



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:37 am BST

PDB ID : 4XZY
Title : Crystal structure of dipeptidyl peptidase 11 (DPP11) from *Porphyromonas gingivalis*
Authors : Sakamoto, Y.; Suzuki, Y.; Iizuka, I.; Tateoka, C.; Roppongi, S.; Fujimoto, M.; Nonaka, T.; Ogasawara, W.; Tanaka, N.
Deposited on : 2015-02-05
Resolution : 2.70 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 ⓘ 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

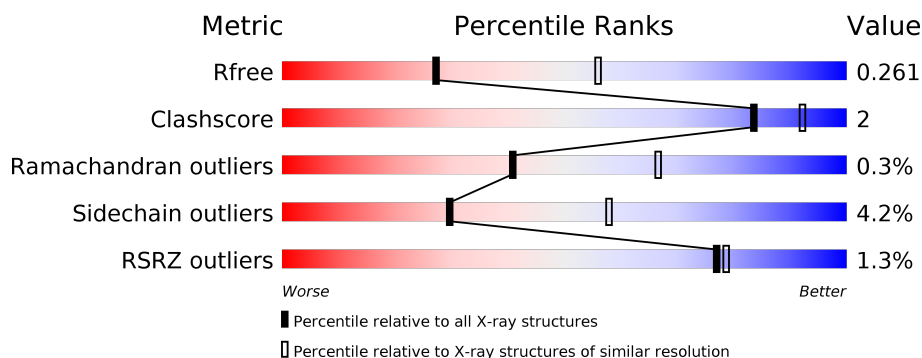
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	720	<div> <div></div> <div>87%</div> <div>9%</div> <div></div> </div>
1	B	720	<div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11544 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 Peptidase S46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5608	3553	970	1058	27			
1	B	699	Total	C	N	O	S	0	1	0
			5618	3558	972	1061	27			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

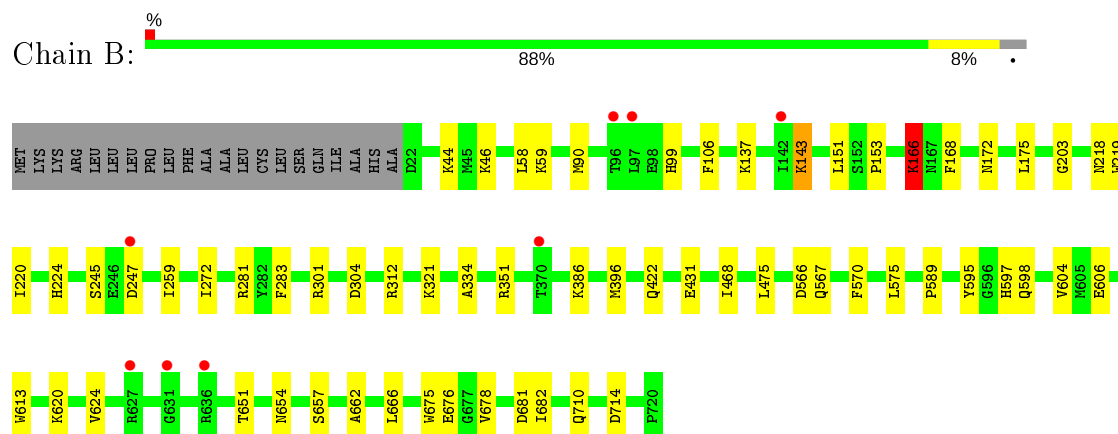
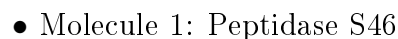
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total	O	0	0
			161	161		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	151	Total	O	0	0
			151	151		

- Molecule 1: Peptidase S46



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.14Å 116.64Å 147.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (40.00-2.70) 93.2 (39.53-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.181 , 0.258 0.188 , 0.261	Depositor DCC
R_{free} test set	2252 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11544	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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:
GOL

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	0.64	1/5733 (0.0%)	0.81	2/7745 (0.0%)
1	B	0.61	0/5743	0.82	3/7757 (0.0%)
All	All	0.63	1/11476 (0.0%)	0.81	5/15502 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	TRP	CB-CG	6.09	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	681	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	392	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	301	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	33	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	351	ARG	NE-CZ-NH1	5.21	122.90	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	LYS	Peptide

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	5608	0	5491	29	0
1	B	5618	0	5498	25	0
2	A	6	0	8	0	0
3	A	161	0	0	2	1
3	B	151	0	0	0	1
All	All	11544	0	10997	53	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 2.

All (53) 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:139:LEU:O	1:A:142:ILE:HG13	1.95	0.66
1:B:589:PRO:HG3	1:B:595:TYR:CE2	2.38	0.58
1:A:302:MET:HE2	1:A:400:GLY:HA2	1.86	0.58
1:B:651:THR:H	1:B:654:ASN:HD22	1.53	0.56
1:A:675:TRP:O	1:A:678:VAL:HG22	2.06	0.56
1:A:348:ARG:HD3	1:A:685:LEU:HD13	1.90	0.53
1:A:101:TYR:HB3	1:A:106:PHE:HB2	1.92	0.52
1:B:620:LYS:O	1:B:624:VAL:HG23	2.10	0.51
1:B:259:ILE:CD1	1:B:666:LEU:HD23	2.41	0.51
1:A:560:LEU:HB3	1:A:569:GLN:HE22	1.75	0.51
1:A:340:GLY:HA3	1:A:678:VAL:HG21	1.93	0.51
1:B:172:ASN:HB3	1:B:175:LEU:HD12	1.92	0.51
1:A:83:ASN:HD22	1:A:85:HIS:CE1	2.30	0.50
1:A:166:LYS:HG2	1:A:167:ASN:HA	1.92	0.50
1:A:352:GLN:OE1	1:A:352:GLN:N	2.42	0.49
1:A:166:LYS:HA	1:A:168:PHE:N	2.26	0.49
1:B:218:ASN:O	1:B:220:ILE:HG12	2.14	0.48
1:B:166:LYS:HA	1:B:168:PHE:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ILE:N	1:B:682:ILE:HD12	2.29	0.48
1:B:597:HIS:CD2	1:B:598:GLN:HB2	2.50	0.47
1:B:396:MET:HG3	1:B:468:ILE:HD11	1.95	0.47
1:A:219:TRP:CD1	3:A:1052:HOH:O	2.68	0.47
1:A:422:GLN:HG3	1:A:516:VAL:HG11	1.98	0.45
1:A:271:MET:HG2	1:A:660:MET:HB2	1.99	0.45
1:B:219:TRP:O	1:B:675:TRP:N	2.50	0.45
1:B:44:LYS:HG2	1:B:662:ALA:HB1	1.99	0.45
1:B:675:TRP:O	1:B:678:VAL:HG13	2.17	0.44
1:A:647:THR:O	1:A:684:TYR:OH	2.34	0.44
1:A:566:ASP:C	1:A:566:ASP:OD1	2.56	0.44
1:B:224:HIS:HB3	1:B:604:VAL:HG22	2.00	0.43
1:B:151:LEU:O	1:B:153:PRO:HD3	2.18	0.43
1:B:166:LYS:HA	1:B:168:PHE:N	2.33	0.43
1:A:348:ARG:CD	1:A:685:LEU:HD13	2.49	0.42
1:A:83:ASN:ND2	1:A:85:HIS:CE1	2.87	0.42
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.83	0.42
1:B:676:GLU:N	1:B:676:GLU:OE1	2.48	0.42
1:A:130:ASP:HA	1:A:189:LEU:HD23	2.01	0.42
1:A:43:LEU:HD11	1:A:45:MET:HG2	2.00	0.42
1:A:543:ARG:HB3	1:A:544:PRO:HD3	2.01	0.42
1:B:272:ILE:HG23	1:B:657:SER:HB3	2.00	0.42
1:A:151:LEU:O	1:A:153:PRO:HD3	2.20	0.42
1:A:272:ILE:HG12	1:A:659:VAL:HG22	2.02	0.42
1:B:281:ARG:HG3	1:B:570:PHE:CE1	2.55	0.42
1:A:590:ARG:HB2	1:B:606:GLU:OE1	2.20	0.41
1:A:340:GLY:CA	1:A:678:VAL:HG21	2.50	0.41
1:B:259:ILE:HD12	1:B:666:LEU:HD23	2.01	0.41
1:B:106:PHE:O	1:B:203:GLY:HA2	2.20	0.41
1:A:425:ASP:HB3	1:A:428:ALA:HB3	2.03	0.41
1:A:24:GLY:HA3	1:A:26:TRP:CE2	2.56	0.40
1:A:569:GLN:HA	3:A:945:HOH:O	2.19	0.40
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.93	0.40
1:B:675:TRP:O	1:B:678:VAL:HG22	2.21	0.40
1:B:710:GLN:NE2	1:B:714:ASP:OD1	2.53	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:924:HOH:O	3:B:820:HOH:O[2_554]	2.19	0.01

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	697/720 (97%)	671 (96%)	25 (4%)	1 (0%)	51	78
1	B	698/720 (97%)	669 (96%)	26 (4%)	3 (0%)	34	60
All	All	1395/1440 (97%)	1340 (96%)	51 (4%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	LYS
1	B	166	LYS
1	B	334	ALA
1	A	372	ARG

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	590/607 (97%)	562 (95%)	28 (5%)	26	54
1	B	591/607 (97%)	570 (96%)	21 (4%)	35	64
All	All	1181/1214 (97%)	1132 (96%)	49 (4%)	30	59

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	59	LYS

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Mol	Chain	Res	Type
1	A	75	SER
1	A	90	MET
1	A	137	LYS
1	A	143	LYS
1	A	162	LYS
1	A	163	LYS
1	A	166	LYS
1	A	175	LEU
1	A	177	VAL
1	A	207	SER
1	A	238	ASN
1	A	247	ASP
1	A	252	LYS
1	A	255	ARG
1	A	304	ASP
1	A	312	ARG
1	A	325	SER
1	A	379	GLU
1	A	504	GLU
1	A	567	GLN
1	A	575	LEU
1	A	598	GLN
1	A	602	ASP
1	A	622	LYS
1	A	632	ARG
1	A	678	VAL
1	B	46	LYS
1	B	59	LYS
1	B	90	MET
1	B	99	HIS
1	B	137	LYS
1	B	143	LYS
1	B	166	LYS
1	B	245	SER
1	B	247	ASP
1	B	283	PHE
1	B	304	ASP
1	B	312	ARG
1	B	321	LYS
1	B	386	LYS
1	B	422	GLN
1	B	431	GLU

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Mol	Chain	Res	Type
1	B	475	LEU
1	B	566	ASP
1	B	567	GLN
1	B	575	LEU
1	B	613	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	218	ASN
1	A	238	ASN
1	A	267	ASN
1	A	307	GLN
1	A	506	GLN
1	A	567	GLN
1	A	569	GLN
1	A	654	ASN
1	B	83	ASN
1	B	146	ASN
1	B	157	GLN
1	B	186	ASN
1	B	307	GLN
1	B	422	GLN
1	B	506	GLN
1	B	597	HIS
1	B	654	ASN

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

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	GOL	A	801	-	5,5,5	0.71	0	5,5,5	0.32	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	GOL	A	801	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	C1-C2-C3-O3
2	A	801	GOL	O2-C2-C3-O3
2	A	801	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	699/720 (97%)	-0.13	10 (1%) 75 77	28, 47, 72, 109	0
1	B	699/720 (97%)	-0.14	8 (1%) 80 82	28, 49, 76, 102	0
All	All	1398/1440 (97%)	-0.13	18 (1%) 77 78	28, 48, 74, 109	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	LYS	3.5
1	A	613	TRP	3.4
1	A	636	ARG	3.3
1	B	97	LEU	3.2
1	A	97	LEU	3.1
1	B	636	ARG	3.1
1	A	142	ILE	2.9
1	A	99	HIS	2.8
1	B	627	ARG	2.8
1	A	247	ASP	2.7
1	A	98	GLU	2.6
1	A	167	ASN	2.3
1	A	237	LYS	2.2
1	B	370	THR	2.2
1	B	142	ILE	2.1
1	B	247	ASP	2.1
1	B	631	GLY	2.1
1	B	96	THR	2.0

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 [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, 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	B-factors(\AA^2)	Q<0.9
2	GOL	A	801	6/6	0.82	0.26	48,54,58,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.