



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 01:20 pm GMT

PDB ID : 1PFQ  
Title : crystal structure of human apo dipeptidyl peptidase IV / CD26  
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Deposited on : 2003-05-27  
Resolution : 1.90 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

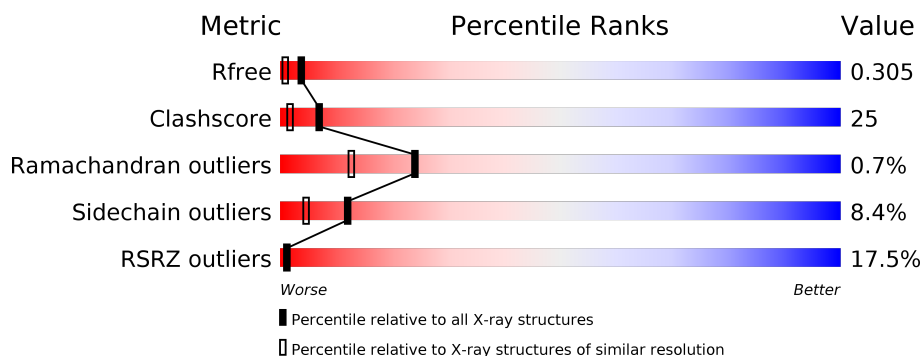
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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. 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	731	<div> <div>16%</div> <div>64%</div> <div>30%</div> <div>5%</div> </div>
1	B	731	<div> <div>19%</div> <div>59%</div> <div>34%</div> <div>6%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

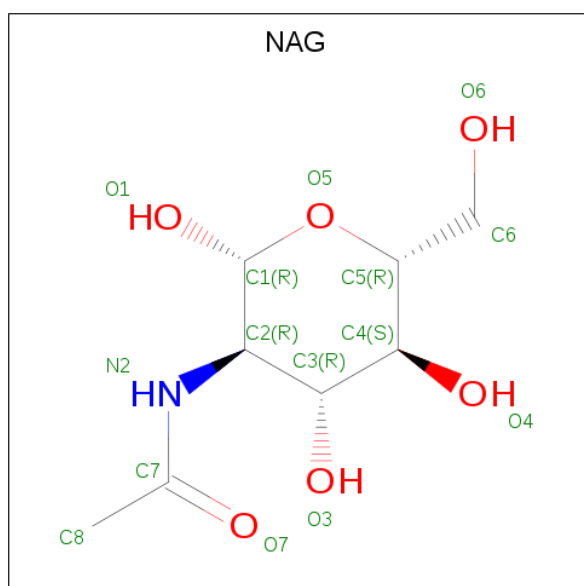
There are 3 unique types of molecules in this entry. The entry contains 12418 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase IV soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			
1	B	725	Total	C	N	O	S	0	0	0
			5926	3801	977	1122	26			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	268	Total 268	O 268	0	0
3	B	204	Total 204	O 204	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.03Å 118.14Å 184.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 29.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-1.90) 98.7 (29.77-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.254 , 0.298 0.264 , 0.305	Depositor DCC
$R_{free}$ test set	11796 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: NAG

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	0.27	0/6136	0.60	27/8344 (0.3%)
1	B	0.26	0/6094	0.60	33/8287 (0.4%)
All	All	0.26	0/12230	0.60	60/16631 (0.4%)

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	B	0	1

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	545	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	725	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	200	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	725	ASP	CB-CG-OD2	5.79	123.51	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	581	ARG	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	5964	0	5683	271	3
1	B	5926	0	5650	314	3
2	A	28	0	26	1	0
2	B	28	0	26	1	0
3	A	268	0	0	26	0
3	B	204	0	0	16	2
All	All	12418	0	11385	573	5

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 25.

The worst 5 of 573 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:517:ILE:HG21	1:A:612:GLN:NE2	1.28	1.45
1:A:517:ILE:CG2	1:A:612:GLN:HE22	1.37	1.36
1:A:198:ILE:HD11	1:A:211:TYR:CE2	1.73	1.22
1:B:544:LEU:HD21	1:B:606:GLN:NE2	1.56	1.20
1:A:150:ASN:ND2	3:A:1095:HOH:O	1.71	1.17

All (5) 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:1043:HOH:O	3:B:1054:HOH:O[3_555]	1.53	0.67
1:A:98:PHE:CZ	1:B:168:TRP:CZ3[1_455]	1.81	0.39
1:A:83:TYR:CD1	1:A:677:GLU:OE1[1_455]	1.89	0.31
1:B:642:SER:O	3:B:1017:HOH:O[1_455]	1.91	0.29
1:A:98:PHE:CZ	1:B:168:TRP:CH2[1_455]	2.12	0.08

## 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	726/731 (99%)	678 (93%)	45 (6%)	3 (0%)	36	25
1	B	721/731 (99%)	667 (92%)	47 (6%)	7 (1%)	17	7
All	All	1447/1462 (99%)	1345 (93%)	92 (6%)	10 (1%)	24	13

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	B	140	ARG
1	B	341	VAL
1	A	98	PHE
1	B	274	ASP

### 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	653/655 (100%)	596 (91%)	57 (9%)	11	4
1	B	647/655 (99%)	595 (92%)	52 (8%)	13	5
All	All	1300/1310 (99%)	1191 (92%)	109 (8%)	12	4

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	642	SER

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Mol	Chain	Res	Type
1	B	69	LEU
1	B	614	SER
1	A	684	ARG
1	A	749	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	ASN
1	B	112	GLN
1	B	612	GLN
1	A	612	GLN
1	A	740	HIS

### 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](#)

4 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	NAG	A	851	1	14,14,15	0.60	0	17,19,21	0.85	1 (5%)
2	NAG	A	853	1	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
2	NAG	B	852	1	14,14,15	0.55	0	17,19,21	0.86	1 (5%)
2	NAG	B	855	1	14,14,15	0.55	0	17,19,21	0.77	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	NAG	A	851	1	-	0/6/23/26	0/1/1/1
2	NAG	A	853	1	-	0/6/23/26	0/1/1/1
2	NAG	B	852	1	-	0/6/23/26	0/1/1/1
2	NAG	B	855	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	853	NAG	O5-C1-C2	-2.97	107.42	111.52
2	B	852	NAG	O5-C5-C6	2.17	110.58	107.15
2	A	851	NAG	O5-C5-C6	2.21	110.64	107.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	853	NAG	1	0
2	B	855	NAG	1	0

## 5.7 Other polymers [i](#)

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 [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	728/731 (99%)	1.04	116 (15%) <b>2</b> <b>2</b>	14, 40, 55, 60	0
1	B	725/731 (99%)	1.26	138 (19%) <b>1</b> <b>1</b>	17, 43, 64, 72	0
All	All	1453/1462 (99%)	1.15	254 (17%) <b>1</b> <b>1</b>	14, 41, 59, 72	0

The worst 5 of 254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ASP	11.2
1	A	95	PHE	10.8
1	B	340	LEU	10.7
1	B	279	VAL	9.1
1	A	766	PRO	8.9

### 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
2	NAG	B	855	14/15	0.63	0.25	68,69,69,69	0
2	NAG	B	852	14/15	0.87	0.14	42,42,44,45	0
2	NAG	A	853	14/15	0.89	0.15	42,43,43,44	0
2	NAG	A	851	14/15	0.90	0.10	48,48,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.