



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:35 PM GMT

PDB ID : 3Q0R  
Title : Crystal structure of the PUMILIO-homology domain from Human PUMILIO2  
in complex with p38alpha NREb  
Authors : Lu, G.; Hall, T.M.T.  
Deposited on : 2010-12-15  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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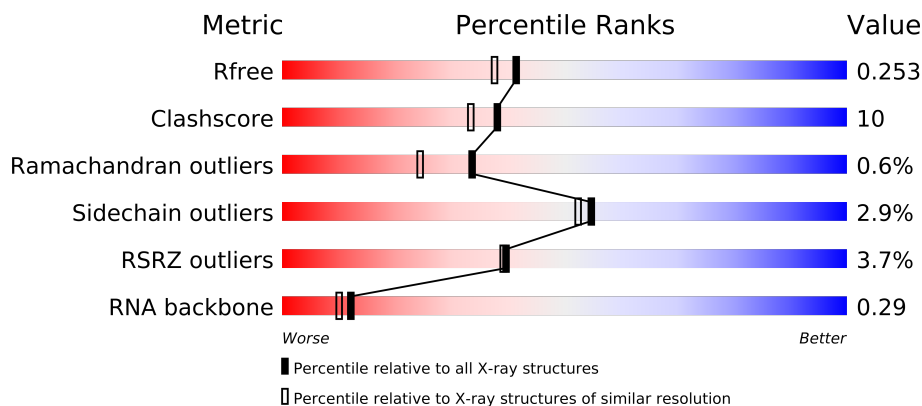
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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)
RNA backbone	1838	1015 (2.96-1.04)

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. 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	351	
2	B	8	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3156 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 Pumilio homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2783	1760	502	503	18			

- Molecule 2 is a RNA chain called 5'-R(UP\*GP\*UP\*AP\*GP\*AP\*UP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			169	77	31	54	7			

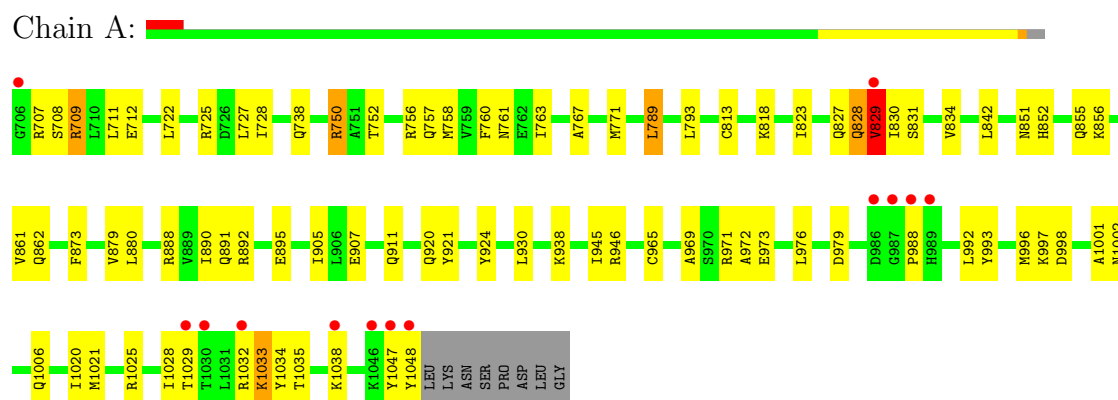
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	190	Total	O	0	0
			190	190		
3	B	14	Total	O	0	0
			14	14		

### 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: Pumilio homolog 2



- Molecule 2: 5'-R(UP\*GP\*UP\*AP\*GP\*AP\*UP\*A)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.48Å 43.12Å 60.61Å 71.93° 85.36° 77.58°	Depositor
Resolution (Å)	27.68 – 2.00 27.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (27.68-2.00) 93.1 (27.68-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.67 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_6)	Depositor
R, $R_{free}$	0.207 , 0.257 0.203 , 0.253	Depositor DCC
$R_{free}$ test set	1104 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 39.0	EDS
Estimated twinning fraction	0.011 for -h,-k,-k+l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21575 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.29	0/2835	0.45	0/3820
2	B	0.58	0/189	1.80	8/293 (2.7%)
All	All	0.32	0/3024	0.65	8/4113 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	A	O3'-P-O5'	-11.94	81.31	104.00
2	B	4	A	OP2-P-O3'	-8.49	86.51	105.20
2	B	4	A	OP1-P-O3'	-8.45	86.61	105.20
2	B	4	A	P-O3'-C3'	7.40	128.58	119.70
2	B	5	G	OP1-P-OP2	7.40	130.70	119.60
2	B	4	A	O4'-C1'-N9	7.12	113.90	108.20
2	B	5	G	O5'-P-OP1	5.69	117.53	110.70
2	B	6	A	N9-C1'-C2'	-5.58	105.86	112.00

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	2783	0	2805	58	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	169	0	87	5	0
3	A	190	0	0	7	0
3	B	14	0	0	0	0
All	All	3156	0	2892	58	1

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 10.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:829:VAL:CG1	1:A:830:ILE:N	2.42	0.83
1:A:1038:LYS:HG2	3:A:5:HOH:O	1.83	0.79
1:A:1032:ARG:HB2	3:A:40:HOH:O	1.83	0.79
1:A:829:VAL:HG12	1:A:830:ILE:H	1.53	0.74
1:A:725:ARG:O	1:A:728:ILE:HG13	1.91	0.70
1:A:829:VAL:HG13	1:A:830:ILE:N	2.06	0.70
1:A:1035:THR:O	1:A:1038:LYS:HG3	1.92	0.70
1:A:861:VAL:HG11	3:A:54:HOH:O	1.93	0.68
1:A:757:GLN:HE21	1:A:761:ASN:HD21	1.41	0.68
1:A:750:ARG:HD3	1:A:750:ARG:O	1.95	0.67
1:A:993:TYR:HA	1:A:996:MET:HE2	1.78	0.65
1:A:852:HIS:HD2	3:A:28:HOH:O	1.80	0.64
1:A:1029:THR:O	1:A:1032:ARG:HB3	1.99	0.62
1:A:722:LEU:HD21	1:A:727:LEU:HD21	1.84	0.58
1:A:767:ALA:O	1:A:771:MET:HG3	2.05	0.57
1:A:972:ALA:O	1:A:976:LEU:HD13	2.06	0.56
1:A:828:GLN:O	1:A:829:VAL:C	2.44	0.55
1:A:789:LEU:HD22	1:A:793:LEU:HG	1.89	0.54
1:A:998:ASP:HB3	1:A:1001:ALA:HB3	1.88	0.54
1:A:827:GLN:O	1:A:828:GLN:C	2.46	0.53
1:A:1025:ARG:HD2	1:A:1048:TYR:OH	2.09	0.52
1:A:760:PHE:O	1:A:763:ILE:HG13	2.11	0.51
1:A:946:ARG:NH1	1:A:976:LEU:HD23	2.24	0.51
1:A:738:GLN:NE2	2:B:8:A:O2'	2.43	0.51
1:A:1002:ASN:O	1:A:1006:GLN:HG3	2.12	0.50
1:A:992:LEU:O	1:A:996:MET:HG3	2.12	0.50
1:A:829:VAL:CG1	1:A:830:ILE:H	2.08	0.49
1:A:708:SER:O	1:A:712:GLU:HG3	2.12	0.49
1:A:842:LEU:HD22	1:A:880:LEU:HD11	1.93	0.49
1:A:971:ARG:NH2	3:A:27:HOH:O	2.45	0.49
1:A:707:ARG:HG3	1:A:711:LEU:HD23	1.95	0.48
1:A:834:VAL:HG21	1:A:861:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:861:VAL:HG12	1:A:862:GLN:N	2.30	0.47
1:A:905:ILE:HD13	3:A:96:HOH:O	2.15	0.46
1:A:1021:MET:HG3	1:A:1047:TYR:CE2	2.51	0.46
1:A:851:ASN:O	1:A:855:GLN:HG3	2.15	0.46
1:A:945:ILE:HG13	1:A:965:CYS:SG	2.56	0.45
1:A:823:ILE:HB	1:A:830:ILE:HD11	1.99	0.45
1:A:930:LEU:O	1:A:938:LYS:HE2	2.17	0.45
1:A:891:GLN:NE2	2:B:4:A:N1	2.51	0.45
1:A:924:TYR:HB3	2:B:4:A:N1	2.32	0.44
1:A:813:CYS:HG	2:B:6:A:H2	1.65	0.44
1:A:891:GLN:O	1:A:895:GLU:HG3	2.17	0.44
1:A:997:LYS:HD2	1:A:1034:TYR:CE1	2.53	0.44
1:A:879:VAL:HG23	3:A:14:HOH:O	2.17	0.44
1:A:709:ARG:HA	1:A:709:ARG:HD2	1.76	0.43
1:A:891:GLN:NE2	2:B:4:A:C2	2.76	0.43
1:A:873:PHE:CD2	1:A:890:ILE:HD11	2.53	0.43
1:A:907:GLU:O	1:A:911:GLN:HG3	2.18	0.42
1:A:1033:LYS:HG2	1:A:1034:TYR:CD1	2.55	0.42
1:A:888:ARG:O	1:A:892:ARG:HG2	2.18	0.42
1:A:828:GLN:O	1:A:831:SER:N	2.52	0.42
1:A:920:GLN:HG3	1:A:921:TYR:CD1	2.55	0.42
1:A:752:THR:O	1:A:756:ARG:HG3	2.19	0.41
1:A:1025:ARG:O	1:A:1028:ILE:HG13	2.19	0.41
1:A:861:VAL:CG1	1:A:862:GLN:N	2.83	0.41
1:A:969:ALA:HB1	1:A:973:GLU:HB2	2.03	0.41
1:A:992:LEU:HD21	1:A:1020:ILE:HG23	2.02	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:A:709:ARG:N	1:A:988:PRO:O[1.544]	2.12	0.08

## 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	341/351 (97%)	333 (98%)	6 (2%)	2 (1%)	33	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	829	VAL
1	A	828	GLN

### 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	307/314 (98%)	298 (97%)	9 (3%)	55	52

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

Mol	Chain	Res	Type
1	A	709	ARG
1	A	750	ARG
1	A	758	MET
1	A	789	LEU
1	A	818	LYS
1	A	829	VAL
1	A	856	LYS
1	A	979	ASP
1	A	1033	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	723	GLN
1	A	730	HIS
1	A	736	GLN
1	A	738	GLN
1	A	761	ASN
1	A	765	GLN
1	A	852	HIS

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Mol	Chain	Res	Type
1	A	864	GLN
1	A	999	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	7/8 (87%)	2 (28%)	1 (14%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	A
2	B	5	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	4	A

## 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, 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	343/351 (97%)	0.07	13 (3%) 38 38	14, 22, 40, 60	0
2	B	8/8 (100%)	-0.44	0 100 100	23, 23, 30, 32	0
All	All	351/359 (97%)	0.06	13 (3%) 39 39	14, 23, 40, 60	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	706	GLY	5.6
1	A	989	HIS	4.4
1	A	986	ASP	4.2
1	A	988	PRO	3.6
1	A	1047	TYR	3.4
1	A	1029	THR	3.3
1	A	1032	ARG	3.1
1	A	1046	LYS	3.1
1	A	1038	LYS	3.0
1	A	1030	THR	2.6
1	A	1048	TYR	2.5
1	A	829	VAL	2.4
1	A	987	GLY	2.1

### 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.