

Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2024 – 04:08 PM EDT

PDB ID	:	8V0E
Title	:	ANK repeat of MIB1
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Deposited on	:	2023-11-17
Resolution	:	2.39 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.39 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	164625	4642 (2.40-2.40)		
Clashscore	180529	5218 (2.40-2.40)		
Ramachandran outliers	177936	5158 (2.40-2.40)		
Sidechain outliers	177891	5159 (2.40-2.40)		
RSRZ outliers	164620	4642 (2.40-2.40)		

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	А	386	3% 80%	9%		11%
1	В	386	17%	11%	•	11%
2	D	5	100%			



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2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5341 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 E3 ubiquitin-protein ligase MIB1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	A 344	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	1 A		2623	1613	497	504	9	0		0
1	В	349	Total	С	Ν	Ο	S	0	0	0
	I B	342	2542	1555	487	491	9			

• Molecule 2 is a protein called Unidentified MIB1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	5	Total 25	C 15	N 5	O 5	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	98	Total O 98 98	0	0
3	В	53	Total O 53 53	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: E3 ubiquitin-protein ligase MIB1

• Molecule 2: Unidentified MIB1 peptide

Chain D:

100%

There are no outlier residues recorded for this chain.



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	79.00Å 137.47Å 96.25Å	Depositor
a, b, c, α , β , γ	90.00° 108.14° 90.00°	Depositor
Bosolution(A)	47.64 - 2.39	Depositor
Resolution (A)	47.64 - 2.39	EDS
% Data completeness	97.7(47.64-2.39)	Depositor
(in resolution range)	98.4(47.64-2.39)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.42 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.207 , 0.244	Depositor
II, II, <i>free</i>	0.208 , 0.245	DCC
R_{free} test set	1887 reflections $(4.89%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.8	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 54.7	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5341	wwPDB-VP
Average B, all atoms $(Å^2)$	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 16.39% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.39	0/2659	0.64	0/3599	
1	В	0.35	0/2576	0.59	1/3489~(0.0%)	
All	All	0.37	0/5235	0.61	1/7088~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	567	LEU	CA-CB-CG	5.85	128.76	115.30

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	А	2623	0	2623	25	0
1	В	2542	0	2458	23	0
2	D	25	0	8	0	0
3	А	98	0	0	5	0
3	В	53	0	0	1	0
All	All	5341	0	5089	48	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 5.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:513:ILE:HD11	1:B:545:VAL:HG13	1.61	0.81	
1:A:620:PRO:HD2	1:A:624:ILE:HD12	1.69	0.75	
1:A:588:ASP:OD2	3:A:801:HOH:O	2.10	0.69	
1:B:620:PRO:HD2	1:B:624:ILE:HD12	1.74	0.69	
1:B:667:GLN:NE2	1:B:675:GLU:OE2	2.28	0.66	
1:A:477:VAL:HG13	1:A:515:VAL:HG21	1.78	0.65	
1:A:793:HIS:ND1	1:A:794:LYS:HG2	2.14	0.63	
1:A:496:ASP:HA	1:A:528:LYS:HD3	1.80	0.62	
1:B:493:GLU:HB3	1:B:497:GLY:HA2	1.81	0.62	
1:B:526:ARG:NH2	1:B:559:GLN:O	2.33	0.62	
1:B:768:ILE:O	1:B:776:PRO:HD3	2.01	0.61	
1:B:621:ARG:HG2	1:B:623:TRP:CH2	2.36	0.61	
1:A:439:ALA:HA	1:A:479:ILE:HD13	1.84	0.60	
1:A:793:HIS:HE1	1:A:794:LYS:HE3	1.66	0.59	
1:B:574:LYS:NZ	3:B:805:HOH:O	2.36	0.57	
1:A:768:ILE:O	1:A:776:PRO:HD3	2.06	0.55	
1:A:503:HIS:HA	1:A:506:PHE:CD2	2.42	0.54	
1:B:510:GLY:O	1:B:514:GLU:HG3	2.07	0.54	
1:B:510:GLY:HA2	1:B:513:ILE:HD12	1.88	0.53	
1:B:703:LEU:HD21	1:B:766:LEU:HD23	1.91	0.51	
1:B:491:GLU:HA	1:B:499:ARG:HD3	1.91	0.51	
1:B:503:HIS:HA	1:B:506:PHE:CD2	2.45	0.50	
1:B:477:VAL:HG22	1:B:481:LYS:HE2	1.94	0.50	
1:A:543:LEU:HD11	1:A:581:VAL:HG21	1.93	0.50	
1:B:719:GLN:O	1:B:723:ASP:HB2	2.12	0.50	
1:A:544:GLN:NE2	3:A:809:HOH:O	2.44	0.49	
1:A:468:MET:HG3	1:A:488:VAL:HG21	1.94	0.49	
1:A:791:LYS:HD2	3:A:857:HOH:O	2.12	0.49	
1:A:662:GLN:HB3	1:A:666:GLN:HA	1.95	0.49	
1:A:793:HIS:CE1	1:A:794:LYS:HE3	2.45	0.49	
1:A:526:ARG:HB3	1:A:530:ARG:HA	1.95	0.47	
1:A:449:ASP:HA	1:A:452:LYS:HE3	1.96	0.47	
1:B:793:HIS:ND1	1:B:794:LYS:HG2	2.30	0.46	
1:B:610:SER:O	1:B:614:VAL:HG23	2.16	0.46	
1:A:770:ASN:OD1	1:A:774:GLN:HG2	2.16	0.46	
1:A:526:ARG:HG3	1:A:530:ARG:HH21	1.80	0.46	
1:A:444:VAL:HG22	1:A:479:ILE:HG13	1.97	0.45	
1:A:609:PRO:HD2	3:A:829:HOH:O	2.18	0.44	
1:A:607:GLY:O	1:A:609:PRO:HD3	2.19	0.42	
1:B:440:ALA:O	1:B:476:HIS:NE2	2.52	0.42	
1:B:629:LYS:NZ	1:B:631:ASP:OD2	2.53	0.42	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:GLN:NE2	1:A:779:LEU:HD21	2.35	0.41
1:A:530:ARG:NE	3:A:812:HOH:O	2.45	0.41
1:B:473:GLN:HG3	1:B:506:PHE:HB2	2.03	0.41
1:B:527:ASN:OD1	1:B:531:GLN:N	2.51	0.41
1:B:770:ASN:OD1	1:B:774:GLN:HG2	2.21	0.41
1:B:567:LEU:HG	1:B:587:ALA:HB1	2.04	0.40
1:A:620:PRO:O	1:A:621:ARG:HG3	2.21	0.40

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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	Perce	entiles
1	А	340/386~(88%)	333~(98%)	7~(2%)	0	100	100
1	В	336/386~(87%)	324 (96%)	12 (4%)	0	100	100
All	All	676/772~(88%)	657 (97%)	19(3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	А	281/314~(90%)	280 (100%)	1 (0%)	89 95



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	$\operatorname{ntil}\epsilon$	\mathbf{s}
1	В	258/314 (82%)	253~(98%)	5(2%)	52	72	
All	All	539/628~(86%)	533 (99%)	6 (1%)	70	84	

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All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	490	VAL
1	В	444	VAL
1	В	446	LYS
1	В	619	LEU
1	В	621	ARG
1	В	712	LEU

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

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 oligosaccharides 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^{th} 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	344/386~(89%)	0.39	13 (3%) 44 42	29, 50, 88, 122	0
1	В	342/386~(88%)	1.20	67 (19%) 4 3	35, 70, 142, 160	0
2	D	0/5	-	-	-	-
All	All	686/777~(88%)	0.79	80 (11%) 10 9	29, 59, 129, 160	0

All (80) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	432	ASN	5.3
1	А	724	VAL	5.3
1	В	747	ALA	5.0
1	В	746	GLY	4.8
1	В	722	GLN	4.7
1	В	724	VAL	4.7
1	В	457	ASP	4.3
1	В	450	LEU	3.9
1	В	447	VAL	3.9
1	В	462	CYS	3.9
1	В	507	GLY	3.9
1	В	430	ASP	3.8
1	В	444	VAL	3.7
1	В	458	VAL	3.7
1	В	436	VAL	3.6
1	В	486	GLN	3.6
1	В	453	ARG	3.6
1	В	435	LEU	3.6
1	В	506	PHE	3.4
1	В	449	ASP	3.4
1	В	451	LEU	3.3
1	В	490	VAL	3.3
1	В	452	LYS	3.2



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Mol	Chain	Res	Type	RSRZ
1	В	454	PRO	3.1
1	В	630	ASP	3.1
1	А	792	CYS	3.1
1	В	718	LEU	3.1
1	В	477	VAL	3.1
1	В	429	GLY	3.0
1	В	479	ILE	2.9
1	В	562	GLU	2.9
1	В	466	THR	2.9
1	В	482	LEU	2.9
1	В	777	LEU	2.8
1	В	768	ILE	2.8
1	В	508	ASP	2.8
1	А	506	PHE	2.7
1	В	504	ALA	2.7
1	А	428	SER	2.7
1	В	439	ALA	2.6
1	А	718	LEU	2.6
1	В	445	ALA	2.6
1	А	750	LYS	2.6
1	В	530	ARG	2.5
1	В	772	LYS	2.5
1	В	467	ALA	2.5
1	В	487	ASN	2.5
1	В	446	LYS	2.4
1	В	794	LYS	2.4
1	А	464	GLY	2.4
1	В	750	LYS	2.4
1	В	470	ALA	2.4
1	А	721	MET	2.3
1	В	791	LYS	2.3
1	В	431	LEU	2.3
1	B	503	HIS	2.3
1	В	484	LEU	2.3
1	A	463	ALA	2.3
1	В	461	GLN	2.3
1	В	468	MET	2.2
1	B	448	GLU	2.2
1	В	529	ARG	2.2
1	В	460	GLY	2.2
1	В	528	LYS	2.2
1	В	440	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	В	521	ALA	2.2
1	В	752	ALA	2.2
1	В	471	ALA	2.2
1	В	456	VAL	2.2
1	В	488	VAL	2.2
1	В	455	ASP	2.2
1	В	793	HIS	2.2
1	А	630	ASP	2.2
1	В	783	PRO	2.1
1	В	789	LEU	2.1
1	А	794	LYS	2.1
1	А	466	THR	2.1
1	В	639	ALA	2.1
1	В	511	ALA	2.0
1	А	465	HIS	2.0

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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 monosaccharides 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.

