

Full wwPDB X-ray Structure Validation Report (i)

Apr 10, 2024 - 04:07 pm BST

PDB ID	:	8RWU
Title	:	ACDC domain of the AP2-I transcription factor from Plasmodium vivax
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Deposited on		
Resolution	:	3.15 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:

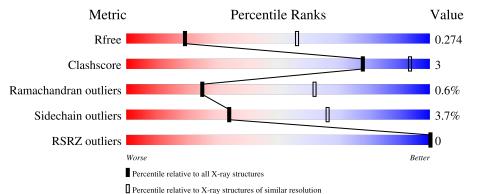
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.15 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	201	41%	·	56%		
1	В	201	37%	5%•	57%		



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1388 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	89	Total	С	Ν	0	S	0	0	0
1	A	89	701	444	118	133	6	0		
1	D	87	Total	С	Ν	0	S	0	0	0
1	D	01	687	437	115	129	6	0	0	0

• Molecule 1 is a protein called AP2 domain transcription factor AP2-I, putative.



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: AP2 domain transcription factor AP2-I, putative

Chain A:	41%	·	56%	
SER LEU ASN GLU GLU GLU GLU GLU ALA ALA	ASP LYS LYS LYS GLU GLU TILE SER MET MET	ASN GLU GLU GLN ASP LEU LEU D60 B82 B82	K123 K123 V128 V132 S148 GLN GLN GLN SER SER SER SER SER SER VAL	SER TYR LEU GLU LEU HIS ASN ASP TYR
GLU ASP ILE ILE HIS ASP LYS CLY SU SN ASN ALA	1HK THR THR ALA SER ASN SER MET GLN GLN ASN ASN MET	ASN SER ASN ASN ASN LEU SER CLN SER SER MET	LYS GLY SER SER ILE ILE HIS MET ASN ASN ASN ASN THR SER ASN VAL SER SER	GLY ASN ALA ALA THR GLY ASN SER SER GLY
HIS ILE SER ASN ALA				
• Molecule 1: A	AP2 domain tran	scription facto	r AP2-I, putative	
Chain B:	37%	5% •	57%	
H P L C K C K C K C K C K C K C K C K C K C				
SECTION SECTIO	ASP LYS LYS GLU GLU GLU TLE SER MET MET	ASN GLU GLN GLN LYS LYS LYS LEU LEU LEU CSO CSO	A81 D82 D82 D82 A81 A81 A88 A88 A88 A88 A88 A88 A88 A88	1130 C133 S148 GLN GLN SER SER
	_	_	ASN ASN ASI MET DB2 ASN ASN SER ASN SER ASN ASN RS6 ASN RS6 ASN R96 CLU 7103 CLU 7103 CLV 7103 SER 1104 CLV 8 CLV 7103 SER 1124	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	78.49Å 78.49Å 123.88Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 - 3.15	Depositor
Resolution (A)	48.62 - 3.15	EDS
% Data completeness	99.7 (48.62-3.15)	Depositor
(in resolution range)	99.8 (48.62-3.15)	EDS
R _{merge}	0.12	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.26 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
D D	0.241 , 0.278	Depositor
R, R_{free}	0.240 , 0.274	DCC
R_{free} test set	357 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	134.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 83.9	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1388	wwPDB-VP
Average B, all atoms $(Å^2)$	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.36% 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).

Mol	Chain		lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.22	0/713	0.36	0/968	
1	В	0.23	0/698	0.34	0/946	
All	All	0.23	0/1411	0.35	0/1914	

There are no bond length outliers.

There are no bond angle outliers.

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	701	0	704	4	0
1	В	687	0	692	6	0
All	All	1388	0	1396	8	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 3.

All (8) 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:A:132:VAL:HG21	1:B:130:ILE:HG23	1.86	0.57	
1:A:147:ASP:OD2	1:B:98:ARG:NH1	2.40	0.54	

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG23	1:B:104:THR:HG23	1.95	0.48
1:B:80:CYS:O	1:B:82:ASP:N	2.46	0.48
1:A:60:ASP:N	1:A:60:ASP:OD1	2.47	0.47
1:B:124:LEU:HG	1:B:127:THR:HB	1.98	0.46
1:B:85:SER:O	1:B:89:LYS:HG2	2.20	0.42
1:A:123:LYS:HG2	1:A:128:TRP:CD2	2.56	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	Pe	erce	entiles
1	А	87/201~(43%)	86~(99%)	1 (1%)	0	1	.00	100
1	В	83/201~(41%)	81~(98%)	1 (1%)	1 (1%)		13	46
All	All	170/402~(42%)	167 (98%)	2(1%)	1 (1%)		25	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	81	ALA

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	82/179~(46%)	80~(98%)	2(2%)	49 76	
1	В	80/179~(45%)	76~(95%)	4 (5%)	24 57	
All	All	162/358~(45%)	156~(96%)	6 (4%)	34 66	

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

Mol	Chain	Res	Type	
1	А	82	ASP	
1	А	98	ARG	
1	В	76	LEU	
1	В	82	ASP	
1	В	124	LEU	
1	В	133	CYS	

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 monosaccharides 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 >	#RSR	Z>2	$OWAB(Å^2)$	Q<0.9
1	А	89/201~(44%)	-0.17	0 100	100	85, 113, 159, 172	0
1	В	87/201 (43%)	-0.03	0 100	100	95, 125, 181, 228	0
All	All	176/402~(43%)	-0.10	0 100	100	85, 121, 171, 228	0

There are no RSRZ outliers to report.

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.

