



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:58 AM GMT

PDB ID : 2JID
Title : Human Dipeptidyl peptidase IV in complex with 1-(3,4-Dimethoxy-phenyl) -
3-m-tolyl-piperidine-4-ylamine
Authors : Hennig, M.; Stihle, M.; Luebbers, T.; Thoma, R.
Deposited on : 2007-02-28
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

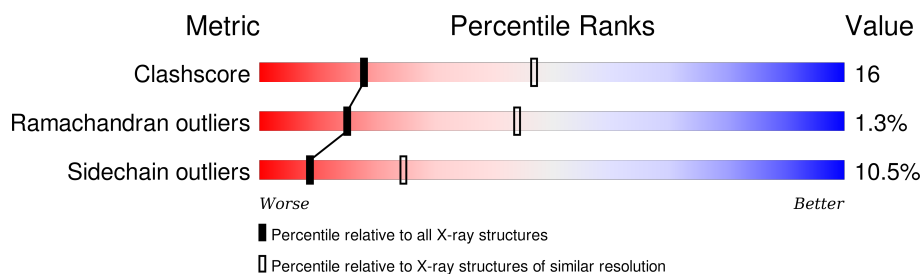
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	736	
1	B	736	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1770	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12214 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

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



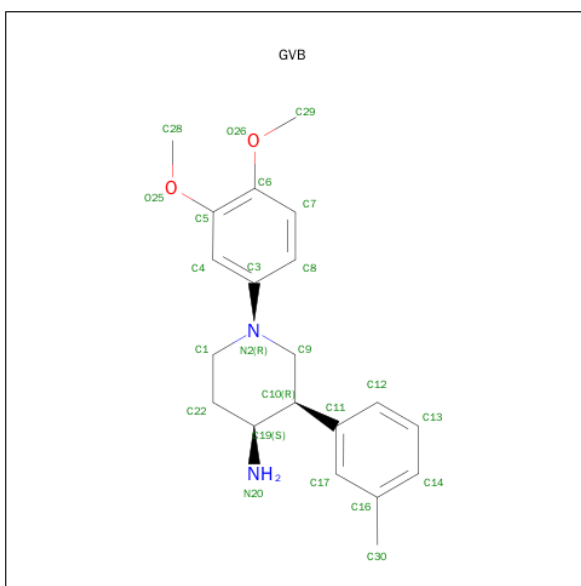
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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 (3R,4S)-1-(3,4-DIMETHOXYPHENYL)-3-(3-METHYLPHENYL)PIPERIDI
N-4-AMINE (three-letter code: GVB) (formula: C₂₀H₂₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	20	2	2		
3	B	1	Total	C	N	O	0	0
			24	20	2	2		

- Molecule 4 is water.

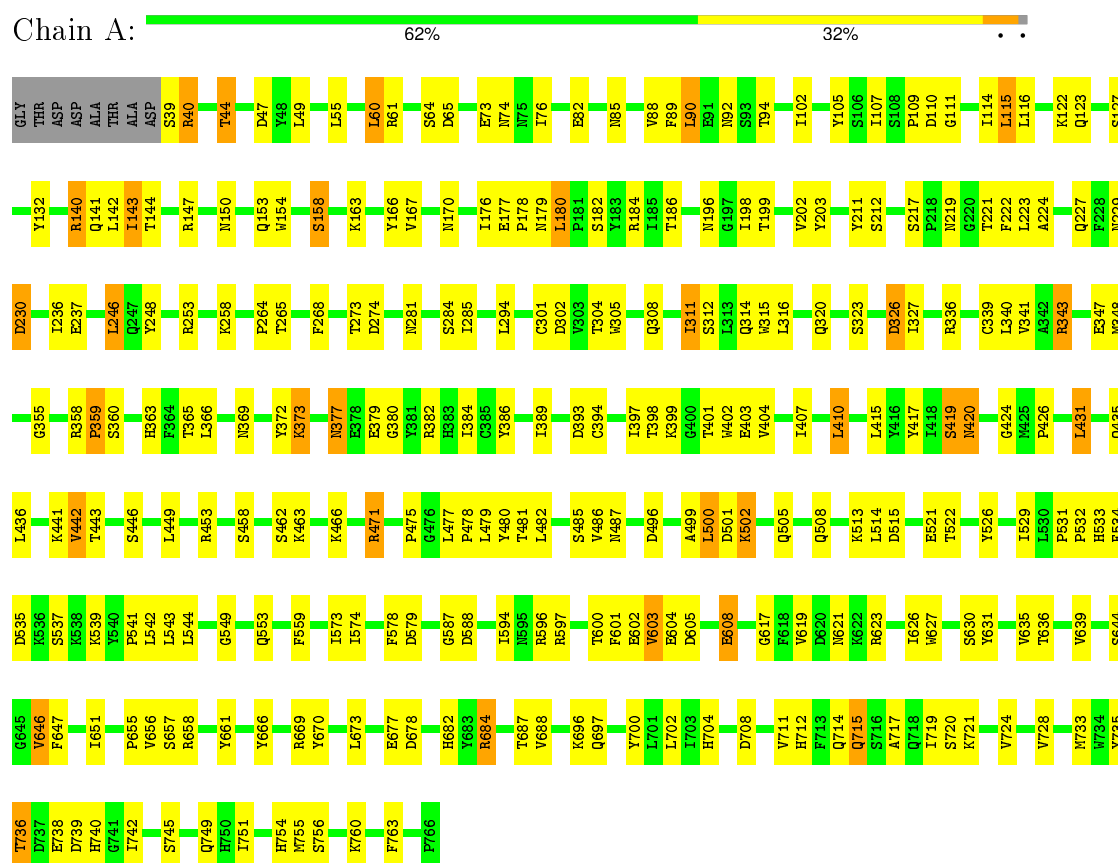
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	73	Total	O	0	0
			73	73		

3 Residue-property plots

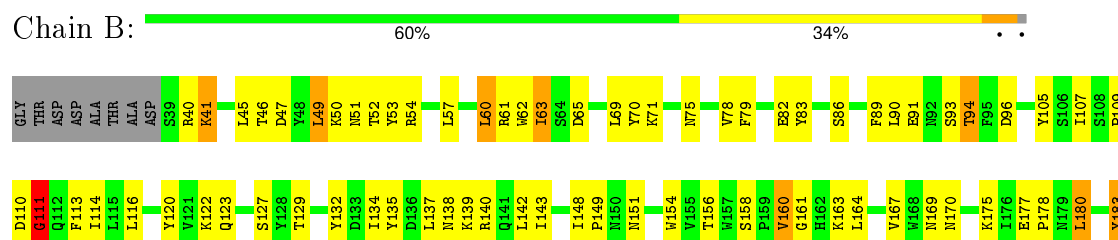
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: DIPEPTIDYL PEPTIDASE 4



• Molecule 1: DIPEPTIDYL PEPTIDASE 4



V698	E699	Y700	N710	N711	H712	F713	Q714	Q715	S716	A717	D725	V726	G727	V728	D729	Y735	T736	G741	I742	Q749	H750	I751	Y752	T753	H754	N755	K760	Q761	C762	F763	S764	L765	F766																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
g599	T600	E602	V603		Q606		R611		S614	K615		F618	V619	D620	N621	K622	R623	I624	A625	H626	H627	S630	V635	T636	S637	N638	V639	K648	C649	G650	S657	R658	D663	V666	R669	T675	D678	N679	L680	D681	H682	V683	R684		T687	F695	K696	Q697																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.25Å 66.82Å 423.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.4 (20.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12214	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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: GVB, 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	0.65	0/6135	0.77	3/8344 (0.0%)
1	B	0.68	1/6135 (0.0%)	0.78	4/8344 (0.0%)
All	All	0.67	1/12270 (0.0%)	0.78	7/16688 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	GLU	CG-CD	5.10	1.59	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	LEU	CA-CB-CG	6.71	130.72	115.30
1	A	60	LEU	CA-CB-CG	6.30	129.79	115.30
1	A	500	LEU	CA-CB-CG	6.21	129.59	115.30
1	B	111	GLY	N-CA-C	5.43	126.68	113.10
1	B	57	LEU	CA-CB-CG	5.34	127.59	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	GLY	Peptide

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	5963	0	5684	196	0
1	B	5963	0	5681	186	0
2	A	56	0	52	10	0
2	B	56	0	52	3	0
3	A	24	0	26	3	0
3	B	24	0	26	5	0
4	A	55	0	0	5	0
4	B	73	0	0	4	0
All	All	12214	0	11521	373	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 16.

The worst 5 of 373 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:229:ASN:HD21	2:B:1769:NAG:C1	1.47	1.26
1:A:281:ASN:HD21	2:A:1769:NAG:C1	1.51	1.23
1:B:351:THR:HG22	1:B:592:HIS:ND1	1.67	1.09
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.30	1.07
1:A:608:GLU:OE1	1:A:608:GLU:HA	1.51	1.02

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	726/736 (99%)	639 (88%)	78 (11%)	9 (1%)	16	47
1	B	726/736 (99%)	637 (88%)	79 (11%)	10 (1%)	14	42
All	All	1452/1472 (99%)	1276 (88%)	157 (11%)	19 (1%)	15	44

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	486	VAL
1	A	73	GLU
1	A	604	GLU
1	B	94	THR

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	653/658 (99%)	584 (89%)	69 (11%)	8	24
1	B	653/658 (99%)	585 (90%)	68 (10%)	9	25
All	All	1306/1316 (99%)	1169 (90%)	137 (10%)	8	24

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	627	TRP
1	B	90	LEU
1	B	620	ASP
1	A	673	LEU
1	B	41	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	697	GLN
1	B	229	ASN
1	B	694	ASN
1	A	715	GLN
1	B	123	GLN

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](#)

10 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	1767	-	14,14,15	0.62	0	15,19,21	1.75	5 (33%)
2	NAG	A	1768	-	14,14,15	0.62	0	15,19,21	1.10	1 (6%)
2	NAG	A	1769	-	14,14,15	0.55	0	15,19,21	0.82	0
2	NAG	A	1770	1	14,14,15	0.51	0	15,19,21	1.69	2 (13%)
3	GVB	A	1771	-	26,26,26	0.61	0	32,36,36	1.01	2 (6%)
2	NAG	B	1767	1	14,14,15	0.58	0	15,19,21	1.77	3 (20%)
2	NAG	B	1768	1	14,14,15	0.61	0	15,19,21	1.40	2 (13%)
2	NAG	B	1769	-	14,14,15	0.89	0	15,19,21	1.70	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1770	1	14,14,15	0.76	1 (7%)	15,19,21	1.43	2 (13%)
3	GVB	B	1771	-	26,26,26	0.58	0	32,36,36	1.09	2 (6%)

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	1767	-	-	1/6/23/26	0/1/1/1
2	NAG	A	1768	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1769	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1770	1	-	0/6/23/26	0/1/1/1
3	GVB	A	1771	-	-	0/12/25/25	0/3/3/3
2	NAG	B	1767	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1768	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1769	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1770	1	1/1/5/7	0/6/23/26	0/1/1/1
3	GVB	B	1771	-	-	0/12/25/25	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1770	NAG	C1-C2	2.46	1.55	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1769	NAG	C2-N2-C7	-3.55	118.48	123.04
2	B	1770	NAG	C3-C4-C5	-3.27	104.49	110.20
2	B	1768	NAG	O3-C3-C4	-2.46	104.79	110.34
2	A	1768	NAG	C1-O5-C5	-2.35	109.27	112.25
2	B	1769	NAG	O6-C6-C5	-2.26	103.87	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1770	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1767	NAG	O7-C7-N2-C2
2	B	1767	NAG	O7-C7-N2-C2
2	B	1767	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1767	NAG	4	0
2	A	1768	NAG	4	0
2	A	1769	NAG	2	0
3	A	1771	GVB	3	0
2	B	1769	NAG	3	0
3	B	1771	GVB	5	0

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.