



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:24 AM UTC

PDB ID : 6EOS / pdb_00006eos
Title : DPP8 - Apo, space group 19
Authors : Ross, B.R.; Huber, R.
Deposited on : 2017-10-10
Resolution : 3.10 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

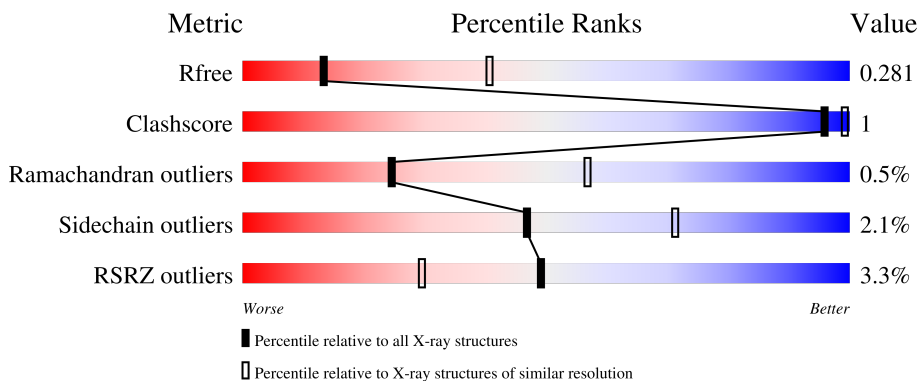
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



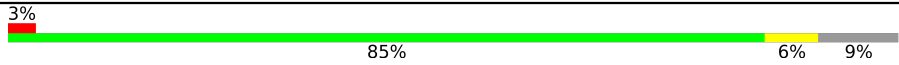
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	898	10% 87% 5% 9%
1	B	898	10% 84% 7% 10%
1	C	898	1% 87% 5% 8%
1	D	898	1% 87% 5% 9%
1	E	898	2% 87% 5% 8%

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Mol	Chain	Length	Quality of chain
1	F	898	 A horizontal bar chart showing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '3%', a large green segment labeled '85%', a small yellow segment labeled '6%', and a small grey segment at the end labeled '9%'. The segments are separated by thin white lines.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 39998 atoms, of which 0 are hydrogens and 0 are deuteriums.

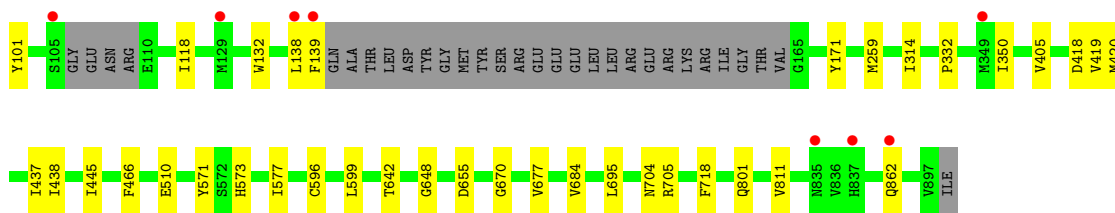
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptidyl peptidase 8.

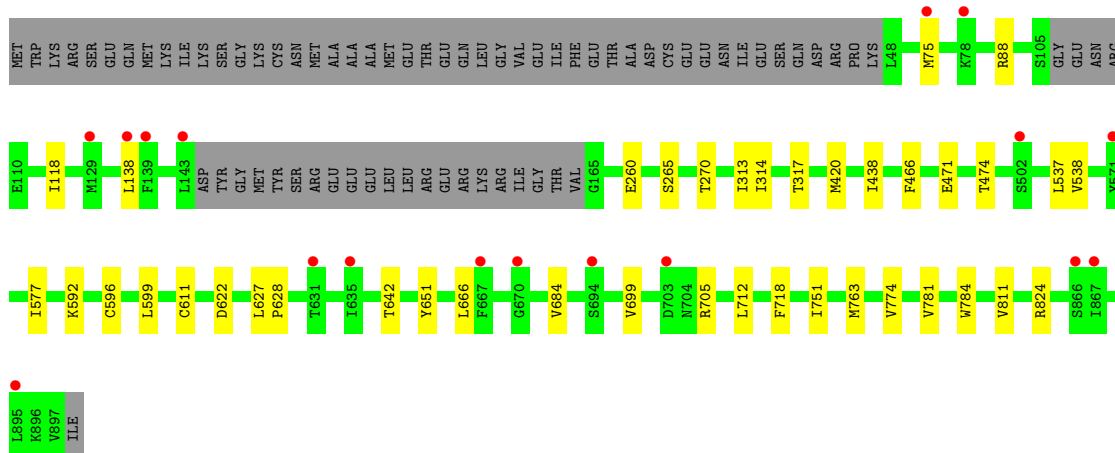
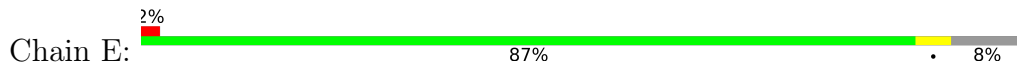
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	815	6620	4257	1107	1230	26	0	0	0
1	C	829	6740	4334	1130	1250	26	0	0	0
1	D	815	6613	4253	1104	1229	27	0	0	0
1	E	825	6697	4308	1118	1243	28	0	0	0
1	F	815	6620	4257	1107	1230	26	0	0	0
1	B	811	6583	4233	1100	1224	26	0	0	0

- Molecule 2 is water.

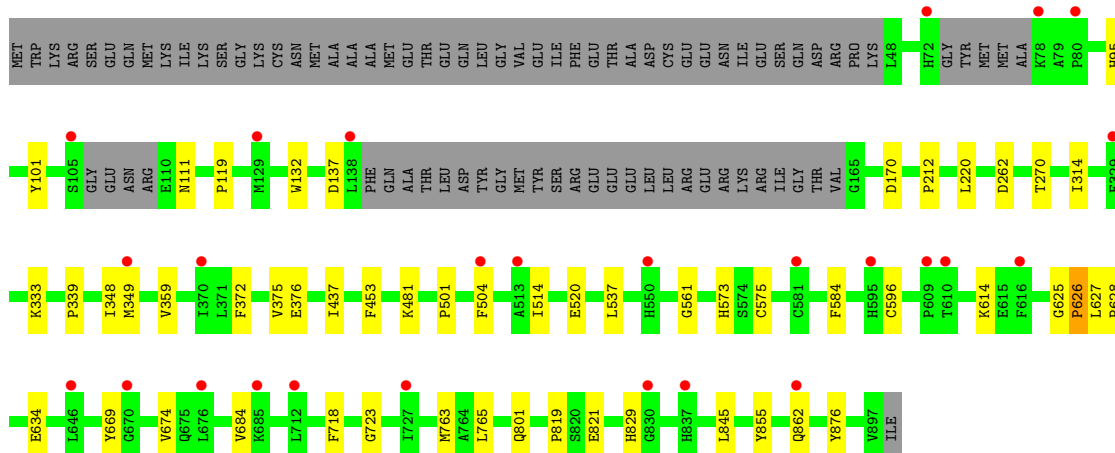
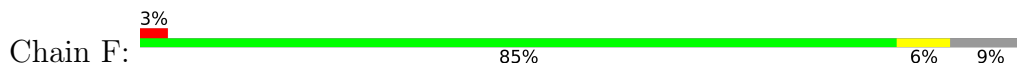
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total 32	O 32	0	0
2	C	23	Total 23	O 23	0	0
2	D	21	Total 21	O 21	0	0
2	E	21	Total 21	O 21	0	0
2	F	20	Total 20	O 20	0	0
2	B	8	Total 8	O 8	0	0



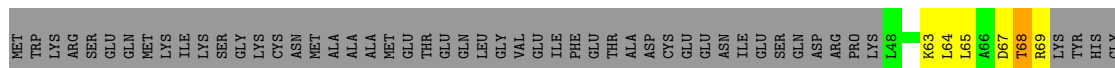
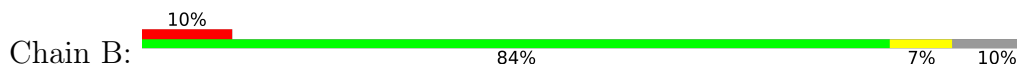
• Molecule 1: Dipeptidyl peptidase 8



• Molecule 1: Dipeptidyl peptidase 8



• Molecule 1: Dipeptidyl peptidase 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.12Å 266.78Å 268.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 3.10 44.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.40-3.10) 99.9 (44.40-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.247 , 0.283 0.247 , 0.281	Depositor DCC
R_{free} test set	9593 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtrriage
Anisotropy	0.549	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.003 for -h,l,k	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	39998	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% 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](#)

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	0.50	1/6805 (0.0%)	0.75	1/9234 (0.0%)
1	B	0.57	0/6766	0.76	0/9182
1	C	0.50	0/6925	0.75	0/9393
1	D	0.51	0/6797	0.74	0/9223
1	E	0.52	0/6885	0.76	0/9343
1	F	0.54	0/6805	0.77	0/9234
All	All	0.53	1/40983 (0.0%)	0.76	1/55609 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	ASP	CA-C	5.89	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	TYR	N-CA-C	-5.29	105.04	112.12

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	6620	0	6439	12	0
1	B	6583	0	6405	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6740	0	6576	15	0
1	D	6613	0	6433	10	0
1	E	6697	0	6515	15	0
1	F	6620	0	6439	15	0
2	A	32	0	0	0	0
2	B	8	0	0	0	0
2	C	23	0	0	0	0
2	D	21	0	0	0	0
2	E	21	0	0	0	0
2	F	20	0	0	0	0
All	All	39998	0	38807	84	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 1.

The worst 5 of 84 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:64:LEU:O	1:A:68:THR:HG23	1.93	0.67
1:F:101:TYR:HH	1:F:132:TRP:CD1	2.14	0.65
1:D:101:TYR:HH	1:D:132:TRP:CD1	2.18	0.62
1:A:333:LYS:HG2	1:A:336:THR:HG23	1.90	0.53
1:E:666:LEU:HD23	1:E:751:ILE:HD12	1.91	0.52

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	807/898 (90%)	767 (95%)	35 (4%)	5 (1%)	21	52
1	B	803/898 (89%)	728 (91%)	70 (9%)	5 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	821/898 (91%)	777 (95%)	42 (5%)	2 (0%)	43	73
1	D	807/898 (90%)	754 (93%)	47 (6%)	6 (1%)	18	49
1	E	819/898 (91%)	765 (93%)	54 (7%)	0	100	100
1	F	807/898 (90%)	750 (93%)	49 (6%)	8 (1%)	12	41
All	All	4864/5388 (90%)	4541 (93%)	297 (6%)	26 (0%)	24	57

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	THR
1	C	158	ARG
1	F	561	GLY
1	A	70	LYS
1	D	138	LEU

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	724/795 (91%)	717 (99%)	7 (1%)	68	79
1	B	720/795 (91%)	697 (97%)	23 (3%)	34	64
1	C	737/795 (93%)	721 (98%)	16 (2%)	45	71
1	D	723/795 (91%)	711 (98%)	12 (2%)	53	74
1	E	731/795 (92%)	717 (98%)	14 (2%)	50	73
1	F	724/795 (91%)	705 (97%)	19 (3%)	40	68
All	All	4359/4770 (91%)	4268 (98%)	91 (2%)	47	71

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	537	LEU
1	B	190	LYS

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Mol	Chain	Res	Type
1	F	596	CYS
1	F	829	HIS
1	B	334	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	862	GLN
1	B	829	HIS
1	B	111	ASN
1	B	315	HIS
1	D	123	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](#)

There are no ligands in this entry.

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, 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	815/898 (90%)	0.13	7 (0%) 81 63	53, 86, 125, 160	0
1	B	811/898 (90%)	0.87	89 (10%) 10 5	69, 123, 159, 189	0
1	C	829/898 (92%)	0.20	12 (1%) 73 53	64, 91, 127, 174	0
1	D	815/898 (90%)	0.15	10 (1%) 76 58	65, 95, 126, 152	0
1	E	825/898 (91%)	0.30	17 (2%) 63 42	66, 94, 135, 185	0
1	F	815/898 (90%)	0.66	26 (3%) 50 30	76, 112, 141, 168	0
All	All	4910/5388 (91%)	0.38	161 (3%) 49 29	53, 98, 141, 189	0

The worst 5 of 161 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	143	LEU	5.7
1	B	189	VAL	5.6
1	B	349	MET	4.6
1	B	179	LEU	4.6
1	A	138	LEU	4.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.