Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 07:41 pm GMT

PDB ID	:	5A50
Title	:	The crystal structure of Arabidopsis thaliana CAR4 in complex with two calcium ions, Zn and Phopho Choline
Authors	:	Diaz, M.; Albert, A.
Deposited on	:	2015-06-16
Resolution	:	2.40 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 ⓘ 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 ⓘ) were used in the production of this report:

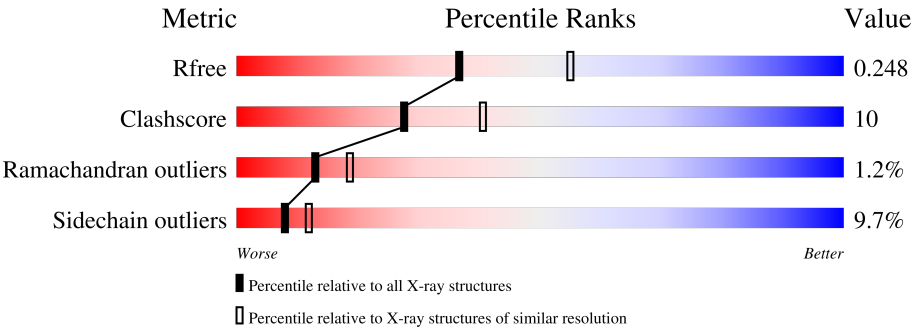
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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%

Mol	Chain	Length	Quality of chain
1	A	177	71% 18% • 7%
2	B	177	69% 20% • • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PC	B	205	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2775 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 AT3G17980.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1305	820	227	251	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	SER	LYS	conflict	UNP Q9LVH4

- Molecule 2 is a protein called AT3G17980.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1302	817	226	252	7			

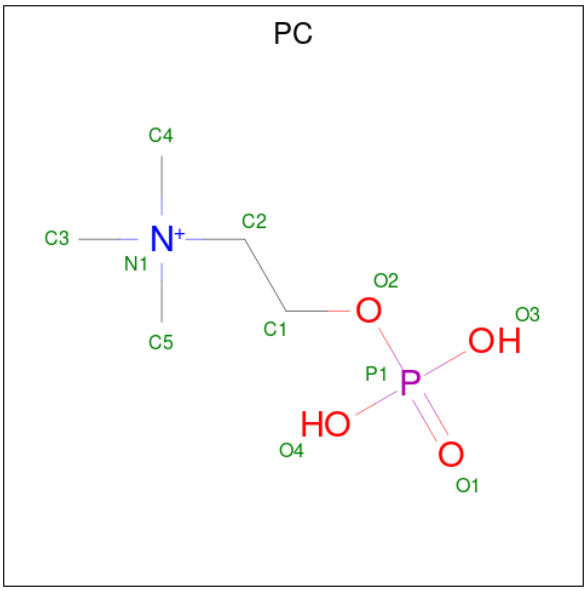
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	192	SER	LYS	conflict	UNP Q9LVH4
B	65	SER	LYS	conflict	UNP Q9LVH4

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

- Molecule 4 is PHOSPHOCHOLINE (three-letter code: PC) (formula: $C_5H_{15}NO_4P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 11 5 1 4 1	0	0
4	B	1	Total C N O P 11 5 1 4 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0

- Molecule 6 is water.

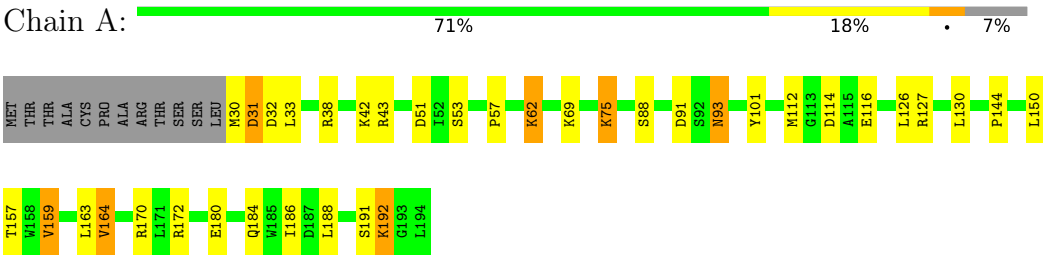
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	64	Total O 64 64	0	0
6	B	77	Total O 77 77	0	0

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. 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. 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.

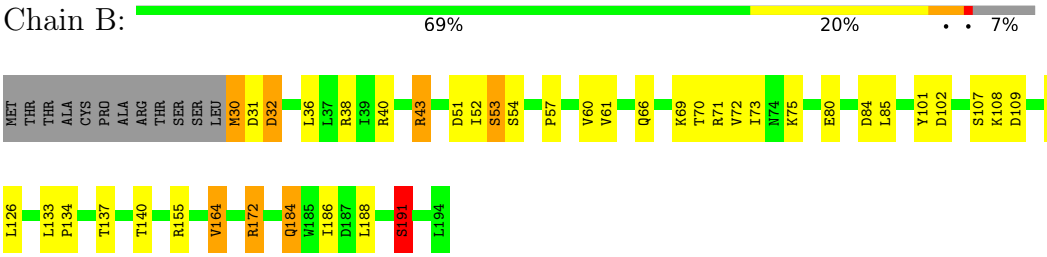
- Molecule 1: AT3G17980

Chain A:



- Molecule 2: AT3G17980

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	35.74Å 89.15Å 112.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 2.40 47.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.56-2.40) 98.0 (47.56-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.195 , 0.245 0.199 , 0.248	Depositor DCC
R_{free} test set	1340 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.0	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	0.94	EDS
Total number of atoms	2775	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2143e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PC, CA

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	0.40	0/1323	0.62	0/1790
2	B	0.44	0/1320	0.62	0/1787
All	All	0.42	0/2643	0.62	0/3577

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

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	1305	0	1336	20	0
2	B	1302	0	1328	31	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	B	22	0	26	8	0
5	B	1	0	0	0	0
6	A	64	0	0	4	1
6	B	77	0	0	9	1
All	All	2775	0	2690	53	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 10.

All (53) 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)
2:B:51:ASP:OD2	6:B:301:HOH:O	1.93	0.87
2:B:69:LYS:HD2	4:B:205:PC:H43	1.58	0.84
2:B:114:ASP:OD2	2:B:172:ARG:NH1	2.12	0.82
1:A:51:ASP:O	1:A:53:SER:N	2.23	0.72
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.53	0.72
1:A:30:MET:HB2	1:A:33:LEU:HG	1.70	0.72
1:A:75:LYS:NZ	6:A:304:HOH:O	2.22	0.71
2:B:75:LYS:NZ	6:B:305:HOH:O	2.23	0.71
2:B:71:ARG:HA	4:B:205:PC:H51	1.73	0.71
2:B:109:ASP:OD1	6:B:303:HOH:O	2.10	0.70
1:A:114:ASP:OD1	1:A:172:ARG:NH1	2.26	0.69
2:B:66:GLN:OE1	6:B:304:HOH:O	2.11	0.68
2:B:72:VAL:O	6:B:302:HOH:O	2.09	0.68
2:B:51:ASP:O	6:B:305:HOH:O	2.12	0.67
2:B:107:SER:O	6:B:303:HOH:O	2.13	0.65
1:A:93:ASN:OD1	1:A:93:ASN:N	2.33	0.62
2:B:164:VAL:HG23	2:B:184:GLN:HG2	1.83	0.61
4:B:203:PC:H41	6:B:313:HOH:O	2.03	0.58
2:B:51:ASP:O	2:B:53:SER:N	2.35	0.58
2:B:72:VAL:HG23	4:B:205:PC:H53	1.89	0.55
2:B:69:LYS:NZ	4:B:205:PC:H21	2.22	0.54
2:B:54:SER:HB3	2:B:75:LYS:HD3	1.89	0.54
1:A:116:GLU:HG2	1:A:172:ARG:HH21	1.70	0.54
1:A:112:MET:O	6:A:301:HOH:O	2.19	0.53
1:A:150:LEU:HB3	1:A:152:GLU:O	2.10	0.51
2:B:30:MET:HA	2:B:32:ASP:H	1.76	0.51
2:B:57:PRO:HA	2:B:101:TYR:O	2.11	0.50
2:B:108:LYS:HA	6:B:313:HOH:O	2.11	0.50
2:B:70:THR:O	4:B:205:PC:H41	2.11	0.49
1:A:38:ARG:HG3	1:A:38:ARG:NH1	2.21	0.48
2:B:133:LEU:HD22	2:B:137:THR:HG21	1.94	0.48
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.79	0.47
2:B:30:MET:CA	2:B:31:ASP:HB2	2.44	0.47
2:B:38:ARG:NH2	2:B:184:GLN:HG3	2.30	0.47
4:B:205:PC:O2	4:B:205:PC:H42	2.16	0.46
2:B:30:MET:HA	2:B:31:ASP:HB2	1.97	0.45
1:A:126:LEU:HG	1:A:163:LEU:HD23	1.99	0.45
1:A:38:ARG:NH2	1:A:186:ILE:HD11	2.32	0.45
2:B:84:ASP:O	2:B:85:LEU:HD23	2.17	0.45
2:B:123:ILE:HA	2:B:126:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:LEU:O	2:B:191:SER:OG	2.24	0.44
2:B:36:LEU:HB2	2:B:186:ILE:HB	2.00	0.44
2:B:69:LYS:HZ3	4:B:205:PC:H21	1.83	0.43
1:A:62:LYS:NZ	6:A:309:HOH:O	2.35	0.43
2:B:60:VAL:HG22	2:B:69:LYS:HB3	2.00	0.43
2:B:133:LEU:HA	2:B:134:PRO:HD3	1.89	0.42
1:A:57:PRO:HA	1:A:101:TYR:O	2.20	0.42
2:B:43:ARG:HD3	2:B:80:GLU:OE2	2.20	0.42
1:A:164:VAL:CG2	1:A:184:GLN:HG2	2.50	0.42
1:A:144:PRO:HD3	1:A:153:GLU:HA	2.02	0.41
1:A:157:THR:HG22	1:A:159:VAL:HG22	2.01	0.41
1:A:180:GLU:OE2	6:A:303:HOH:O	2.22	0.41
1:A:31:ASP:HA	1:A:192:LYS:HD2	2.03	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)
6:A:349:HOH:O	6:B:357:HOH:O[2_555]	2.14	0.06

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	163/177 (92%)	150 (92%)	11 (7%)	2 (1%)	13	19
2	B	163/177 (92%)	155 (95%)	6 (4%)	2 (1%)	13	19
All	All	326/354 (92%)	305 (94%)	17 (5%)	4 (1%)	13	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	191	SER
2	B	191	SER
2	B	52	ILE

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	A	150/160 (94%)	135 (90%)	15 (10%)	7 11
2	B	150/160 (94%)	136 (91%)	14 (9%)	9 13
All	All	300/320 (94%)	271 (90%)	29 (10%)	8 12

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	42	LYS
1	A	43	ARG
1	A	62	LYS
1	A	69	LYS
1	A	75	LYS
1	A	88	SER
1	A	91	ASP
1	A	93	ASN
1	A	127	ARG
1	A	130	LEU
1	A	159	VAL
1	A	164	VAL
1	A	188	LEU
1	A	192	LYS
2	B	30	MET
2	B	32	ASP
2	B	40	ARG
2	B	43	ARG
2	B	53	SER

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Mol	Chain	Res	Type
2	B	61	VAL
2	B	73	ILE
2	B	102	ASP
2	B	140	THR
2	B	155	ARG
2	B	164	VAL
2	B	172	ARG
2	B	184	GLN
2	B	191	SER

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

Mol	Chain	Res	Type
1	A	82	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PC	B	203	-	10,10,10	0.97	0	15,15,15	0.87	0
4	PC	B	205	5	10,10,10	1.14	0	15,15,15	0.82	0

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	Link	Chirals	Torsions	Rings
4	PC	B	203	-	-	2/8/8/8	-
4	PC	B	205	5	-	3/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	203	PC	O2-C1-C2-N1
4	B	205	PC	C1-O2-P1-O1
4	B	205	PC	C1-O2-P1-O3
4	B	205	PC	C1-O2-P1-O4
4	B	203	PC	C1-O2-P1-O1

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	203	PC	1	0
4	B	205	PC	7	0

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.