

Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 - 02:20 am BST

:	4NT1
:	Crystal structure of apo-form of Arabidopsis ACD11 (accelerated-cell-death
	11) at 1.8 Angstrom resolution
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	2013-11-29
:	1.80 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 following versions of software and data (see references (1)) were used in the production of this report:

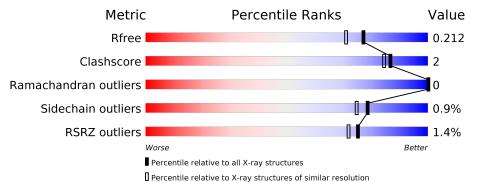
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950(1.80-1.80)
Clashscore	141614	6793(1.80-1.80)
Ramachandran outliers	138981	6697(1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850(1.80-1.80)

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 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	207	93%	•	·
1	В	207	91%	6%	•
1	С	207	91%	6%	·
1	D	207	2% 91%	• 6	%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6976 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	Λ	200	Total	С	Ν	Ο	S	0	9	0
	A	200	1549	993	266	280	10	0	3	0
1	В	200	Total	С	Ν	Ο	S	0	6	0
	D	200	1577	1012	269	286	10	0	0	0
1	С	200	Total	С	Ν	Ο	S	0	4	0
	U	200	1566	1004	266	286	10	0	4	0
1	п	105	Total	С	Ν	Ο	S	0	6	0
		195	1530	984	262	274	10	0	6	0

• Molecule 1 is a protein called accelerated-cell-death 11.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP 064587
В	0	SER	-	EXPRESSION TAG	UNP 064587
С	0	SER	-	EXPRESSION TAG	UNP 064587
D	0	SER	-	EXPRESSION TAG	UNP 064587

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atom	.s	ZeroOcc	AltConf
2	А	1	Total 1 1	Na 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	192	Total O 192 192	0	0
3	В	198	Total O 198 198	0	0
3	С	180	Total O 180 180	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	183	Total O 183 183	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

- Chain A: 93% SER MET ALA ASP GLU GLU • Molecule 1: accelerated-cell-death 11 Chain B: 91% 6% SER MET ALA ASP SER SER GLU • Molecule 1: accelerated-cell-death 11 Chain C: 91% 6% SER MET ALA ASP SER SER ALA • Molecule 1: accelerated-cell-death 11 Chain D: 91% 6% SER MET ALA ASP SER GLU GLU GLEU GLEV ASP
- Molecule 1: accelerated-cell-death 11



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.76Å 77.01 Å 154.72 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.82 - 1.80	Depositor
Resolution (A)	33.82 - 1.80	EDS
% Data completeness	95.0 (33.82-1.80)	Depositor
(in resolution range)	94.0 (33.82-1.80)	EDS
R _{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.11 (at 1.79 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R R.	0.174 , 0.213	Depositor
R, R_{free}	0.172 , 0.212	DCC
R_{free} test set	3912 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	24.0	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 41.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6976	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.56% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, KCX

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/1578	0.45	0/2133	
1	В	0.33	0/1614	0.49	0/2181	
1	С	0.30	0/1596	0.45	0/2159	
1	D	0.32	0/1564	0.49	0/2113	
All	All	0.32	0/6352	0.47	0/8586	

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	1549	0	1595	5	0
1	В	1577	0	1631	12	0
1	С	1566	0	1606	13	0
1	D	1530	0	1596	4	0
2	А	1	0	0	0	0
3	А	192	0	0	0	0
3	В	198	0	0	3	0
3	С	180	0	0	2	0
3	D	183	0	0	1	0
All	All	6976	0	6428	27	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 2.

All (27) close contacts	within the	same	$\operatorname{asymmetric}$	unit a	are listed	below,	sorted by	v their cl	ash
magnitude.									

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:55:LYS:HZ1	1:C:92:ARG:HH22	1.42	0.68
1:B:55:LYS:NZ	1:C:92:ARG:HH22	1.92	0.67
1:D:102:LEU:HD12	1:D:105:LYS:HE3	1.81	0.63
1:A:156:TYR:O	1:C:201[A]:GLN:HG3	2.00	0.62
1:B:55:LYS:HZ1	1:C:92:ARG:NH2	2.00	0.59
1:B:93[A]:LYS:HD2	3:B:355:HOH:O	2.06	0.55
1:C:84:LYS:HE3	3:C:411:HOH:O	2.06	0.54
1:D:149[A]:LYS:HG3	1:D:150:ALA:N	2.22	0.54
1:B:129:ASP:HB2	1:B:130:PRO:HD3	1.91	0.52
1:A:164:LEU:HA	1:A:167:MET:HE3	1.97	0.47
1:B:55:LYS:HZ3	1:C:92:ARG:HH12	1.63	0.47
1:A:152:SER:HB2	1:B:52:ILE:HD13	1.97	0.46
1:C:52:ILE:HG23	3:C:381:HOH:O	2.13	0.46
1:B:55:LYS:NZ	1:C:92:ARG:NH2	2.58	0.46
1:B:145:TRP:CE3	1:B:149:LYS:HD2	2.53	0.44
1:C:169:LYS:HA	1:C:169:LYS:HD3	1.87	0.43
1:A:164:LEU:HA	1:A:167:MET:CE	2.50	0.42
1:D:132[A]:THR:HG23	3:D:381:HOH:O	2.19	0.42
1:B:8:LYS:HA	3:B:306:HOH:O	2.18	0.42
1:B:93[A]:LYS:HE3	3:B:361:HOH:O	2.20	0.42
1:C:52:ILE:HD11	1:C:156:TYR:CE1	2.55	0.42
1:C:153:LEU:O	1:C:156:TYR:HD1	2.03	0.41
1:B:61:TYR:CD1	1:B:107:GLY:HA3	2.55	0.41
1:C:21:ALA:HA	1:C:24[B]:VAL:HG22	2.03	0.41
1:A:8:LYS:HB3	1:A:11:ARG:HG3	2.03	0.41
1:D:44:SER:HB2	1:D:45:PRO:HD3	2.02	0.40
1:C:129:ASP:HB2	1:C:130:PRO:HD3	2.02	0.40

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	ers Percentile	
1	А	200/207~(97%)	197~(98%)	3(2%)	0	100	100
1	В	203/207~(98%)	200~(98%)	3~(2%)	0	100	100
1	С	201/207~(97%)	198~(98%)	3~(2%)	0	100	100
1	D	198/207~(96%)	195~(98%)	3(2%)	0	100	100
All	All	802/828~(97%)	790~(98%)	12 (2%)	0	100	100

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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	169/174~(97%)	167~(99%)	2(1%)	71	65	
1	В	174/174~(100%)	172~(99%)	2(1%)	73	68	
1	С	171/174~(98%)	170~(99%)	1 (1%)	86	84	
1	D	168/174~(97%)	166~(99%)	2(1%)	71	65	
All	All	682/696~(98%)	675~(99%)	7 (1%)	78	71	

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	103	ARG
1	А	105	LYS
1	В	10	LEU
1	В	105	LYS
1	С	105	LYS
1	D	149[A]	LYS
1	D	149[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	А	25	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Chain Res	Chain	Bos	Link	B	Bond lengths			Bond angles			
		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2			
1	KCX	С	64	1	7,11,12	1.03	1 (14%)	4,12,14	1.18	0		
1	KCX	D	64	1	7,8,12	0.53	0	3,8,14	0.31	0		
1	KCX	А	64	1	$7,\!8,\!12$	0.58	0	3,8,14	0.34	0		
1	KCX	В	64	1	7,11,12	1.02	1 (14%)	4,12,14	1.65	1 (25%)		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	\mathbf{Link}	Chirals	Torsions	Rings
1	KCX	С	64	1	-	1/7/10/12	-
1	KCX	D	64	1	-	1/6/7/12	-
1	KCX	А	64	1	-	0/6/7/12	-
1	KCX	В	64	1	-	0/7/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	64	KCX	CE-NZ	2.24	1.50	1.45
1	В	64	KCX	CE-NZ	2.22	1.50	1.45



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	64	KCX	CE-NZ-CX	-2.80	118.21	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
1	С	64	KCX	CG-CD-CE-NZ
1	D	64	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	А	199/207~(96%)	-0.56	1 (0%) 91 89	17, 25, 36, 53	0
1	В	199/207~(96%)	-0.37	1 (0%) 91 89	16, 23, 38, 51	0
1	С	199/207~(96%)	-0.47	5 (2%) 57 52	17, 26, 40, 54	0
1	D	194/207~(93%)	-0.50	4 (2%) 63 59	17, 24, 40, 65	0
All	All	791/828~(95%)	-0.48	11 (1%) 75 72	16, 25, 39, 65	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	27	PRO	4.6
1	С	156	TYR	3.6
1	В	7	ASP	3.5
1	С	28	ASN	3.3
1	D	198	LEU	3.1
1	А	7	ASP	2.8
1	D	199	SER	2.7
1	D	7	ASP	2.5
1	D	6	ALA	2.3
1	С	52	ILE	2.2
1	С	26	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
1	KCX	С	64	12/13	0.94	0.09	$22,\!27,\!40,\!41$	0

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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	KCX	D	64	9/13	0.95	0.11	$21,\!22,\!32,\!33$	0
1	KCX	В	64	12/13	0.97	0.09	$16,\!18,\!24,\!25$	0
1	KCX	А	64	9/13	0.98	0.09	$19,\!21,\!33,\!34$	0

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6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({f A}^2)$	Q<0.9
2	NA	А	301	1/1	0.82	0.19	$54,\!54,\!54,\!54$	0

6.5 Other polymers (i)

There are no such residues in this entry.

