



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2IWP / pdb_00002iwp
Title : 12th PDZ domain of Multiple PDZ Domain Protein MPDZ
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Deposited on : 2006-07-03
Resolution : 2.15 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 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
Xtriage (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

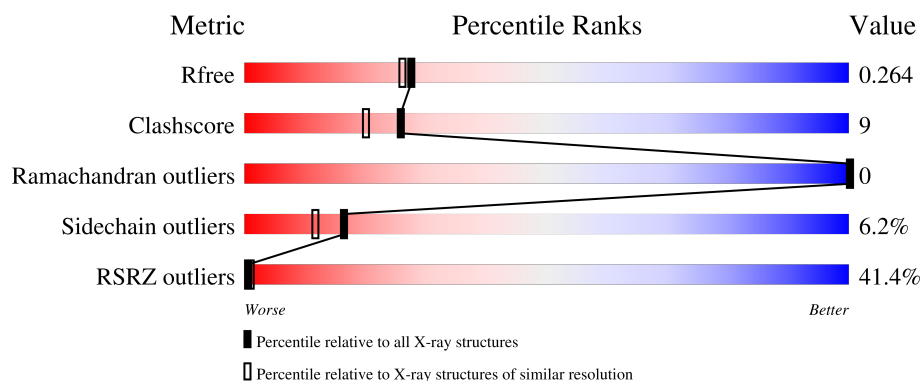
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	120	25% 61% 14% • 23%
1	B	120	43% 70% 16% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1401 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 MULTIPLE PDZ DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			643	397	110	130	6			
1	B	106	Total	C	N	O	S	0	0	0
			734	454	127	146	7			

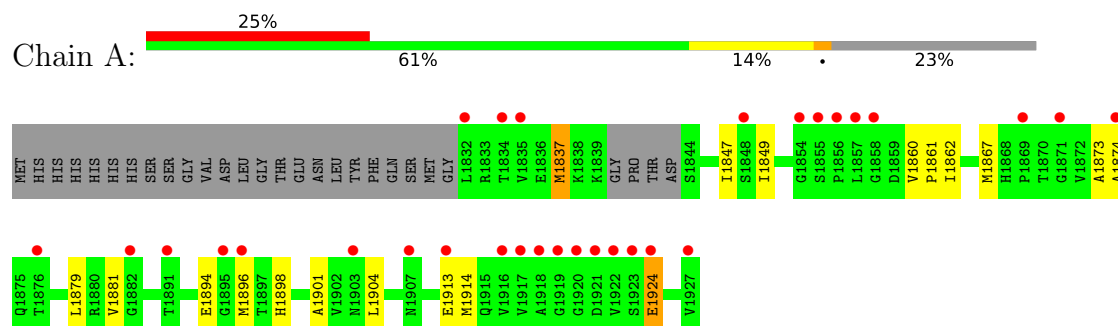
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	9	Total	O	0	0
			9	9		

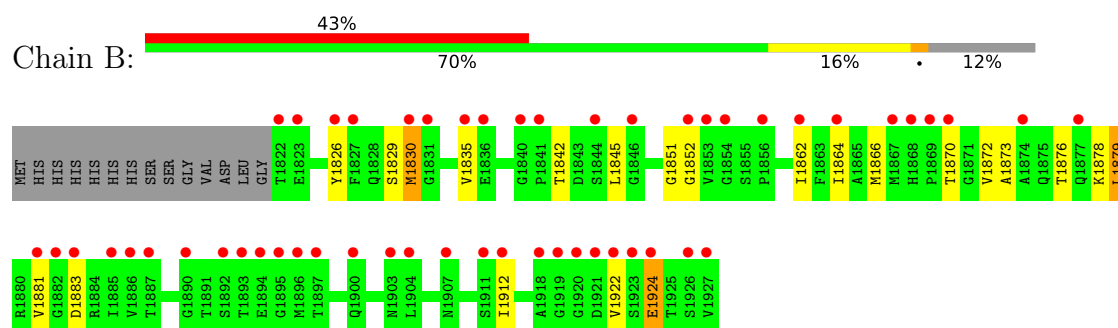
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

• Molecule 1: MULTIPLE PDZ DOMAIN PROTEIN



• Molecule 1: MULTIPLE PDZ DOMAIN PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.71Å 88.10Å 73.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.83 – 2.15 57.83 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (57.83-2.15) 99.3 (57.83-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.270 0.228 , 0.264	Depositor DCC
R_{free} test set	687 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1401	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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	0.98	0/647	0.97	0/874
1	B	0.92	0/742	1.03	1/1006 (0.1%)
All	All	0.95	0/1389	1.00	1/1880 (0.1%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1830	MET	N-CA-C	7.79	122.98	113.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1830	MET	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	643	0	650	12	0
1	B	734	0	717	16	0
2	A	15	0	0	0	0
2	B	9	0	0	0	0
All	All	1401	0	1367	26	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 9.

All (26) 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:1896:MET:HE1	1:A:1904:LEU:HD23	1.70	0.73
1:B:1851:GLY:C	1:B:1862:ILE:HD13	2.24	0.63
1:A:1847:ILE:HG22	1:A:1867:MET:HG2	1.82	0.60
1:B:1852:GLY:HA3	1:B:1862:ILE:HD11	1.85	0.57
1:B:1873:ALA:HB1	1:B:1879:LEU:HD23	1.89	0.53
1:A:1867:MET:HE3	1:A:1874:ALA:HB2	1.89	0.53
1:B:1851:GLY:O	1:B:1862:ILE:HD13	2.09	0.53
1:B:1852:GLY:CA	1:B:1862:ILE:HD11	2.39	0.52
1:B:1835:VAL:HG11	1:B:1876:THR:HG21	1.92	0.51
1:B:1845:LEU:HD21	1:B:1912:ILE:HD12	1.91	0.51
1:B:1842:THR:O	1:B:1842:THR:HG22	2.10	0.51
1:A:1924:GLU:OE2	1:B:1866:MET:SD	2.68	0.50
1:B:1835:VAL:CG1	1:B:1876:THR:HG21	2.40	0.50
1:A:1860:VAL:O	1:A:1861:PRO:C	2.53	0.49
1:B:1852:GLY:CA	1:B:1862:ILE:CD1	2.90	0.48
1:B:1826:TYR:O	1:B:1829:SER:OG	2.30	0.48
1:B:1876:THR:HG22	1:B:1878:LYS:H	1.79	0.47
1:B:1864:ILE:HD12	1:B:1883:ASP:HB2	1.97	0.47
1:A:1862:ILE:CD1	1:A:1901:ALA:HB2	2.46	0.46
1:A:1862:ILE:HD13	1:A:1901:ALA:CB	2.45	0.46
1:A:1881:VAL:HG12	1:B:1866:MET:HE3	1.97	0.45
1:B:1881:VAL:HG11	1:B:1924:GLU:HG2	1.99	0.44
1:A:1896:MET:HE1	1:A:1904:LEU:CD2	2.45	0.42
1:A:1873:ALA:HB1	1:A:1879:LEU:HD12	2.02	0.42
1:A:1849:ILE:O	1:A:1898:HIS:HE1	2.03	0.41
1:A:1837:MET:HE1	1:A:1914:MET:HE3	2.03	0.41

There are no symmetry-related clashes.

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	88/120 (73%)	88 (100%)	0	0	100	100
1	B	104/120 (87%)	100 (96%)	4 (4%)	0	100	100
All	All	192/240 (80%)	188 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	70/97 (72%)	66 (94%)	4 (6%)	18	14
1	B	76/97 (78%)	71 (93%)	5 (7%)	15	10
All	All	146/194 (75%)	137 (94%)	9 (6%)	16	12

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1837	MET
1	A	1894	GLU
1	A	1913	GLU
1	A	1924	GLU
1	B	1870	THR
1	B	1872	VAL
1	B	1879	LEU
1	B	1922	VAL

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Mol	Chain	Res	Type
1	B	1924	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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	92/120 (76%)	1.67	30 (32%)  	42, 55, 64, 71	0
1	B	106/120 (88%)	2.15	52 (49%)  	48, 56, 65, 68	0
All	All	198/240 (82%)	1.93	82 (41%)  	42, 56, 66, 71	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1841	PRO	6.6
1	B	1822	THR	6.1
1	B	1920	GLY	5.7
1	B	1874	ALA	5.0
1	B	1840	GLY	4.6
1	A	1855	SER	4.5
1	B	1921	ASP	4.5
1	B	1919	GLY	4.5
1	B	1922	VAL	4.4
1	B	1877	GLN	4.3
1	A	1913	GLU	4.2
1	A	1927	VAL	4.2
1	A	1858	GLY	3.9
1	B	1903	ASN	3.8
1	A	1919	GLY	3.7
1	B	1882	GLY	3.4
1	A	1903	ASN	3.4
1	B	1897	THR	3.3
1	B	1831	GLY	3.3
1	A	1921	ASP	3.2
1	A	1882	GLY	3.2
1	A	1895	GLY	3.1
1	A	1876	THR	3.1
1	A	1871	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1907	ASN	3.0
1	A	1922	VAL	3.0
1	B	1846	GLY	2.9
1	B	1830	MET	2.9
1	B	1836	GLU	2.9
1	B	1907	ASN	2.9
1	B	1904	LEU	2.8
1	B	1870	THR	2.8
1	B	1895	GLY	2.8
1	B	1896	MET	2.8
1	A	1856	PRO	2.8
1	B	1869	PRO	2.8
1	B	1912	ILE	2.8
1	B	1886	VAL	2.8
1	B	1854	GLY	2.8
1	B	1826	TYR	2.8
1	A	1848	SER	2.7
1	B	1890	GLY	2.7
1	A	1891	THR	2.7
1	A	1923	SER	2.7
1	A	1832	LEU	2.7
1	B	1867	MET	2.6
1	B	1853	VAL	2.6
1	A	1916	VAL	2.5
1	B	1864	ILE	2.5
1	B	1927	VAL	2.5
1	B	1868	HIS	2.5
1	A	1834	THR	2.5
1	B	1892	SER	2.5
1	A	1918	ALA	2.4
1	B	1918	ALA	2.4
1	B	1911	SER	2.4
1	B	1893	THR	2.4
1	A	1874	ALA	2.4
1	A	1835	VAL	2.4
1	B	1835	VAL	2.4
1	B	1856	PRO	2.4
1	B	1924	GLU	2.3
1	B	1900	GLN	2.3
1	A	1917	VAL	2.3
1	B	1894	GLU	2.3
1	B	1844	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1926	SER	2.2
1	A	1920	GLY	2.2
1	B	1923	SER	2.2
1	B	1823	GLU	2.2
1	B	1881	VAL	2.2
1	B	1852	GLY	2.2
1	A	1857	LEU	2.2
1	A	1924	GLU	2.1
1	B	1883	ASP	2.1
1	A	1896	MET	2.1
1	A	1869	PRO	2.1
1	B	1887	THR	2.0
1	B	1862	ILE	2.0
1	B	1885	ILE	2.0
1	B	1827	PHE	2.0
1	A	1854	GLY	2.0

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 [i](#)

There are no such residues in this entry.