



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:14 am GMT

PDB ID : 3B4M
Title : Crystal Structure of Human PABPN1 RRM
Authors : Ge, H.; Zhou, D.; Teng, M.; Niu, L.
Deposited on : 2007-10-24
Resolution : 2.82 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

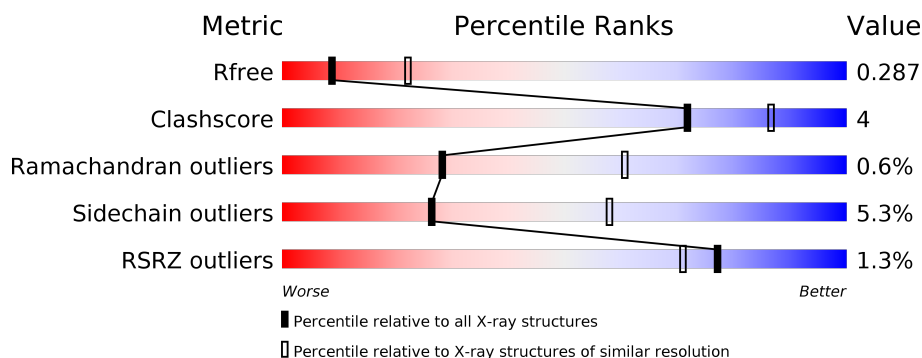
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	100719	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

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. 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	96	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>17%</div> </div> </div>
1	B	96	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>17%</div> </div> </div>
1	C	96	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	96	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>18%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2522 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 Polyadenylate-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	16	0	0
			625	393	112	118	2			
1	B	80	Total	C	N	O	S	11	0	0
			625	393	112	118	2			
1	C	80	Total	C	N	O	S	6	0	0
			625	393	112	118	2			
1	D	79	Total	C	N	O	S	21	0	0
			614	387	108	117	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	LEU	-	EXPRESSION TAG	UNP Q86U42
A	256	GLU	-	EXPRESSION TAG	UNP Q86U42
A	257	HIS	-	EXPRESSION TAG	UNP Q86U42
A	258	HIS	-	EXPRESSION TAG	UNP Q86U42
A	259	HIS	-	EXPRESSION TAG	UNP Q86U42
A	260	HIS	-	EXPRESSION TAG	UNP Q86U42
A	261	HIS	-	EXPRESSION TAG	UNP Q86U42
A	262	HIS	-	EXPRESSION TAG	UNP Q86U42
B	255	LEU	-	EXPRESSION TAG	UNP Q86U42
B	256	GLU	-	EXPRESSION TAG	UNP Q86U42
B	257	HIS	-	EXPRESSION TAG	UNP Q86U42
B	258	HIS	-	EXPRESSION TAG	UNP Q86U42
B	259	HIS	-	EXPRESSION TAG	UNP Q86U42
B	260	HIS	-	EXPRESSION TAG	UNP Q86U42
B	261	HIS	-	EXPRESSION TAG	UNP Q86U42
B	262	HIS	-	EXPRESSION TAG	UNP Q86U42
C	255	LEU	-	EXPRESSION TAG	UNP Q86U42
C	256	GLU	-	EXPRESSION TAG	UNP Q86U42
C	257	HIS	-	EXPRESSION TAG	UNP Q86U42
C	258	HIS	-	EXPRESSION TAG	UNP Q86U42
C	259	HIS	-	EXPRESSION TAG	UNP Q86U42

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Chain	Residue	Modelled	Actual	Comment	Reference
C	260	HIS	-	EXPRESSION TAG	UNP Q86U42
C	261	HIS	-	EXPRESSION TAG	UNP Q86U42
C	262	HIS	-	EXPRESSION TAG	UNP Q86U42
D	255	LEU	-	EXPRESSION TAG	UNP Q86U42
D	256	GLU	-	EXPRESSION TAG	UNP Q86U42
D	257	HIS	-	EXPRESSION TAG	UNP Q86U42
D	258	HIS	-	EXPRESSION TAG	UNP Q86U42
D	259	HIS	-	EXPRESSION TAG	UNP Q86U42
D	260	HIS	-	EXPRESSION TAG	UNP Q86U42
D	261	HIS	-	EXPRESSION TAG	UNP Q86U42
D	262	HIS	-	EXPRESSION TAG	UNP Q86U42

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	7	Total O 7 7	0	0
2	C	12	Total O 12 12	0	0
2	D	5	Total O 5 5	0	0

- Molecule 1: Polyadenylate-binding protein 2



MET
G169
S197
L204
F215
I218
D222
E224
D233
E234
R240
Q241
R243
THR
ASN
ARG
PRO
GLY
ILE
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

MET	GLU	VAL	LEU	ILE	GLY	PRO	ARG	ASN	THR
A169	V176	Y181	T184	E187	L188	E189	H193	S197	T202
P212	K213	A216	Y217	I218	K223	T228	S229	L230	R238
R248	H249	L250	L251	L252	L253	L254	L255	L256	L257

MET	GLU	A169	Y175	T184	A185	E186	T202	I203	L204	F215	A216	Y217	T218	D222	D233	E234	R238	G239	R240	K247	ARG	THR	ASN	ARG	ARG	PRO	GLY	ILE	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HTS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	59.34Å 59.34Å 80.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.58 – 2.82 31.71 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.58-2.82) 99.9 (31.71-2.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.290 0.231 , 0.287	Depositor DCC
R_{free} test set	354 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 15.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.470 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2522	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% 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	0.57	0/637	0.68	1/856 (0.1%)
1	B	0.55	0/637	0.64	0/856
1	C	0.57	0/637	0.67	0/856
1	D	0.53	0/626	0.64	1/842 (0.1%)
All	All	0.56	0/2537	0.66	2/3410 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	222	ASP	CB-CG-OD2	5.16	122.94	118.30

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	625	0	611	2	0
1	B	625	0	611	2	0
1	C	625	0	611	11	0
1	D	614	0	598	6	0
2	A	9	0	0	0	0
2	B	7	0	0	0	0
2	C	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
All	All	2522	0	2431	19	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 4.

All (19) 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:C:223:LYS:HD2	1:C:223:LYS:H	1.42	0.85
1:C:223:LYS:CD	1:C:223:LYS:H	2.09	0.65
1:C:223:LYS:HD2	1:C:223:LYS:N	2.15	0.57
1:D:233:ASP:OD2	1:D:234:GLU:N	2.38	0.57
1:A:211:HIS:O	1:A:240:ARG:NH2	2.31	0.56
1:A:176:VAL:HG21	1:A:218:ILE:HD12	1.86	0.56
1:C:184:THR:HG22	1:D:184:THR:CG2	2.36	0.55
1:C:187:GLU:OE1	1:C:238:ARG:HD2	2.12	0.50
1:C:189:GLU:OE2	1:C:193:HIS:CD2	2.65	0.50
1:B:204:LEU:HD13	1:B:215:PHE:CE1	2.50	0.47
1:C:184:THR:HG22	1:D:184:THR:HG22	1.96	0.47
1:C:189:GLU:OE2	1:C:193:HIS:HD2	1.97	0.45
1:B:233:ASP:O	1:B:234:GLU:HB2	2.17	0.44
1:C:202:THR:O	1:C:216:ALA:HA	2.17	0.44
1:D:204:LEU:HD13	1:D:215:PHE:CE1	2.53	0.43
1:D:238:ARG:HH11	1:D:238:ARG:HG2	1.84	0.43
1:C:176:VAL:HG21	1:C:218:ILE:HD12	2.00	0.42
1:C:181:TYR:HB2	1:C:212:PRO:O	2.21	0.41
1:D:202:THR:O	1:D:216:ALA:HA	2.21	0.41

There are no symmetry-related clashes.

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	78/96 (81%)	74 (95%)	4 (5%)	0	100	100
1	B	78/96 (81%)	73 (94%)	5 (6%)	0	100	100
1	C	78/96 (81%)	75 (96%)	1 (1%)	2 (3%)	6	20
1	D	77/96 (80%)	75 (97%)	2 (3%)	0	100	100
All	All	311/384 (81%)	297 (96%)	12 (4%)	2 (1%)	28	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	TYR
1	C	230	LEU

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	66/81 (82%)	64 (97%)	2 (3%)	46	79
1	B	66/81 (82%)	61 (92%)	5 (8%)	15	39
1	C	66/81 (82%)	62 (94%)	4 (6%)	22	51
1	D	65/81 (80%)	62 (95%)	3 (5%)	31	64
All	All	263/324 (81%)	249 (95%)	14 (5%)	26	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	TYR
1	A	228	THR
1	B	197	SER
1	B	222	ASP
1	B	224	GLU
1	B	240	ARG
1	B	241	GLN
1	C	197	SER
1	C	213	LYS

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Mol	Chain	Res	Type
1	C	223	LYS
1	C	228	THR
1	D	175	TYR
1	D	186	GLU
1	D	240	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	C	178	ASN
1	C	193	HIS
1	C	199	ASN
1	D	199	ASN

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, 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	80/96 (83%)	-0.35	1 (1%) 77 71	24, 33, 41, 45	7 (8%)
1	B	80/96 (83%)	-0.22	1 (1%) 77 71	26, 43, 55, 57	5 (6%)
1	C	80/96 (83%)	-0.40	1 (1%) 77 71	23, 34, 43, 48	4 (5%)
1	D	79/96 (82%)	-0.25	1 (1%) 77 71	25, 40, 53, 55	7 (8%)
All	All	319/384 (83%)	-0.31	4 (1%) 77 71	23, 35, 52, 57	23 (7%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ILE	2.5
1	B	218	ILE	2.3
1	D	218	ILE	2.3
1	C	218	ILE	2.2

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.