



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:59 PM GMT

PDB ID : 4B6H  
Title : Structure of hDcp1a in complex with proline rich sequence of PNRC2  
Authors : Lai, T.; Song, H.  
Deposited on : 2012-08-13  
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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

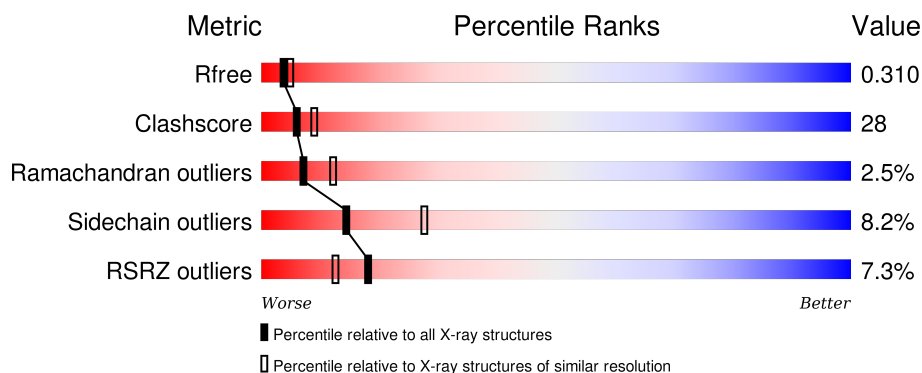
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	134	<div> <div>2%</div> <div>52%</div> <div>40%</div> <div>• •</div> </div>
1	B	134	<div> <div>10%</div> <div>41%</div> <div>28%</div> <div>6%</div> <div>25%</div> </div>
2	C	135	<div> <div>• 6% •</div> <div>89%</div> </div>
2	D	135	<div> <div>• 5% •</div> <div>90%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2152 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 MRNA-DECAPPING ENZYME 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1052	673	177	196	6			
1	B	101	Total	C	N	O	S	0	0	1
			823	535	134	150	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	EXPRESSION TAG	UNP Q9NPI6
A	-2	ALA	-	EXPRESSION TAG	UNP Q9NPI6
A	-1	ASP	-	EXPRESSION TAG	UNP Q9NPI6
A	0	LEU	-	EXPRESSION TAG	UNP Q9NPI6
B	-3	MET	-	EXPRESSION TAG	UNP Q9NPI6
B	-2	ALA	-	EXPRESSION TAG	UNP Q9NPI6
B	-1	ASP	-	EXPRESSION TAG	UNP Q9NPI6
B	0	LEU	-	EXPRESSION TAG	UNP Q9NPI6

- Molecule 2 is a protein called PROLINE-RICH NUCLEAR RECEPTOR COACTIVATOR 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	0	0	1
			109	73	19	17			
2	D	14	Total	C	N	O	0	0	1
			102	68	18	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	MET	-	EXPRESSION TAG	UNP Q9NPJ4
C	-12	GLY	-	EXPRESSION TAG	UNP Q9NPJ4
C	-11	SER	-	EXPRESSION TAG	UNP Q9NPJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	SER	-	EXPRESSION TAG	UNP Q9NPJ4
C	-9	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
C	-8	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
C	-7	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
C	-6	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
C	-5	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
C	-4	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
C	-3	SER	-	EXPRESSION TAG	UNP Q9NPJ4
C	-2	GLN	-	EXPRESSION TAG	UNP Q9NPJ4
C	-1	ASP	-	EXPRESSION TAG	UNP Q9NPJ4
C	0	PRO	-	EXPRESSION TAG	UNP Q9NPJ4
D	-13	MET	-	EXPRESSION TAG	UNP Q9NPJ4
D	-12	GLY	-	EXPRESSION TAG	UNP Q9NPJ4
D	-11	SER	-	EXPRESSION TAG	UNP Q9NPJ4
D	-10	SER	-	EXPRESSION TAG	UNP Q9NPJ4
D	-9	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
D	-8	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
D	-7	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
D	-6	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
D	-5	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
D	-4	HIS	-	EXPRESSION TAG	UNP Q9NPJ4
D	-3	SER	-	EXPRESSION TAG	UNP Q9NPJ4
D	-2	GLN	-	EXPRESSION TAG	UNP Q9NPJ4
D	-1	ASP	-	EXPRESSION TAG	UNP Q9NPJ4
D	0	PRO	-	EXPRESSION TAG	UNP Q9NPJ4

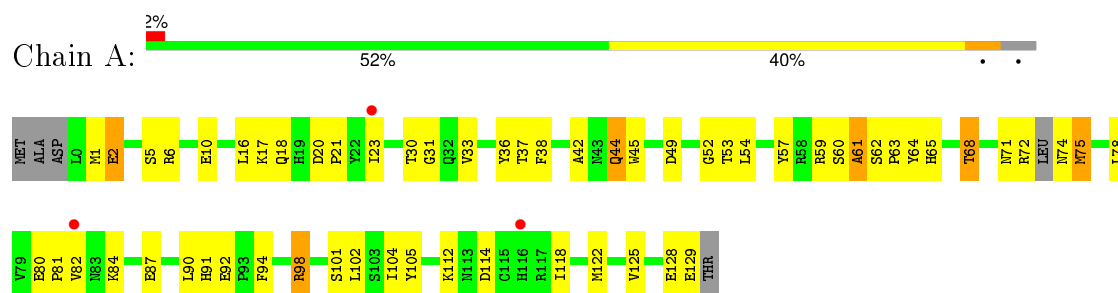
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	25	Total O 25 25	0	0
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	0	0

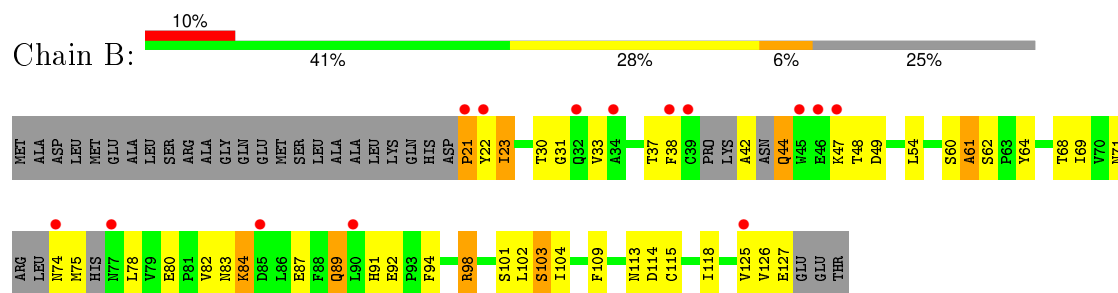
### 3 Residue-property plots

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.

#### • Molecule 1: MRNA-DECAPPING ENZYME 1A



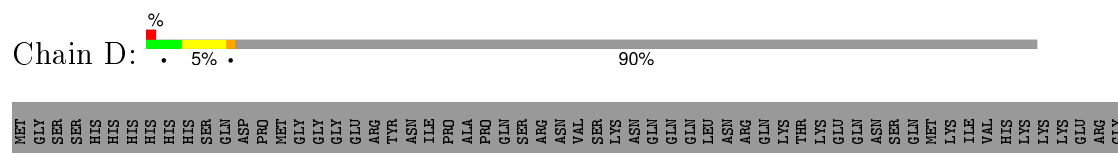
#### • Molecule 1: MRNA-DECAPPING ENZYME 1A



#### • Molecule 2: PROLINE-RICH NUCLEAR RECEPTOR COACTIVATOR 2



#### • Molecule 2: PROLINE-RICH NUCLEAR RECEPTOR COACTIVATOR 2



HIS	GLY	TYR	ASN	SER	SER	ALA	ALA	ALA	TRP	GLN	ALA	MET	GLN	ASN	GLY	GLY	LYS	ASN	LYS	ASN	PHE	PRO	ASN	ASN	GLN	SER	TRP	ASN	SER	SER	LEU	SER	GLY	PRO	ARG	LEU	LEU	PHE	LYS	SER	GLN	ALA	ASN	GLN	ASN	TYR	ALA	GLY	ALA	LYS	PHE	SER	GLU	PRO	P102	S103	PRO	S105	V106
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L107	P108	S112	H113	W114	V115	P116	VAL	SER	PHE	ASN	PRO
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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.09Å 97.64Å 109.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 2.60 72.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.93-2.60) 97.6 (72.93-2.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.1_357)	Depositor
R, $R_{free}$	0.234 , 0.285 0.271 , 0.310	Depositor DCC
$R_{free}$ test set	1261 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 86.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 12620 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	0/1077	0.61	0/1459
1	B	0.47	0/842	0.68	1/1140 (0.1%)
2	C	0.66	1/116 (0.9%)	0.71	0/162
2	D	0.65	1/107 (0.9%)	0.51	0/147
All	All	0.47	2/2142 (0.1%)	0.64	1/2908 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	115	VAL	C-N	-5.62	1.23	1.34
2	C	115	VAL	C-N	-5.45	1.23	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21	PRO	CA-N-CD	-8.92	99.01	111.50

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	1052	0	1023	57	2
1	B	823	0	794	48	1
2	C	109	0	109	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	102	0	101	11	0
3	A	34	0	0	10	3
3	B	25	0	0	16	0
3	C	4	0	0	0	0
3	D	3	0	0	2	0
All	All	2152	0	2027	117	3

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 28.

The worst 5 of 117 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:71:ASN:HB3	1:B:74:ASN:O	1.35	1.25
1:A:75:MET:O	1:A:75:MET:HE2	1.54	1.07
1:A:75:MET:O	1:A:75:MET:CE	2.03	1.07
1:A:72:ARG:NH2	3:A:2017:HOH:O	1.87	1.05
1:A:57:TYR:HE2	1:A:68:THR:HG22	1.20	1.02

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:OE2	3:A:2032:HOH:O[7_445]	2.00	0.20
1:A:1:MET:CG	3:A:2017:HOH:O[3_555]	2.00	0.20
1:A:1:MET:CB	3:A:2017:HOH:O[3_555]	2.04	0.16

## 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	125/134 (93%)	115 (92%)	8 (6%)	2 (2%)	12	24
1	B	92/134 (69%)	84 (91%)	5 (5%)	3 (3%)	5	7
2	C	13/135 (10%)	9 (69%)	3 (23%)	1 (8%)	1	1
2	D	10/135 (7%)	9 (90%)	1 (10%)	0	100	100
All	All	240/538 (45%)	217 (90%)	17 (7%)	6 (2%)	7	12

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	105	SER
1	B	31	GLY
1	A	61	ALA
1	B	61	ALA
1	B	23	ILE

### 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	114/118 (97%)	107 (94%)	7 (6%)	23	46
1	B	90/118 (76%)	83 (92%)	7 (8%)	16	30
2	C	14/117 (12%)	11 (79%)	3 (21%)	1	2
2	D	13/117 (11%)	11 (85%)	2 (15%)	3	5
All	All	231/470 (49%)	212 (92%)	19 (8%)	14	27

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	68	THR
1	B	84	LYS
2	C	105	SER
1	B	44	GLN
2	C	107	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	65	HIS
2	D	113	HIS

### 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	129/134 (96%)	0.81	3 (2%) 64 57	49, 73, 107, 138	0
1	B	101/134 (75%)	1.10	14 (13%) 4 2	56, 87, 127, 168	0
2	C	15/135 (11%)	0.78	1 (6%) 21 15	65, 80, 114, 124	0
2	D	14/135 (10%)	1.14	1 (7%) 19 13	82, 115, 132, 146	0
All	All	259/538 (48%)	0.94	19 (7%) 18 12	49, 81, 124, 168	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	TYR	5.0
1	B	21	PRO	4.1
1	B	38	PHE	3.5
1	B	39	CYS	3.3
1	A	23	ILE	3.1

### 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 carbohydrates 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.