



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:56 pm BST

PDB ID : 6AZC  
Title : Crystal structure of Physcomitrella patens KAI2-like E S166A  
Authors : Burger, M.; Lee, H.J.; Chory, J.  
Deposited on : 2017-09-11  
Resolution : 2.00 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](mailto: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 ⓘ symbol.

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

MolProbity	:	4.02b-467
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

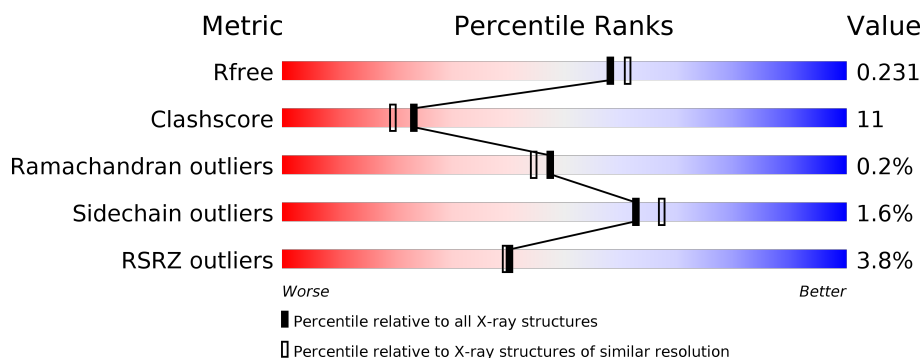
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	272	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	272	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4243 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 Pp-KAI2-like E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2039	1313	338	379	9			
1	B	263	Total	C	N	O	S	0	1	0
			2044	1317	338	379	10			

There are 6 discrepancies between the modelled and reference sequences:

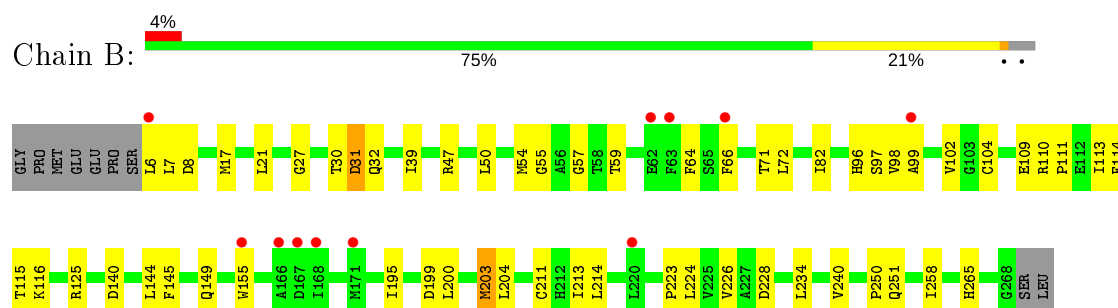
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP A9ST85
A	0	PRO	-	cloning artifact	UNP A9ST85
A	166	ALA	SER	engineered mutation	UNP A9ST85
B	-1	GLY	-	cloning artifact	UNP A9ST85
B	0	PRO	-	cloning artifact	UNP A9ST85
B	166	ALA	SER	engineered mutation	UNP A9ST85

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	85	Total	O	0	0
			85	85		
2	B	75	Total	O	0	0
			75	75		

**i**

- Molecule 1: Pp-KAI2-like E



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.93Å 121.82Å 46.91Å 90.00° 91.54° 90.00°	Depositor
Resolution (Å)	46.89 – 2.00 46.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.89-2.00) 91.1 (46.89-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.49 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.220 , 0.253 0.205 , 0.231	Depositor DCC
$R_{free}$ test set	1712 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.0	Xtriage
Anisotropy	1.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 25.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.129 for l,k,-h 0.207 for h,-k,-l 0.137 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.26	0/2089	0.45	0/2844
1	B	0.25	0/2097	0.44	0/2854
All	All	0.26	0/4186	0.44	0/5698

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	A	2039	0	2016	48	0
1	B	2044	0	2025	44	0
2	A	85	0	0	15	1
2	B	75	0	0	19	0
All	All	4243	0	4041	92	1

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 11.

All (92) 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:B:6:LEU:HD23	1:B:7:LEU:H	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLY:O	2:A:301:HOH:O	1.81	0.95
1:A:130:ARG:NH1	2:A:302:HOH:O	1.99	0.93
1:B:214:LEU:O	2:B:301:HOH:O	1.97	0.82
1:A:55:GLY:H	1:A:59:THR:HG21	1.48	0.78
1:B:6:LEU:CD2	1:B:7:LEU:H	1.96	0.77
1:B:6:LEU:HD23	1:B:7:LEU:N	2.01	0.76
1:B:6:LEU:HD21	1:B:82:ILE:HG12	1.67	0.76
1:B:211:CYS:SG	2:B:374:HOH:O	2.44	0.75
1:B:104:CYS:SG	2:B:374:HOH:O	2.47	0.73
1:A:68:ARG:O	2:A:303:HOH:O	2.07	0.72
1:A:96:HIS:ND1	2:A:309:HOH:O	2.22	0.71
1:B:116:LYS:O	2:B:302:HOH:O	2.07	0.70
1:A:6:LEU:O	2:A:304:HOH:O	2.08	0.69
1:A:167:ASP:OD1	1:A:168:ILE:N	2.27	0.68
1:B:96:HIS:N	2:B:310:HOH:O	2.28	0.67
1:B:71:THR:O	2:B:303:HOH:O	2.13	0.65
1:A:72:LEU:HD12	1:A:200:LEU:HD11	1.78	0.64
1:A:22:VAL:HG22	1:A:92:ILE:HB	1.77	0.64
1:B:6:LEU:O	2:B:305:HOH:O	2.15	0.64
1:A:48:VAL:HA	2:A:314:HOH:O	1.98	0.63
1:A:148:MET:HG2	1:A:155:TRP:CD2	2.33	0.63
1:B:99:ALA:HB3	2:B:310:HOH:O	1.97	0.62
1:A:22:VAL:HB	2:A:314:HOH:O	1.99	0.61
1:A:250:PRO:HB2	1:A:258:ILE:HD11	1.82	0.61
1:B:228:ASP:OD1	2:B:306:HOH:O	2.16	0.61
1:B:110:ARG:HB3	1:B:113:ILE:HG12	1.84	0.59
1:B:140:ASP:HA	2:B:320:HOH:O	2.02	0.59
1:A:13:ARG:NH1	2:A:319:HOH:O	2.36	0.58
1:B:72:LEU:HD12	1:B:200:LEU:HD11	1.84	0.58
1:B:114:PHE:HD2	2:B:314:HOH:O	1.87	0.58
1:A:263:LYS:NZ	2:A:321:HOH:O	2.37	0.57
1:B:66:PHE:O	2:B:307:HOH:O	2.16	0.57
1:A:101:MET:HB3	1:A:200:LEU:HD12	1.88	0.56
1:B:223:PRO:HG2	1:B:226:VAL:HG23	1.88	0.55
1:A:105:LEU:O	2:A:306:HOH:O	2.18	0.54
1:A:110:ARG:HB3	1:A:113:ILE:HG12	1.90	0.54
1:B:250:PRO:HB2	1:B:258:ILE:HD11	1.87	0.54
1:B:6:LEU:CG	1:B:7:LEU:H	2.17	0.54
1:B:115:THR:HG22	2:B:327:HOH:O	2.06	0.53
1:A:38:VAL:HG22	1:A:259:ILE:HG12	1.91	0.53
1:B:145:PHE:O	1:B:149:GLN:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:OG1	1:B:31:ASP:N	2.41	0.52
1:A:59:THR:O	1:A:61:PRO:HD3	2.11	0.51
1:B:27:GLY:HA3	1:B:97:SER:HB3	1.93	0.51
1:A:264:ARG:NH1	2:A:326:HOH:O	2.42	0.51
1:A:44:ASP:OD1	2:A:307:HOH:O	2.19	0.51
1:A:145:PHE:O	1:A:149:GLN:HG3	2.11	0.51
1:A:186:ASP:O	2:A:305:HOH:O	2.19	0.51
1:B:125:ARG:NH1	1:B:199:ASP:OD2	2.42	0.50
1:A:178:ARG:O	1:A:182:ASN:ND2	2.40	0.50
1:B:111:PRO:HA	2:B:314:HOH:O	2.11	0.50
1:A:167:ASP:O	1:A:173:VAL:HG21	2.12	0.50
1:A:6:LEU:O	1:A:8:ASP:N	2.43	0.49
1:A:30:THR:OG1	1:A:31:ASP:N	2.45	0.49
1:A:116:LYS:NZ	1:A:268:GLY:O	2.44	0.49
1:B:116:LYS:NZ	1:B:265:HIS:O	2.41	0.49
1:A:27:GLY:HA2	1:A:98:VAL:HG12	1.95	0.48
1:A:109:GLU:HA	2:B:307:HOH:O	2.13	0.48
1:A:144:LEU:O	1:A:148:MET:HG3	2.13	0.48
1:B:99:ALA:HA	1:B:102:VAL:HB	1.95	0.48
1:A:22:VAL:HA	1:A:92:ILE:O	2.15	0.47
1:B:8:ASP:OD1	2:B:308:HOH:O	2.20	0.47
1:A:56:ALA:O	1:A:59:THR:HG22	2.15	0.46
1:B:39:ILE:HD11	1:B:50:LEU:HD21	1.98	0.46
1:A:148:MET:HE1	1:A:189:PHE:HA	1.97	0.45
1:A:184:ARG:HG2	1:A:186:ASP:OD1	2.16	0.45
1:A:148:MET:CE	1:A:189:PHE:HA	2.46	0.45
1:B:203:MET:HE2	1:B:204:LEU:HD23	1.99	0.44
1:A:153:LYS:HB2	1:A:181:PHE:CE1	2.53	0.44
1:B:21:LEU:HD23	1:B:47:ARG:HB3	2.00	0.44
1:B:204:LEU:HB3	1:B:234:LEU:HD12	1.99	0.44
1:B:98:VAL:HG21	1:B:195:ILE:HG12	1.99	0.44
1:B:32:GLN:HG2	2:B:321:HOH:O	2.19	0.43
1:B:55:GLY:H	1:B:59:THR:HG21	1.84	0.43
1:A:15:VAL:O	1:A:48:VAL:N	2.38	0.42
1:A:254:SER:O	1:A:258:ILE:HD13	2.20	0.42
1:B:144:LEU:HG	1:B:155:TRP:HE1	1.84	0.42
1:A:61:PRO:O	1:A:184:ARG:NH1	2.52	0.42
1:A:265:HIS:CD2	2:A:326:HOH:O	2.71	0.42
1:A:158:GLY:C	1:A:161:PRO:HD2	2.40	0.42
1:A:263:LYS:NZ	2:A:317:HOH:O	2.33	0.42
1:A:21:LEU:HD23	1:A:47:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG13	1:A:49:ILE:HG12	2.02	0.41
1:B:109:GLU:OE2	2:B:309:HOH:O	2.21	0.41
1:A:250:PRO:HB2	1:A:258:ILE:CD1	2.50	0.41
1:B:96:HIS:CD2	1:B:251:GLN:HE22	2.38	0.41
1:B:224:LEU:HD12	1:B:224:LEU:HA	1.91	0.41
1:B:54:MET:HG3	1:B:64:PHE:HD1	1.86	0.41
1:B:213:ILE:HB	1:B:240:VAL:HG22	2.03	0.41
1:B:57:GLY:N	2:B:304:HOH:O	2.14	0.40
1:A:219:ASP:HB3	1:A:222:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:HOH:O	2:A:355:HOH:O[1_554]	2.19	0.01

## 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	261/272 (96%)	254 (97%)	6 (2%)	1 (0%)	34	30
1	B	262/272 (96%)	257 (98%)	5 (2%)	0	100	100
All	All	523/544 (96%)	511 (98%)	11 (2%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO

### 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	225/233 (97%)	221 (98%)	4 (2%)	59	63
1	B	226/233 (97%)	223 (99%)	3 (1%)	69	74
All	All	451/466 (97%)	444 (98%)	7 (2%)	62	67

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

Mol	Chain	Res	Type
1	A	31	ASP
1	A	170	SER
1	A	171	MET
1	A	234	LEU
1	B	17	MET
1	B	31	ASP
1	B	203	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	174	GLN
1	B	53	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 [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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	263/272 (96%)	0.60	9 (3%) 45 44	6, 15, 30, 56	0
1	B	263/272 (96%)	0.61	11 (4%) 36 35	7, 16, 30, 52	0
All	All	526/544 (96%)	0.60	20 (3%) 40 39	6, 16, 30, 56	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	ILE	5.8
1	B	6	LEU	4.7
1	A	166	ALA	4.3
1	B	66	PHE	4.1
1	A	167	ASP	4.0
1	B	166	ALA	4.0
1	B	99	ALA	3.7
1	B	168	ILE	3.2
1	B	62	GLU	2.9
1	A	220	LEU	2.9
1	A	189	PHE	2.8
1	A	165	GLY	2.7
1	A	155	TRP	2.3
1	B	63	PHE	2.3
1	B	167	ASP	2.3
1	B	155	TRP	2.2
1	B	171	MET	2.2
1	A	6	LEU	2.2
1	A	63	PHE	2.1
1	B	220	LEU	2.1

## 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.