



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:18 PM GMT

PDB ID : 3Q0S
Title : Crystal structure of the PUMILIO-homology domain from Human PUMILIO2
in complex with erk2 NRE
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

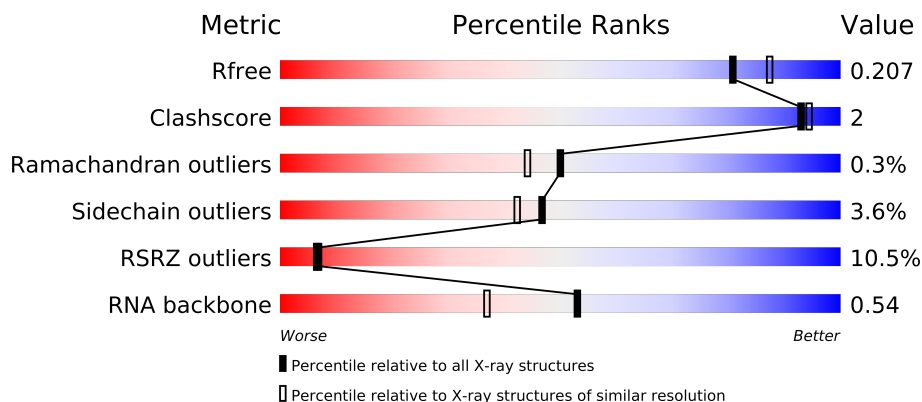
The following versions of software and data (see [references](#)) were used in the production of this report:

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)
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 ≥ 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 3083 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*CP*AP*UP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			164	75	27	55	7			

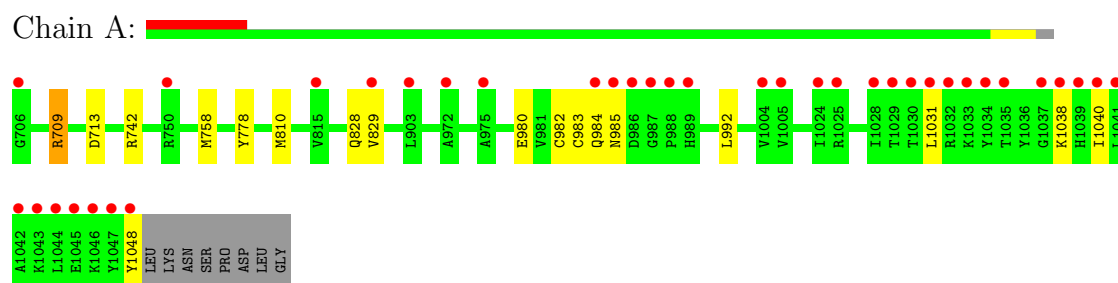
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	8	Total	O	0	0
			8	8		

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*CP*AP*UP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.40Å 45.36Å 97.80Å 90.00° 125.26° 90.00°	Depositor
Resolution (Å)	24.00 – 2.00 24.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (24.00-2.00) 98.8 (24.03-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_6)	Depositor
R, R_{free}	0.207 , 0.249 0.212 , 0.207	Depositor DCC
R_{free} test set	1403 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 59.6	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 27924 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3083	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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	0.33	0/2835	0.47	1/3820 (0.0%)
2	B	0.53	0/182	1.08	0/281
All	All	0.34	0/3017	0.54	1/4101 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	985	ASN	CB-CA-C	-8.02	94.36	110.40

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	0	4	0
2	B	164	0	87	1	0
3	A	128	0	0	1	0
3	B	8	0	0	0	0
All	All	3083	0	87	4	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 2.

All (4) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:980:GLU:O	1:A:984:GLN:CG	2.62	0.47
1:A:742:ARG:CG	3:A:111:HOH:O	2.62	0.47
1:A:709:ARG:NH1	1:A:713:ASP:OD1	2.48	0.47
1:A:778:TYR:CE2	2:B:8:C:C4	3.09	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	341/351 (97%)	328 (96%)	12 (4%)	1 (0%)	50	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1038	LYS

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%)	296 (96%)	11 (4%)	47	42

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	709	ARG
1	A	758	MET

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Mol	Chain	Res	Type
1	A	810	MET
1	A	828	GLN
1	A	829	VAL
1	A	982	CYS
1	A	983	CYS
1	A	992	LEU
1	A	1031	LEU
1	A	1040	ILE
1	A	1048	TYR

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	7/8 (87%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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	343/351 (97%)	0.74	37 (10%) 6 6	27, 45, 126, 168	0
2	B	8/8 (100%)	-0.29	0 100 100	39, 41, 55, 78	0
All	All	351/359 (97%)	0.71	37 (10%) 7 6	27, 45, 126, 168	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	985	ASN	14.9
1	A	1037	GLY	12.0
1	A	1046	LYS	12.0
1	A	986	ASP	9.4
1	A	1047	TYR	8.6
1	A	1044	LEU	8.5
1	A	1045	GLU	8.1
1	A	984	GLN	8.0
1	A	989	HIS	7.4
1	A	1033	LYS	7.0
1	A	706	GLY	6.8
1	A	1029	THR	6.4
1	A	1039	HIS	6.2
1	A	1038	LYS	6.1
1	A	1042	ALA	5.9
1	A	1031	LEU	5.5
1	A	972	ALA	5.4
1	A	1048	TYR	5.2
1	A	987	GLY	4.9
1	A	1041	LEU	4.9
1	A	1032	ARG	4.5
1	A	1040	ILE	4.4
1	A	1030	THR	4.2
1	A	1034	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1004	VAL	3.6
1	A	1028	ILE	3.2
1	A	1024	ILE	3.1
1	A	1025	ARG	3.0
1	A	1005	VAL	2.7
1	A	975	ALA	2.6
1	A	1035	THR	2.5
1	A	988	PRO	2.4
1	A	750	ARG	2.2
1	A	903	LEU	2.2
1	A	815	VAL	2.1
1	A	1043	LYS	2.0
1	A	829	VAL	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.