



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2020 – 09:42 pm BST

PDB ID : 5TR7  
Title : Crystal structure of a putative D-alanyl-D-alanine carboxypeptidase from *Vibrio cholerae* O1 biovar eltor str. N16961  
Authors : Filippova, E.V.; Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Dubrovskaya, I.; Shatsman, S.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2016-10-25  
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11



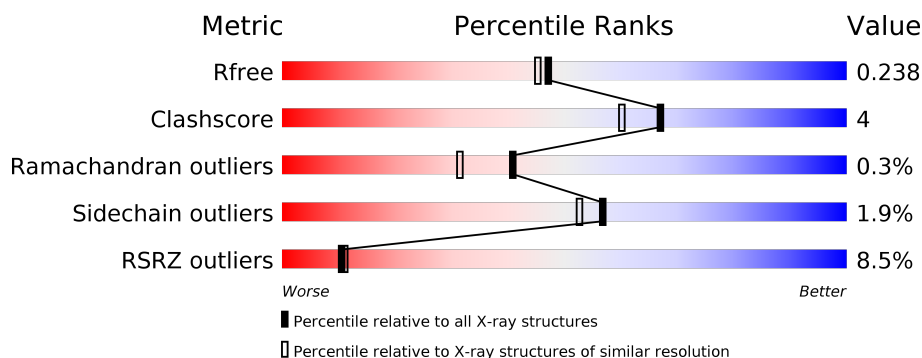
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 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  $\leq 5\%$ . 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	341	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>6%</div> <div>26%</div> </div> </div>
1	B	341	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>9%</div> <div>27%</div> </div> </div>
1	C	341	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>6%</div> <div>26%</div> </div> </div>



## 2 Entry composition [i](#)

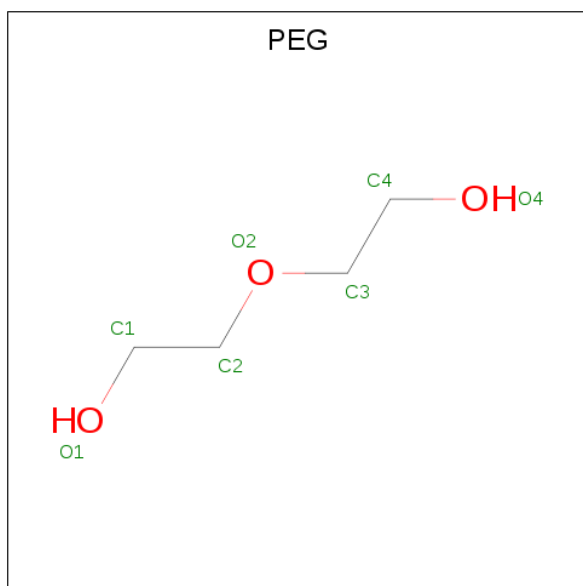
There are 5 unique types of molecules in this entry. The entry contains 5902 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanyl-D-alanine carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1930	1210	326	382	12			
1	B	249	Total	C	N	O	S	0	0	0
			1912	1200	324	376	12			
1	C	251	Total	C	N	O	S	0	1	0
			1936	1213	327	384	12			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

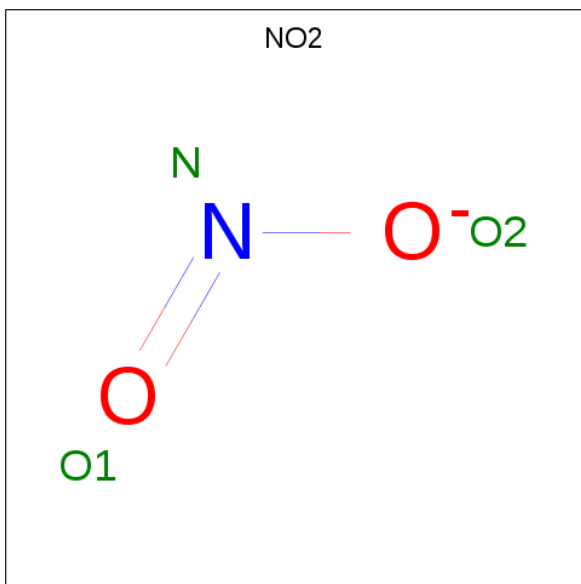
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			3	1	2		
3	A	1	Total	N	O	0	0
			3	1	2		
3	C	1	Total	N	O	0	0
			3	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	38	Total	O	0	0
			38	38		
5	C	17	Total	O	0	0
			17	17		







THR  
ALA  
SER  
PHE  
VAL  
LEU  
GLU  
LYS  
GLN  
LEU  
LYS  
ALA  
PRO  
LEU  
LYS  
LYS  
GLY  
ASP  
ILE  
VAL  
GLY  
THR  
LEU  
TYR  
TYR  
GLN  
LEU  
ALA  
GLY  
ASN  
ASP  
ILE  
ALA  
GLN  
TYR  
PRO  
LEU  
LEU  
ALA  
LEU  
GLU  
ASP  
VAL  
GLN  
GLU



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.75Å 88.75Å 85.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.05 29.05 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.05) 100.0 (29.05-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.191 , 0.238 0.193 , 0.238	Depositor DCC
$R_{free}$ test set	2246 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.043 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5902	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, NO2

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	0.95	2/1965 (0.1%)	1.10	8/2656 (0.3%)
1	B	0.87	1/1947 (0.1%)	1.02	5/2631 (0.2%)
1	C	0.91	1/1971 (0.1%)	1.08	6/2664 (0.2%)
All	All	0.91	4/5883 (0.1%)	1.07	19/7951 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLU	CD-OE1	8.36	1.34	1.25
1	A	157	SER	CB-OG	-5.99	1.34	1.42
1	B	198	GLU	CD-OE1	5.67	1.31	1.25
1	C	203	SER	CB-OG	-5.58	1.35	1.42

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	A	193	ARG	NE-CZ-NH1	13.41	127.00	120.30
1	C	193	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	173	ASP	CB-CA-C	-9.37	91.67	110.40
1	A	198	GLU	CG-CD-OE2	-8.19	101.92	118.30

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	1930	0	1885	11	0
1	B	1912	0	1871	22	0
1	C	1936	0	1889	15	0
2	A	7	0	10	0	0
2	B	14	0	20	0	0
2	C	7	0	10	0	0
3	A	6	0	0	0	0
3	C	3	0	0	0	0
4	B	6	0	8	0	0
5	A	26	0	0	2	0
5	B	38	0	0	1	0
5	C	17	0	0	0	0
All	All	5902	0	5693	45	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 4.

The worst 5 of 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:A:193:ARG:HD2	1:A:194:ASP:OD1	1.73	0.89
1:C:193:ARG:HD2	1:C:194:ASP:OD1	1.79	0.82
1:B:114:THR:HG21	5:B:512:HOH:O	1.84	0.78
1:B:167:THR:HB	1:C:224:LYS:HE2	1.67	0.76
1:C:217:ARG:HB2	1:C:233:THR:HG21	1.71	0.72

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	249/341 (73%)	244 (98%)	4 (2%)	1 (0%)	34	24
1	B	247/341 (72%)	241 (98%)	5 (2%)	1 (0%)	34	24
1	C	250/341 (73%)	244 (98%)	6 (2%)	0	100	100
All	All	746/1023 (73%)	729 (98%)	15 (2%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	B	109	PHE

### 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	209/283 (74%)	204 (98%)	5 (2%)	49	42
1	B	207/283 (73%)	203 (98%)	4 (2%)	57	53
1	C	210/283 (74%)	207 (99%)	3 (1%)	67	65
All	All	626/849 (74%)	614 (98%)	12 (2%)	57	53

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	60	THR
1	B	114	THR
1	C	95	LYS
1	A	198	GLU
1	B	268	LYS

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 ⓘ

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 ⓘ

8 ligands 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	$\# Z  > 2$
2	PEG	B	402	-	6,6,6	0.47	0	5,5,5	0.32	0
3	NO2	A	402	-	1,2,2	0.14	0	0,1,1	0.00	-
3	NO2	C	402	-	1,2,2	0.10	0	0,1,1	0.00	-
2	PEG	B	401	-	6,6,6	0.48	0	5,5,5	0.41	0
2	PEG	C	401	-	6,6,6	0.46	0	5,5,5	0.28	0
4	GOL	B	403	-	5,5,5	0.31	0	5,5,5	0.48	0
2	PEG	A	401	-	6,6,6	0.55	0	5,5,5	0.31	0
3	NO2	A	403	-	1,2,2	0.06	0	0,1,1	0.00	-

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	PEG	C	401	-	-	2/4/4/4	-
2	PEG	B	401	-	-	1/4/4/4	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	B	402	-	-	1/4/4/4	-
4	GOL	B	403	-	-	0/4/4/4	-
2	PEG	A	401	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	PEG	O1-C1-C2-O2
2	B	402	PEG	O2-C3-C4-O4
2	A	401	PEG	O2-C3-C4-O4
2	A	401	PEG	C1-C2-O2-C3
2	C	401	PEG	O2-C3-C4-O4

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<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	251/341 (73%)	0.15	20 (7%)	12 13	46, 61, 87, 125	0
1	B	249/341 (73%)	0.20	20 (8%)	12 13	42, 61, 93, 125	0
1	C	251/341 (73%)	0.27	24 (9%)	8 8	51, 64, 93, 109	0
All	All	751/1023 (73%)	0.20	64 (8%)	10 11	42, 62, 92, 125	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	ALA	6.7
1	B	231	ILE	4.9
1	B	175	PRO	4.6
1	A	244	VAL	4.1
1	C	231	ILE	4.1

### 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<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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NO2	A	402	3/3	0.71	0.18	80,80,87,100	0
2	PEG	B	402	7/7	0.73	0.33	89,95,100,100	0
2	PEG	A	401	7/7	0.81	0.26	78,90,103,104	0
3	NO2	C	402	3/3	0.87	0.09	87,87,89,92	0
4	GOL	B	403	6/6	0.88	0.13	73,82,86,87	0
2	PEG	B	401	7/7	0.91	0.12	52,64,69,75	0
2	PEG	C	401	7/7	0.91	0.07	67,70,72,72	0
3	NO2	A	403	3/3	0.91	0.13	68,68,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.