



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:45 PM UTC

PDB ID : 1J2E / pdb_00001j2e
Title : Crystal structure of Human Dipeptidyl peptidase IV
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Deposited on : 2002-12-30
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

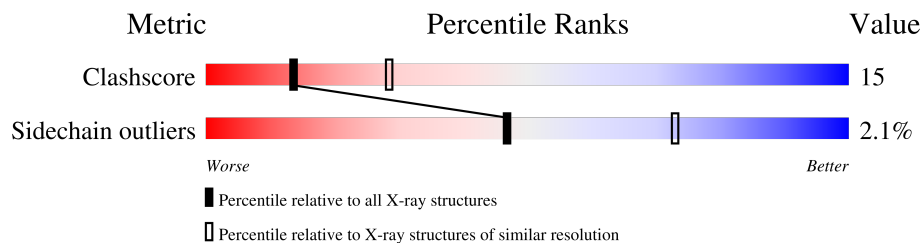
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	740	
1	B	740	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12355 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	729	5971	3831	983	1131	26	0	0	0
1	B	729	5971	3831	983	1131	26	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	HIS	-	expression tag	UNP P27487
A	768	HIS	-	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
B	767	HIS	-	expression tag	UNP P27487
B	768	HIS	-	expression tag	UNP P27487
B	769	HIS	-	expression tag	UNP P27487
B	770	HIS	-	expression tag	UNP P27487
B	771	HIS	-	expression tag	UNP P27487
B	772	HIS	-	expression tag	UNP P27487

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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		
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		
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	136	Total	O	0	0
			136	136		
3	B	137	Total	O	0	0
			137	137		

F222	F223	A224	Y225	L236	E237	Y241	E244	Y248	R253	A259	M263	F268	F269	M281	L285	Q296	P290	A291	S292	M293	L294	I295	L300	M305	Q308	W315	I319	Q320	V324	M325	D326	Y330	D331	E332	S333	S334	G335	R336	M337	C339				
I340	V341	A342	R343	E361	L366	E378	E379	Q388	I397	T398	E403	Y414	I418	G428	R429	M430	C454	S458	V459	S460	F461	S462	K463	K466	Y467	Y468	Q469	L470	R471	C472	L477	P478	H483	S484	S485	K489	L494	L500	D501	L504	Q505			
R506	V507	Q508	K512	K513	I517	I518	L519	M520	E521	Y526	Q527	M528	P531	D535	K538	K539	Y540	P541	L542	V546	Y547	A548	M562	W563	A564	T565	A568	E571	I574	Y585	I594	M595	R596	R597	L598	G599	T600	F601	E602	V603	E604	T605	Q606	Q612
F618	V619	D620	R623	I624	A625	I626	S630	Y631	Y634	W635	T636	L640	G650	V656	S657	R658	W659	E660	Y661	Y666	R669	Y670	M671	H682	E693	K696	I703	M710	Q714	V724	D725	V726	F730	Q731	A732	M733	W734	H740	G741	I742	A743	S744		
I751	M755	I759	K760	P766	HIS	HIS	HIS	HIS	HIS	HIS																																		

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.04Å 125.92Å 136.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.4 (10.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX	Depositor
R, R_{free}	0.249 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12355	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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:
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	0.40	0/6143	0.90	25/8355 (0.3%)
1	B	0.40	0/6143	0.90	21/8355 (0.3%)
All	All	0.40	0/12286	0.90	46/16710 (0.3%)

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	SER	N-CA-C	-8.06	97.08	109.24
1	B	300	LEU	N-CA-C	-7.44	97.11	109.46
1	A	300	LEU	N-CA-C	-7.42	97.16	108.96
1	B	656	VAL	N-CA-C	-7.12	98.05	108.87
1	A	656	VAL	N-CA-C	-7.11	99.74	109.55

There are no chirality outliers.

There are no planarity outliers.

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	5971	0	5684	177	0
1	B	5971	0	5683	175	0
2	A	70	0	65	2	0
2	B	70	0	65	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	136	0	0	0	0
3	B	137	0	0	2	0
All	All	12355	0	11497	343	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 15.

The worst 5 of 343 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:219:ASN:H	1:B:308:GLN:HE22	1.07	0.99
1:B:72:GLN:HG3	1:B:73:GLU:H	1.27	0.98
1:B:293:MET:HE3	1:B:324:VAL:HG12	1.46	0.97
1:B:528:MET:HE2	1:B:574:ILE:HG21	1.50	0.94
1:A:219:ASN:H	1:A:308:GLN:HE22	1.11	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	654/663 (99%)	644 (98%)	10 (2%)	57 80
1	B	654/663 (99%)	637 (97%)	17 (3%)	40 68
All	All	1308/1326 (99%)	1281 (98%)	27 (2%)	47 73

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	133	ASP
1	B	326	ASP
1	B	696	LYS
1	B	263	ASN
1	B	339	CYS

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

Mol	Chain	Res	Type
1	B	612	GLN
1	B	679	ASN
1	B	748	HIS
1	A	562	ASN
1	A	506	ASN

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 oligosaccharides 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	B	906	1	14,14,15	0.48	0	17,19,21	0.70	0
2	NAG	A	904	1	14,14,15	0.54	0	17,19,21	0.92	1 (5%)
2	NAG	B	907	1	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
2	NAG	A	901	1	14,14,15	0.53	0	17,19,21	0.70	0
2	NAG	A	905	1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
2	NAG	B	908	1	14,14,15	0.50	0	17,19,21	0.76	1 (5%)
2	NAG	B	909	1	14,14,15	0.56	0	17,19,21	0.59	0
2	NAG	B	910	1	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
2	NAG	A	902	1	14,14,15	0.51	0	17,19,21	0.71	0
2	NAG	A	903	1	14,14,15	0.44	0	17,19,21	0.75	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	B	906	1	-	3/6/23/26	0/1/1/1
2	NAG	A	904	1	-	0/6/23/26	0/1/1/1
2	NAG	B	907	1	-	3/6/23/26	0/1/1/1
2	NAG	A	901	1	-	3/6/23/26	0/1/1/1
2	NAG	A	905	1	-	2/6/23/26	0/1/1/1
2	NAG	B	908	1	-	2/6/23/26	0/1/1/1
2	NAG	B	909	1	-	4/6/23/26	0/1/1/1
2	NAG	B	910	1	-	2/6/23/26	0/1/1/1
2	NAG	A	902	1	-	2/6/23/26	0/1/1/1
2	NAG	A	903	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	905	NAG	C4-C3-C2	-3.59	105.75	111.02
2	B	907	NAG	C2-N2-C7	-2.81	119.13	122.90
2	A	905	NAG	C2-N2-C7	-2.77	119.19	122.90
2	B	910	NAG	C2-N2-C7	-2.48	119.58	122.90
2	B	908	NAG	C2-N2-C7	-2.29	119.84	122.90

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	NAG	C8-C7-N2-C2
2	A	901	NAG	O7-C7-N2-C2
2	A	902	NAG	C8-C7-N2-C2
2	A	902	NAG	O7-C7-N2-C2
2	A	903	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	905	NAG	1	0
2	B	909	NAG	2	0
2	B	910	NAG	1	0
2	A	902	NAG	1	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.