



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:21 PM GMT

PDB ID : 2IOL
Title : Crystal structure of the C-terminal MA3 domain of Pdcd4 (mouse); form 1
Authors : Wlodawer, A.; LaRonde-LeBlanc, N.A.
Deposited on : 2006-10-10
Resolution : 2.00 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

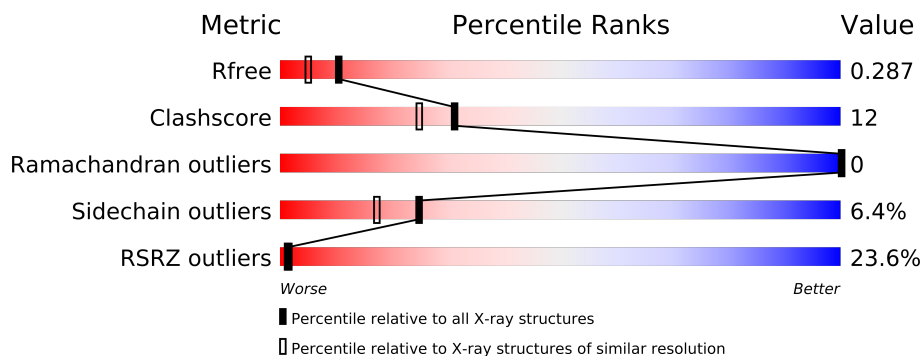
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	150	
1	B	150	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2110 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Programmed Cell Death 4, Pdcd4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	Se	0	0	0
			1030	662	166	195	3	4			
1	B	127	Total	C	N	O	S	Se	0	0	0
			1030	662	166	195	3	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	MSE	MET	MODIFIED RESIDUE	UNP Q61823
A	370	MSE	MET	MODIFIED RESIDUE	UNP Q61823
A	382	MSE	MET	MODIFIED RESIDUE	UNP Q61823
A	401	MSE	MET	MODIFIED RESIDUE	UNP Q61823
B	333	MSE	MET	MODIFIED RESIDUE	UNP Q61823
B	370	MSE	MET	MODIFIED RESIDUE	UNP Q61823
B	382	MSE	MET	MODIFIED RESIDUE	UNP Q61823
B	401	MSE	MET	MODIFIED RESIDUE	UNP Q61823

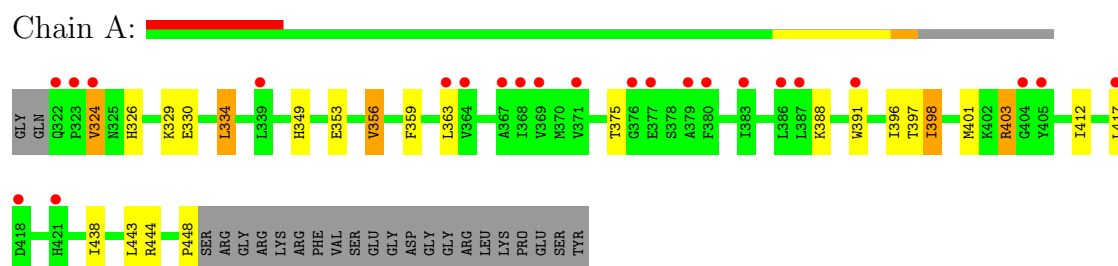
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	14	Total	O	0	0
			14	14		

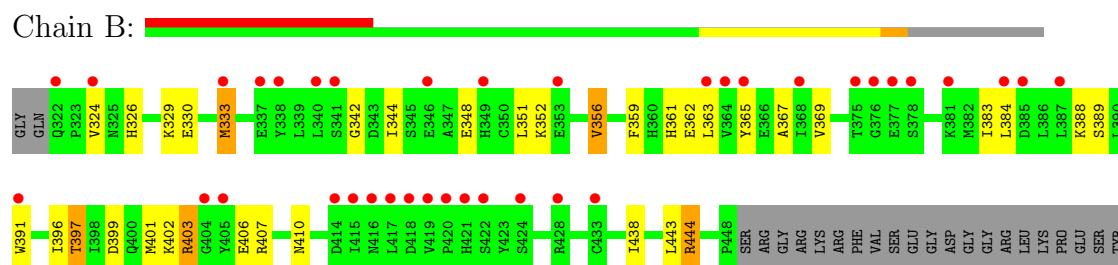
3 Residue-property plots i

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.

- Molecule 1: Programmed Cell Death 4, Pdcd4



- Molecule 1: Programmed Cell Death 4, Pdcd4



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.65Å 64.65Å 164.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 28.39 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.00) 98.0 (28.39-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.259 , 0.297 0.252 , 0.287	Depositor DCC
R_{free} test set	1381 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	EDS
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27191 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2110	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.66	0/1047	0.72	1/1409 (0.1%)
1	B	0.81	5/1047 (0.5%)	0.76	2/1409 (0.1%)
All	All	0.74	5/2094 (0.2%)	0.74	3/2818 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	GLY	C-O	10.58	1.40	1.23
1	B	342	GLY	C-N	6.91	1.50	1.34
1	B	333	MSE	CG-SE	6.41	2.17	1.95
1	B	329	LYS	CD-CE	5.93	1.66	1.51
1	B	329	LYS	CE-NZ	5.34	1.62	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	B	444	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	334	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1030	0	1028	20	0
1	B	1030	0	1028	30	0
2	A	36	0	0	1	0
2	B	14	0	0	5	0
All	All	2110	0	2056	48	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:333:MSE:SE	1:B:333:MSE:CE	2.16	1.44
1:B:333:MSE:CG	1:B:333:MSE:SE	2.17	1.42
1:B:391:TRP:CD1	1:B:401:MSE:HE3	1.98	0.97
1:B:391:TRP:HD1	1:B:401:MSE:HE3	1.37	0.82
1:A:349:HIS:O	1:A:353:GLU:HG3	1.79	0.81
1:B:348:GLU:O	1:B:352:LYS:HG2	1.88	0.73
1:A:397:THR:HG23	2:A:39:HOH:O	1.90	0.72
1:B:359:PHE:CZ	1:B:362:GLU:HG3	2.25	0.71
1:A:403:ARG:CG	1:A:403:ARG:HH11	2.04	0.70
1:B:344:ILE:HG21	1:B:389:SER:OG	1.97	0.65
1:A:375:THR:N	1:B:410:ASN:HD21	1.95	0.64
1:A:375:THR:H	1:B:410:ASN:HD21	1.47	0.62
1:B:391:TRP:HD1	1:B:401:MSE:CE	2.11	0.62
1:B:326:HIS:O	1:B:330:GLU:HG2	1.99	0.62
1:A:396:ILE:CG2	1:A:401:MSE:HG2	2.30	0.62
1:B:388:LYS:CE	2:B:38:HOH:O	2.47	0.61
1:B:333:MSE:SE	1:B:333:MSE:CB	2.99	0.61
1:B:396:ILE:CG2	1:B:401:MSE:HE2	2.37	0.55
1:A:396:ILE:HG22	1:A:401:MSE:HG2	1.89	0.55
1:B:388:LYS:HE3	2:B:38:HOH:O	2.06	0.55
1:A:356:VAL:HG13	1:A:356:VAL:O	2.07	0.55
1:B:402:LYS:O	1:B:406:GLU:HG3	2.08	0.54
1:A:324:VAL:HG11	1:A:329:LYS:HE2	1.90	0.54
1:A:326:HIS:O	1:A:330:GLU:HG2	2.08	0.53
1:A:403:ARG:CG	1:A:403:ARG:NH1	2.73	0.50
1:A:403:ARG:HG2	1:A:403:ARG:HH11	1.77	0.50
1:A:356:VAL:HG13	1:A:359:PHE:HB3	1.93	0.49
1:A:403:ARG:HG3	1:A:403:ARG:HH11	1.76	0.49
1:B:397:THR:HB	2:B:24:HOH:O	2.13	0.49
1:A:391:TRP:HB2	1:A:401:MSE:HE3	1.95	0.48
1:B:356:VAL:HG13	1:B:359:PHE:HB3	1.94	0.48
1:A:396:ILE:HG21	1:A:401:MSE:HG2	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:388:LYS:HE2	2:B:38:HOH:O	2.13	0.48
1:B:356:VAL:O	1:B:356:VAL:CG1	2.62	0.47
1:B:384:LEU:HG	2:B:34:HOH:O	2.12	0.47
1:A:398:ILE:O	1:A:398:ILE:HD13	2.16	0.46
1:B:351:LEU:HD22	1:B:363:LEU:HD13	1.98	0.45
1:B:396:ILE:HG22	1:B:401:MSE:HE2	1.99	0.45
1:B:362:GLU:HG2	1:B:407:ARG:HH12	1.84	0.43
1:B:361:HIS:CG	1:B:403:ARG:HG2	2.53	0.43
1:B:388:LYS:HA	1:B:438:ILE:HG21	2.01	0.43
1:B:365:TYR:O	1:B:369:VAL:HG23	2.18	0.43
1:B:388:LYS:HE2	1:B:388:LYS:HB3	1.87	0.42
1:A:388:LYS:HA	1:A:438:ILE:HG21	2.02	0.42
1:A:412:ILE:HG21	1:A:448:PRO:HG2	2.03	0.41
1:B:356:VAL:HG13	1:B:359:PHE:CB	2.51	0.40
1:B:367:ALA:HB1	1:B:383:ILE:HG23	2.03	0.40
1:A:334:LEU:C	1:A:334:LEU:HD23	2.42	0.40

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	125/150 (83%)	125 (100%)	0	0	100	100
1	B	125/150 (83%)	123 (98%)	2 (2%)	0	100	100
All	All	250/300 (83%)	248 (99%)	2 (1%)	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	118/133 (89%)	110 (93%)	8 (7%)	22	15
1	B	118/133 (89%)	111 (94%)	7 (6%)	28	20
All	All	236/266 (89%)	221 (94%)	15 (6%)	25	17

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	VAL
1	A	356	VAL
1	A	363	LEU
1	A	398	ILE
1	A	403	ARG
1	A	417	LEU
1	A	443	LEU
1	A	444	ARG
1	B	324	VAL
1	B	356	VAL
1	B	397	THR
1	B	399	ASP
1	B	403	ARG
1	B	443	LEU
1	B	444	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	410	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

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	127/150 (84%)	1.08	23 (18%) 2 2	43, 51, 57, 59	0
1	B	127/150 (84%)	1.81	37 (29%) 1 1	41, 52, 59, 61	0
All	All	254/300 (84%)	1.45	60 (23%) 1 1	41, 51, 59, 61	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	11.2
1	A	324	VAL	7.8
1	B	419	VAL	7.2
1	B	340	LEU	7.2
1	B	421	HIS	6.1
1	B	415	ILE	6.0
1	B	322	GLN	5.8
1	B	377	GLU	5.7
1	B	324	VAL	5.2
1	B	418	ASP	5.0
1	B	341	SER	5.0
1	B	420	PRO	4.9
1	B	376	GLY	4.8
1	B	333	MSE	4.3
1	A	368	ILE	4.3
1	A	421	HIS	4.2
1	B	424	SER	4.1
1	B	364	VAL	4.0
1	B	378	SER	3.9
1	B	375	THR	3.7
1	B	422	SER	3.7
1	B	381	LYS	3.4
1	A	387	LEU	3.4
1	B	346	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	368	ILE	3.3
1	B	391	TRP	3.2
1	A	364	VAL	3.2
1	B	353	GLU	3.1
1	A	363	LEU	3.0
1	A	322	GLN	3.0
1	A	386	LEU	3.0
1	A	383	ILE	2.9
1	A	371	VAL	2.9
1	B	349	HIS	2.9
1	A	367	ALA	2.8
1	B	387	LEU	2.8
1	B	405	TYR	2.7
1	A	323	PRO	2.5
1	B	363	LEU	2.5
1	B	338	TYR	2.5
1	B	337	GLU	2.5
1	A	377	GLU	2.5
1	A	404	GLY	2.4
1	B	404	GLY	2.4
1	A	417	LEU	2.4
1	B	433	CYS	2.3
1	B	416	ASN	2.3
1	B	384	LEU	2.3
1	A	380	PHE	2.3
1	A	418	ASP	2.3
1	A	405	TYR	2.2
1	A	339	LEU	2.2
1	A	369	VAL	2.2
1	B	414	ASP	2.2
1	A	379	ALA	2.2
1	A	391	TRP	2.1
1	B	385	ASP	2.1
1	B	428	ARG	2.1
1	A	376	GLY	2.0
1	B	365	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.