wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:46 PM BST

PDB ID	:	3J4R
EMDB ID:	:	EMD-5756
Title	:	Pseudo-atomic model of the AKAP18-PKA Complex in a linear conformation derived from electron microscopy
Authors	:	Reichow, S.L.; Gonen, T.
Deposited on	:	2013-09-25
Resolution	:	35.00 Å(reported)
Based on PDB ID	:	2IZX, 2VFL, 2QVS

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

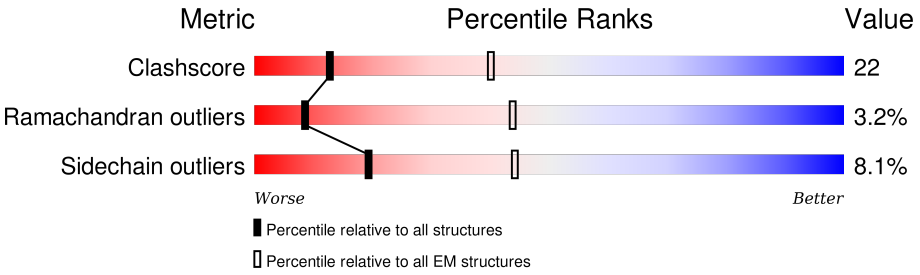
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 35.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	A	353	53% 12% • 35%
2	B	402	55% 34% 6% 5%
2	C	402	56% 33% 6% 5%
3	D	351	57% 29% 5% • 7%
3	E	351	58% 28% 5% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12906 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 A-kinase anchor protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	1	0
			1836	1180	312	336	8		

- Molecule 2 is a protein called cAMP-dependent protein kinase type II-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	382	Total	C	N	O	S	0	0
			3018	1888	514	601	15		
2	C	382	Total	C	N	O	S	0	0
			3018	1888	514	601	15		

- Molecule 3 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

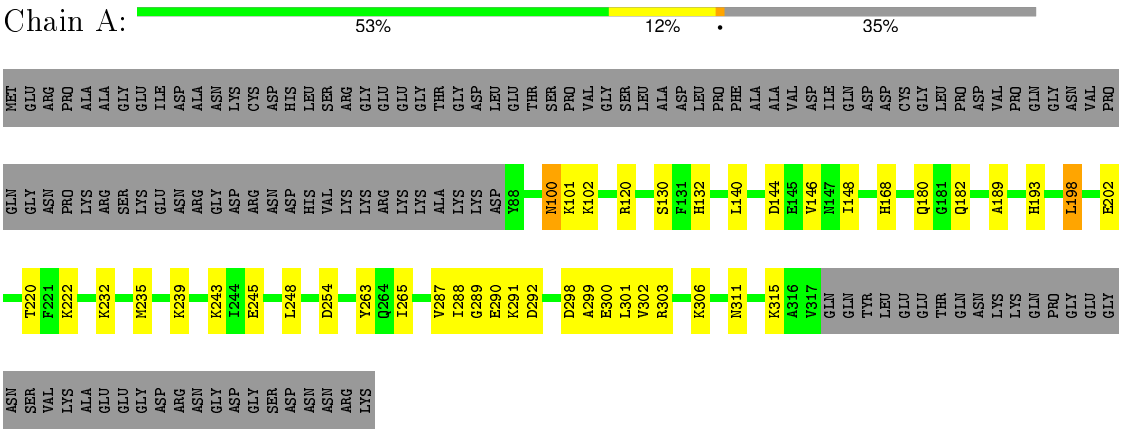
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	325	Total	C	N	O	S	0	0
			2517	1632	430	450	5		
3	E	325	Total	C	N	O	S	0	0
			2517	1632	430	450	5		

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 errors 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.

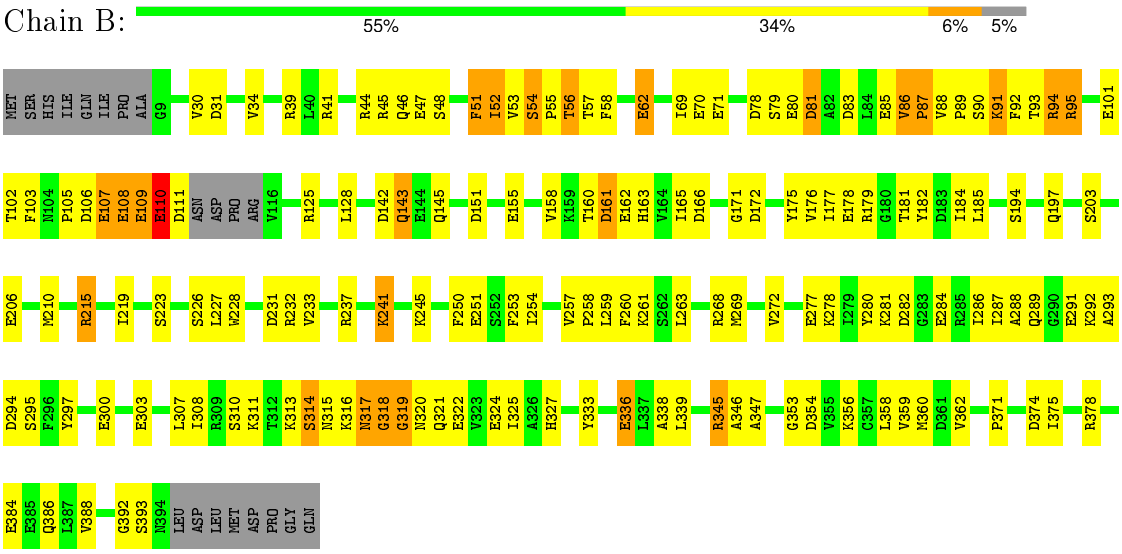
- Molecule 1: A-kinase anchor protein 18

Chain A:



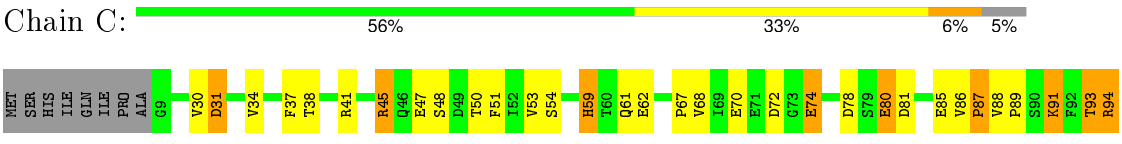
- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit

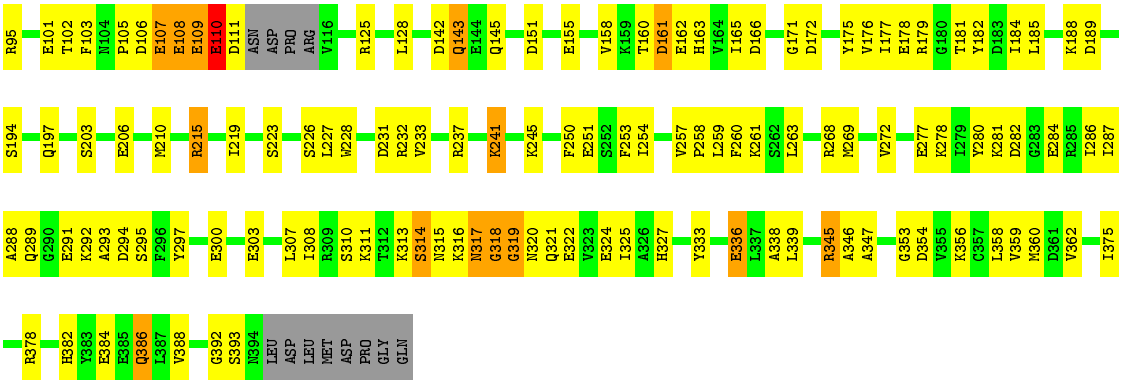
Chain B:



- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit

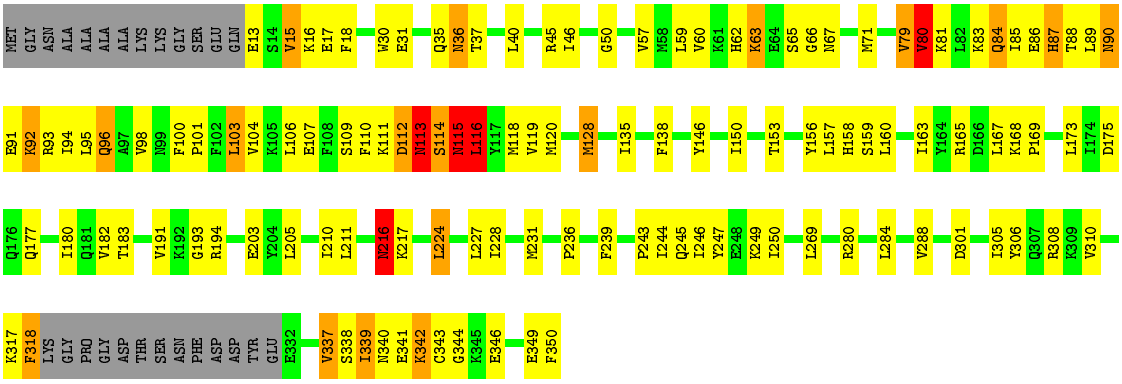
Chain C:





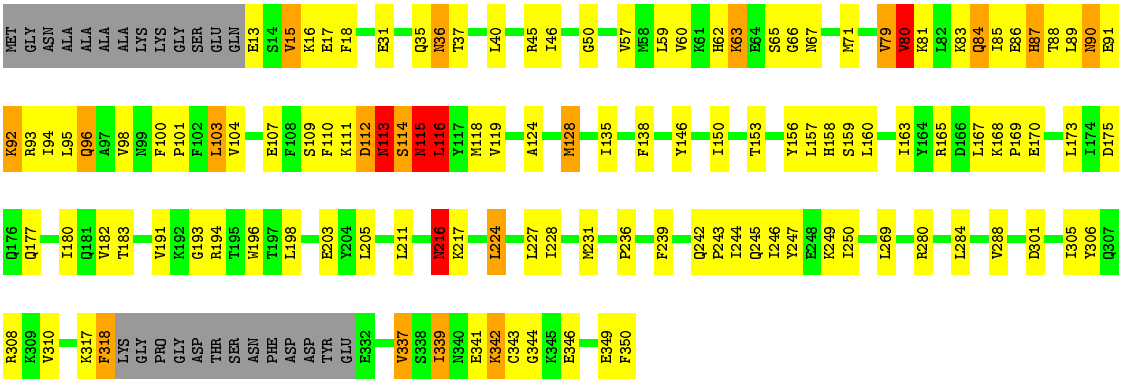
• Molecule 3: cAMP-dependent protein kinase catalytic subunit alpha

Chain D:



• Molecule 3: cAMP-dependent protein kinase catalytic subunit alpha

Chain E:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	1000	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each Micrograph	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	52000	Depositor
Image detector	CCD Gatan	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.50	0/1872	0.58	0/2518
2	B	0.50	0/3065	0.73	8/4135 (0.2%)
2	C	0.52	1/3065 (0.0%)	0.74	7/4135 (0.2%)
3	D	0.38	0/2581	0.80	14/3498 (0.4%)
3	E	0.38	0/2581	0.80	14/3498 (0.4%)
All	All	0.46	1/13164 (0.0%)	0.74	43/17784 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	87	PRO	N-CD	-5.68	1.39	1.47

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	116	LEU	CA-C-O	11.07	143.34	120.10
3	E	116	LEU	CA-C-O	11.06	143.32	120.10
3	E	116	LEU	CA-C-N	-10.74	93.56	117.20
3	D	116	LEU	CA-C-N	-10.74	93.57	117.20
3	E	114	SER	CA-C-N	-9.85	95.53	117.20

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	1836	0	1893	56	0
2	B	3018	0	2929	151	0
2	C	3018	0	2929	143	0
3	D	2517	0	2349	109	0
3	E	2517	0	2349	112	0
All	All	12906	0	12449	551	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 22.

The worst 5 of 551 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:34:VAL:CG2	2:C:41:ARG:HD3	1.55	1.35
2:B:34:VAL:HG21	2:C:41:ARG:CD	1.57	1.34
2:B:86:VAL:HB	2:B:87:PRO:HD3	1.17	1.15
1:A:289:GLY:HA2	1:A:292:ASP:HB2	1.30	1.14
2:B:92:PHE:HA	2:B:93:THR:HB	1.34	1.09

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 PDB entries followed by that with respect to all EM entries.

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	229/353 (65%)	223 (97%)	6 (3%)	0	100	100
2	B	378/402 (94%)	353 (93%)	15 (4%)	10 (3%)	7	45
2	C	378/402 (94%)	353 (93%)	15 (4%)	10 (3%)	7	45
3	D	321/351 (92%)	277 (86%)	28 (9%)	16 (5%)	3	31
3	E	321/351 (92%)	277 (86%)	28 (9%)	16 (5%)	3	31
All	All	1627/1859 (88%)	1483 (91%)	92 (6%)	52 (3%)	8	41

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	109	GLU
2	B	310	SER
2	B	314	SER
2	B	317	ASN
2	B	319	GLY

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 PDB entries followed by that with respect to all EM entries.

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	202/302 (67%)	196 (97%)	6 (3%)	48 77
2	B	330/357 (92%)	296 (90%)	34 (10%)	9 37
2	C	330/357 (92%)	296 (90%)	34 (10%)	9 37
3	D	240/306 (78%)	223 (93%)	17 (7%)	18 55
3	E	240/306 (78%)	223 (93%)	17 (7%)	18 55
All	All	1342/1628 (82%)	1234 (92%)	108 (8%)	19 50

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	74	GLU
2	C	143	GLN
3	E	103	LEU
2	C	80	GLU
2	C	91	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	197	GLN
3	D	62	HIS
3	E	177	GLN
2	C	327	HIS

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Mol	Chain	Res	Type
3	D	35	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.