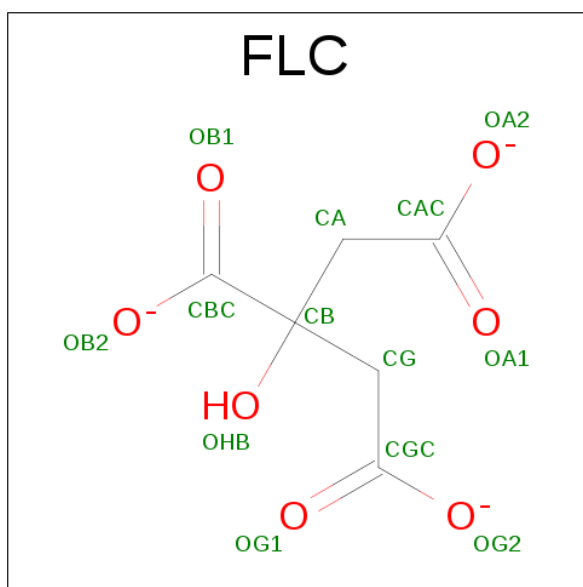
- Molecule 1 is a protein called Peptidyl-tRNA hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	196	Total	C	H	N	O	S	0	2	0
			2874	956	1380	262	270	6			
1	B	197	Total	C	H	N	O	S	0	0	0
			2824	938	1352	261	268	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	see sequence details	UNP Q9KQ21
A	0	ALA	-	see sequence details	UNP Q9KQ21
A	1	MET	-	expression tag	UNP Q9KQ21
A	2	VAL	-	expression tag	UNP Q9KQ21
B	-1	GLY	-	see sequence details	UNP Q9KQ21
B	0	ALA	-	see sequence details	UNP Q9KQ21
B	1	MET	-	expression tag	UNP Q9KQ21
B	2	VAL	-	expression tag	UNP Q9KQ21

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total	O	0	0
			179	179		
3	B	152	Total	O	0	0
			152	152		

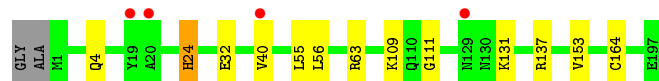
3 Residue-property plots [i](#)

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: Peptidyl-tRNA hydrolase



- Molecule 1: Peptidyl-tRNA hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.72Å 73.63Å 124.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.55 – 1.63 32.55 – 1.63	Depositor EDS
% Data completeness (in resolution range)	91.0 (32.55-1.63) 90.3 (32.55-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.171 , 0.211 0.169 , 0.210	Depositor DCC
R_{free} test set	1897 reflections (4.03%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6047	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.01 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.5567e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, FLC

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	0.53	0/1522	0.63	0/2053
1	B	0.49	0/1491	0.61	0/2017
All	All	0.51	0/3013	0.62	0/4070

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1494	1380	1483	7	0
1	B	1472	1352	1446	9	0
2	B	13	5	5	0	0
3	A	179	0	0	0	1
3	B	152	0	0	4	0
All	All	3310	2737	2934	16	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 3.

All (16) 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:32:GLU:OE1	3:B:301:HOH:O	2.08	0.72
1:B:109:LYS:HE3	1:B:137:ARG:HD2	1.71	0.71
1:B:164:CSO:OD	3:B:302:HOH:O	2.10	0.67
1:A:88:LYS:HG3	1:A:91:GLU:OE1	2.07	0.54
1:A:33:GLU:OE2	1:A:36:ARG:NH2	2.43	0.49
1:A:109:LYS:HE3	1:A:111:GLY:O	2.12	0.49
1:A:55:LEU:HD11	1:A:57:ILE:HD11	2.00	0.43
1:B:56:LEU:HD13	3:B:319:HOH:O	2.18	0.43
1:A:26:ALA:HA	1:A:29:TRP:CE3	2.55	0.42
1:B:40:VAL:HG21	1:B:55:LEU:HD23	2.02	0.42
1:A:7:LYS:HE2	1:A:91:GLU:OE2	2.20	0.41
1:B:111:GLY:HA2	1:B:131:LYS:O	2.20	0.41
1:B:24:HIS:CG	1:B:153:VAL:HG12	2.56	0.41
1:B:63:ARG:NH2	3:B:304:HOH:O	2.52	0.41
1:B:24:HIS:ND1	1:B:153:VAL:CG1	2.84	0.41
1:A:13:ALA:HB2	1:A:28:ALA:HB2	2.03	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)
3:A:251:HOH:O	3:A:344:HOH:O 4_466]	2.18	0.02

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	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
1	B	194/199 (98%)	192 (99%)	2 (1%)	0	100	100
All	All	389/398 (98%)	386 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	145/158 (92%)	142 (98%)	3 (2%)	61	32
1	B	140/158 (89%)	138 (99%)	2 (1%)	74	52
All	All	285/316 (90%)	280 (98%)	5 (2%)	66	41

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	40	VAL
1	A	55	LEU
1	B	4	GLN
1	B	24	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	A	164	1	3,6,7	0.44	0	2,6,8	1.41	0
1	CSO	B	164	1	3,6,7	0.59	0	2,6,8	1.56	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	164	1	-	0/1/5/7	0/0/0/0
1	CSO	B	164	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	CSO	O-C-CA	-2.01	120.32	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	164	CSO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FLC	B	201	-	3,12,12	0.92	0	3,17,17	1.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	B	201	-	-	0/6/16/16	0/0/0/0

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 ⓘ

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	195/199 (97%)	0.13	9 (4%)	36 32	20, 29, 44, 71	1 (0%)
1	B	196/199 (98%)	0.06	4 (2%)	68 69	22, 32, 51, 75	0
All	All	391/398 (98%)	0.10	13 (3%)	50 48	20, 30, 47, 75	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	TYR	5.4
1	A	2	VAL	4.2
1	B	20	ALA	4.2
1	A	59	SER	3.9
1	A	197	GLU	3.1
1	B	40	VAL	2.7
1	A	144	GLY	2.7
1	A	12	LEU	2.5
1	A	27	GLY	2.4
1	A	28	ALA	2.2
1	A	159	ALA	2.2
1	A	58	ASN	2.1
1	B	129	ASN	2.0

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

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, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
1	CSO	B	164	7/8	0.95	0.07	-	27,28,40,42	0
1	CSO	A	164	7/8	0.95	0.07	-	26,27,42,49	0

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. 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, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
2	FLC	B	201	13/13	0.87	0.17	1.31	28,34,41,43	2

6.5 Other polymers [i](#)

There are no such residues in this entry.