wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:51 PM GMT

PDB ID	:	1QX5
Title	:	Crystal structure of apoCalmodulin
Authors	:	Schumacher, M.A.; Crum, M.; Miller, M.C.
Deposited on	:	2003-09-04
Resolution	:	2.54 Å(reported)

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

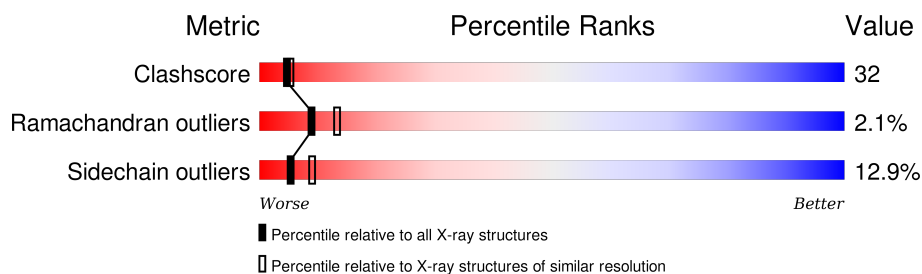|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.54 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	Percentile Ranks	Value
Clashscore		32
Ramachandran outliers		2.1%
Sidechain outliers		12.9%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

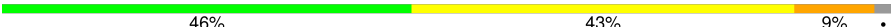| Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	148	46% 44% 7% ••
1	D	148	43% 45% 9% ••
1	I	148	49% 39% 10% ••
1	J	148	53% 36% 8% •
1	K	148	47% 43% 6% ••
1	R	148	50% 40% 9% ••
1	T	148	49% 45% ••

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Mol	Chain	Length	Quality of chain
1	Y	148	46% 43% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9333 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 Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	145	Total 1146	C 702	N 184	O 251	S 9	0	0	0
1	I	145	Total 1146	C 702	N 184	O 251	S 9	0	0	0
1	B	145	Total 1146	C 702	N 184	O 251	S 9	0	0	0
1	J	144	Total 1138	C 698	N 183	O 248	S 9	0	0	0
1	K	143	Total 1129	C 693	N 181	O 246	S 9	0	0	0
1	T	145	Total 1146	C 702	N 184	O 251	S 9	0	0	0
1	R	147	Total 1161	C 711	N 187	O 254	S 9	0	0	0
1	Y	145	Total 1146	C 702	N 184	O 251	S 9	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	26	Total 26	O 26	0	0
2	D	24	Total 24	O 24	0	0
2	I	30	Total 30	O 30	0	0
2	J	15	Total 15	O 15	0	0
2	K	20	Total 20	O 20	0	0
2	R	30	Total 30	O 30	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	T	7	Total 7	O 7	0	0
2	Y	23	Total 23	O 23	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: Calmodulin

Chain D:

- Molecule 1: Calmodulin

Chain I:

- Molecule 1: Calmodulin

Chain B:

- Molecule 1: Calmodulin

Chain J:

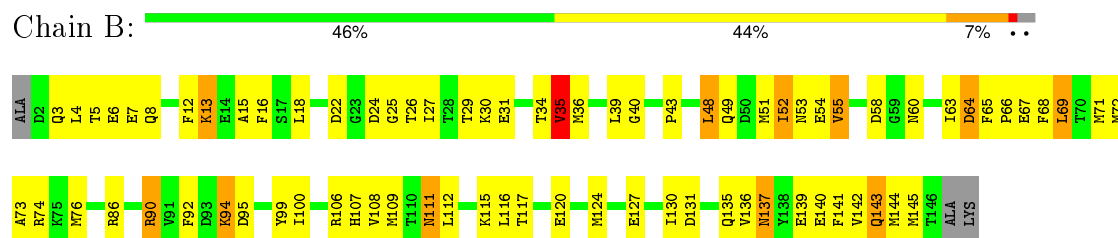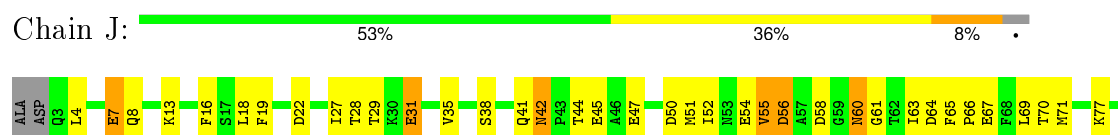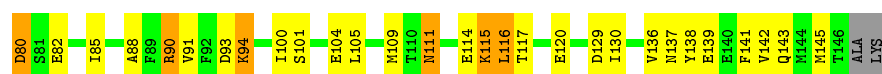D80 S81 E82 I85 A88 F89 R90 V91 F92 D93 K94 I100 S101 E104 L105 M109 T110 N111 E114 K115 L116 T117 E120 D129 I130 V136 N137 Y138 E139 F140 F141 V142 Q143 M144 M145 T146 ALA LYS

● Molecule 1: Calmodulin

Chain K:

47%   43%   6% • •

ALA ASP GLN L4 T5 E6 E7 Q8 E11 F12 F16 F19 D20 K21 D22 G23 D24 G25 T26 I27 T28 T29 K30 E31 L32 V35 M36 R37 S38 G40 Q41 N42 P43 L48 Q49 D50 M51 I52 N53 E54 V55 D56 A57 D58 G59 N60 I63 D64 F65 P66 E67 F68 L69

M72 A73 R74 K75 M76 T79 E84 I85 A88 F89 R90 V91 F92 D93 K94 N97 G98 Y99 A103 E104 L105 R106 H107 V108 N111 T117 D118 E119 E120 M124 Q135 E140 M144 M145 T146 ALA LYS

● Molecule 1: Calmodulin

Chain T:

49%   45%   • •

ALA D2 Q3 L4 T5 I9 K13 F19 D22 G23 D24 G25 T26 I27 T28 T29 K30 E31 L32 G33 T34 V35 M36 R37 S38 Q41 N42 P43 T44 E47 D50 M51 I52 N53 E54 V55 D56 T62 I63 D64 F65 P66 E67 M72 A73 R74 E83 E84 I85 R86

E87 R90 D93 K94 D95 G96 N97 G98 Y99 E104 L105 R106 H107 V108 N111 L112 K115 L116 T117 D118 E119 E120 V121 D122 E123 M124 I125 I130 D131 Q135 V136 N137 Y138 V142 M145 T146 ALA LYS

● Molecule 1: Calmodulin

Chain R:

50%   40%   9% ••

ALA D2 Q3 L4 T5 E6 E7 Q8 E14 L18 K21 D22 G23 D24 G25 T26 I27 T28 T29 K30 E31 V35 T44 E45 A46 E47 L48 Q49 D50 M51 I52 N53 E54 V55 D56 A57 D58 G59 N60 I63 D64 F65 P66 E67 F68 L69 T70 M71 M72 A73 R74 K75 M76 K77

S81 E82 E83 E84 I85 R86 R90 K94 N97 G98 Y99 H107 V108 M109 T110 N111 E114 K115 L116 E119 E120 V121 D122 E123 M124 I125 R126 D129 I130 D131 G134 Q135 V136 N137 Y138 E139 E140 F141 M144 M145 T146 A147 K148

● Molecule 1: Calmodulin

Chain Y:

46%   43%   9% •

ALA D2 Q3 L4 Q8 I9 L18 F19 D20 K21 D22 G23 D24 G25 T26 I27 T28 T29 K30 E31 G40 Q41 N42 P43 T44 E47 L48 Q49 D50 M51 I52 N53 E54 V55 D56 A57 D58 G59 N60 I63 D64 F65 P66 M71 M72 A73 R74 K75 M76 K77 D80 E83

E84 E87 R90 V91 F92 D93 K94 N97 G98 Y99 I100 S101 L105 R106 H107 N111 E114 K115 L116 T117 D118 E119 E120 E123 M124 I125 D129 I130 D131 G132 D133 G134 Q135 V136 N137 Y138 E139 E140 M144 M145 T146 ALA LYS

4   Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	146.00Å 146.00Å 78.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.39 – 2.54	Depositor
% Data completeness (in resolution range)	98.5 (66.39-2.54)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9333	wwPDB-VP
Average B, all atoms (Å²)	70.0	wwPDB-VP

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	B	0.83	2/1158 (0.2%)	0.83	0/1555
1	D	0.87	1/1158 (0.1%)	0.87	2/1555 (0.1%)
1	I	1.01	0/1158	1.06	8/1555 (0.5%)
1	J	0.68	0/1150	0.73	1/1544 (0.1%)
1	K	0.82	0/1141	0.82	1/1532 (0.1%)
1	R	0.93	1/1173 (0.1%)	0.92	1/1573 (0.1%)
1	T	0.59	0/1158	0.68	1/1555 (0.1%)
1	Y	0.77	0/1158	0.87	4/1555 (0.3%)
All	All	0.82	4/9254 (0.0%)	0.85	18/12424 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	R	0	1
1	Y	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	GLU	CG-CD	6.67	1.61	1.51
1	R	83	GLU	CG-CD	5.80	1.60	1.51
1	B	35	VAL	CA-CB	5.67	1.66	1.54
1	B	15	ALA	CA-CB	5.19	1.63	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	106	ARG	NE-CZ-NH2	-7.73	116.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	37	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	Y	131	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	I	131	ASP	CB-CG-OD1	7.36	124.93	118.30
1	R	129	ASP	CB-CG-OD1	-6.13	112.79	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	92	PHE	Sidechain
1	R	99	TYR	Sidechain
1	Y	138	TYR	Sidechain

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	B	1146	0	1070	89	0
1	D	1146	0	1070	83	0
1	I	1146	0	1070	63	0
1	J	1138	0	1066	67	0
1	K	1129	0	1058	93	0
1	R	1161	0	1088	77	0
1	T	1146	0	1070	74	0
1	Y	1146	0	1070	66	0
2	B	26	0	0	1	0
2	D	24	0	0	2	0
2	I	30	0	0	2	0
2	J	15	0	0	2	0
2	K	20	0	0	2	0
2	R	30	0	0	1	0
2	T	7	0	0	2	0
2	Y	23	0	0	2	0
All	All	9333	0	8562	566	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 32.

The worst 5 of 566 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:94:LYS:HG3	1:K:94:LYS:HG2	1.39	1.04
1:K:4:LEU:HD21	1:K:73:ALA:HA	1.39	1.04
1:D:44:THR:HG21	1:I:131:ASP:OD2	1.59	1.03
1:R:124:MET:HA	1:R:144:MET:HE1	1.42	1.01
1:J:90:ARG:HG2	1:J:90:ARG:HH11	1.24	1.01

There are no symmetry-related clashes.

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	B	143/148 (97%)	131 (92%)	11 (8%)	1 (1%)	26	44
1	D	143/148 (97%)	131 (92%)	9 (6%)	3 (2%)	9	13
1	I	143/148 (97%)	130 (91%)	10 (7%)	3 (2%)	9	13
1	J	142/148 (96%)	125 (88%)	14 (10%)	3 (2%)	9	13
1	K	141/148 (95%)	123 (87%)	12 (8%)	6 (4%)	3	3
1	R	145/148 (98%)	135 (93%)	5 (3%)	5 (3%)	5	5
1	T	143/148 (97%)	128 (90%)	13 (9%)	2 (1%)	14	23
1	Y	143/148 (97%)	129 (90%)	13 (9%)	1 (1%)	26	44
All	All	1143/1184 (96%)	1032 (90%)	87 (8%)	24 (2%)	9	13

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	ASP
1	I	55	VAL
1	T	96	GLY

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Mol	Chain	Res	Type
1	R	55	VAL
1	R	147	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	B	125/126 (99%)	106 (85%)	19 (15%)	3	6
1	D	125/126 (99%)	105 (84%)	20 (16%)	3	5
1	I	125/126 (99%)	105 (84%)	20 (16%)	3	5
1	J	124/126 (98%)	106 (86%)	18 (14%)	4	6
1	K	123/126 (98%)	113 (92%)	10 (8%)	15	26
1	R	126/126 (100%)	112 (89%)	14 (11%)	8	13
1	T	125/126 (99%)	115 (92%)	10 (8%)	15	26
1	Y	125/126 (99%)	107 (86%)	18 (14%)	4	6
All	All	998/1008 (99%)	869 (87%)	129 (13%)	5	9

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	J	90	ARG
1	Y	77	LYS
1	J	7	GLU
1	J	42	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	137	ASN
1	K	97	ASN
1	Y	53	ASN

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Mol	Chain	Res	Type
1	K	42	ASN
1	K	53	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 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.