



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 24, 2017 – 04:20 PM EDT

PDB ID : 4CKG
EMDB ID: : EMD-2546
Title : Helical reconstruction of ACAP1(BAR-PH domain) decorated membrane tubules by cryo-electron microscopy
Authors : Pang, X.Y.; Fan, J.; Zhang, Y.; Zhang, K.; Gao, B.Q.; Ma, J.; Li, J.; Deng, Y.C.; Zhou, Q.J.; Hsu, V.; Sun, F.
Deposited on : unknown
Resolution : 12.00 Å(reported)
Based on PDB ID : 4NSW

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

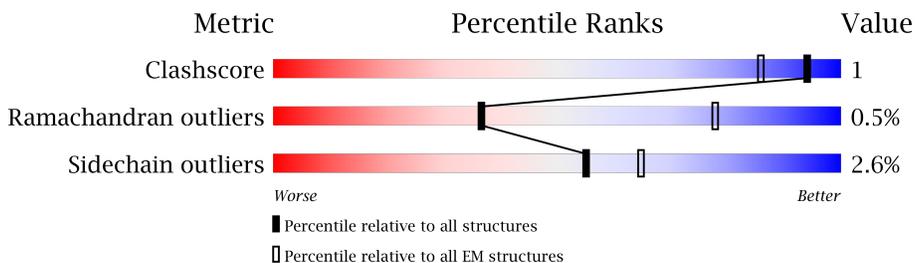
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	382	 70% 22% . .
1	B	382	 73% 18% . 5%
1	C	382	 70% 23% . .
1	D	382	 73% 17% . 5%

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 11682 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 ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	369	2941	1841	539	548	13	0	1
1	B	363	2900	1813	533	541	13	0	1
1	C	369	2941	1841	539	548	13	0	1
1	D	363	2900	1813	533	541	13	0	1

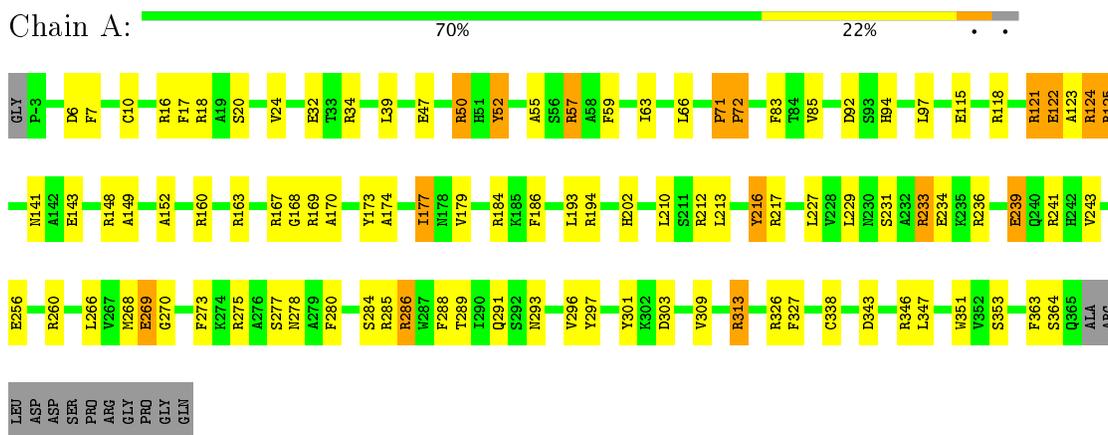
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q15027
A	-3	PRO	-	expression tag	UNP Q15027
A	-2	LEU	-	expression tag	UNP Q15027
A	-1	GLY	-	expression tag	UNP Q15027
A	0	SER	-	expression tag	UNP Q15027
B	-4	GLY	-	expression tag	UNP Q15027
B	-3	PRO	-	expression tag	UNP Q15027
B	-2	LEU	-	expression tag	UNP Q15027
B	-1	GLY	-	expression tag	UNP Q15027
B	0	SER	-	expression tag	UNP Q15027
C	-4	GLY	-	expression tag	UNP Q15027
C	-3	PRO	-	expression tag	UNP Q15027
C	-2	LEU	-	expression tag	UNP Q15027
C	-1	GLY	-	expression tag	UNP Q15027
C	0	SER	-	expression tag	UNP Q15027
D	-4	GLY	-	expression tag	UNP Q15027
D	-3	PRO	-	expression tag	UNP Q15027
D	-2	LEU	-	expression tag	UNP Q15027
D	-1	GLY	-	expression tag	UNP Q15027
D	0	SER	-	expression tag	UNP Q15027

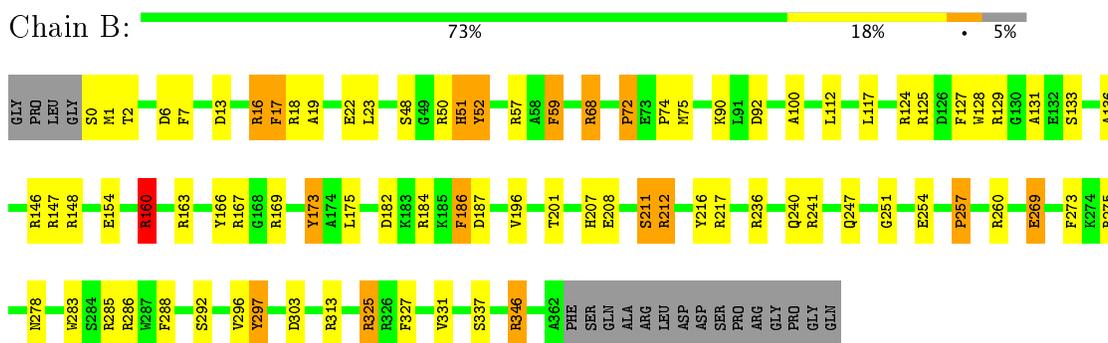
3 Residue-property plots

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

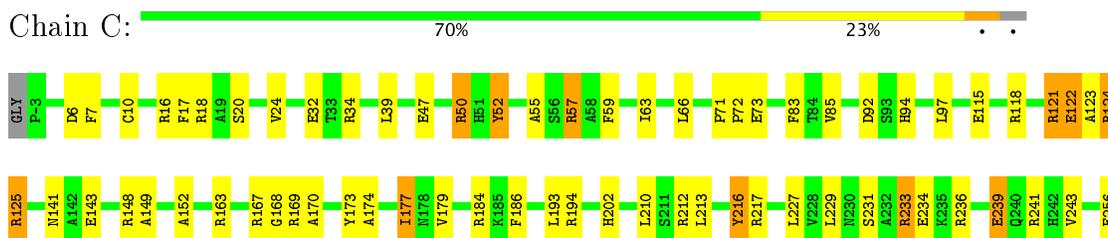
- Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

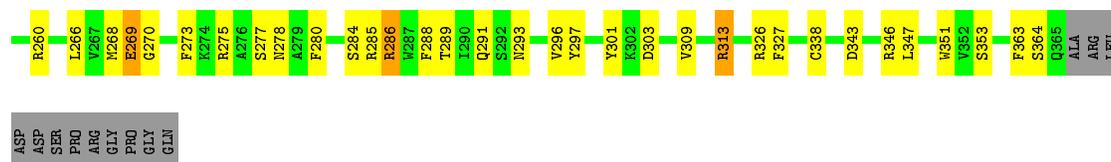


- Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1



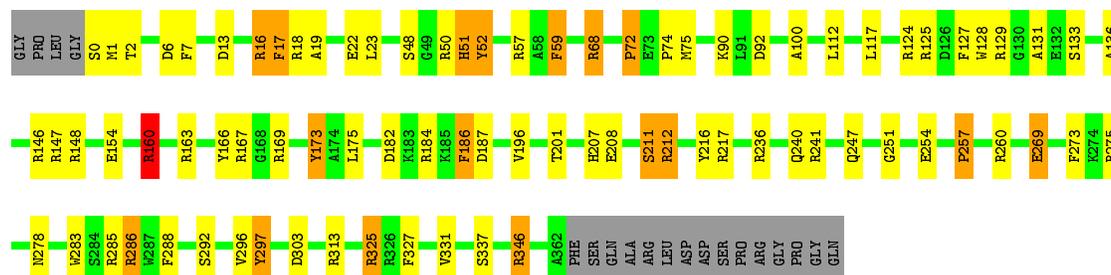
- Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1





- Molecule 1: ARF-GAP WITH COILED-COIL, ANK REPEAT AND PH DOMAIN-CONTAINING PROTEIN 1

Chain D: 73% 17% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	367	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125418	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

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 >2	RMSZ	# Z >2
1	A	1.69	26/2990 (0.9%)	2.00	82/4024 (2.0%)
1	B	1.69	18/2947 (0.6%)	2.00	74/3966 (1.9%)
1	C	1.69	27/2990 (0.9%)	2.00	82/4024 (2.0%)
1	D	1.69	20/2947 (0.7%)	2.00	75/3966 (1.9%)
All	All	1.69	91/11874 (0.8%)	2.00	313/15980 (2.0%)

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	A	0	12
1	B	0	15
1	C	0	12
1	D	0	15
All	All	0	54

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	SER	CA-CB	8.69	1.66	1.52
1	D	337	SER	CA-CB	8.60	1.65	1.52
1	A	280	PHE	CB-CG	-7.74	1.38	1.51
1	C	280	PHE	CB-CG	-7.72	1.38	1.51
1	A	297	TYR	CG-CD1	7.40	1.48	1.39

The worst 5 of 313 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ARG	NE-CZ-NH1	16.76	128.68	120.30
1	C	163	ARG	NE-CZ-NH1	16.62	128.61	120.30
1	D	50	ARG	NE-CZ-NH2	14.46	127.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH2	-14.37	113.12	120.30
1	C	18	ARG	NE-CZ-NH2	-14.32	113.14	120.30

There are no chirality outliers.

5 of 54 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	ARG	Sidechain
1	A	50	ARG	Sidechain
1	A	52	TYR	Sidechain
1	A	57	ARG	Sidechain
1	A	71	PRO	Peptide

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	2941	0	2960	20	0
1	B	2900	0	2922	5	0
1	C	2941	0	2959	19	0
1	D	2900	0	2922	6	0
All	All	11682	0	11763	33	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 1.

The worst 5 of 33 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:A:122:GLU:OE1	1:C:125:ARG:NH2	1.60	1.35
1:A:125:ARG:NH2	1:C:122:GLU:OE1	1.72	1.20
1:A:122:GLU:CD	1:C:125:ARG:NH2	1.91	1.20
1:A:122:GLU:OE1	1:C:122:GLU:OE1	1.60	1.20
1:A:125:ARG:NH2	1:C:122:GLU:CD	1.96	1.17

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	367/382 (96%)	354 (96%)	12 (3%)	1 (0%)	44	81
1	B	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	22	67
1	C	367/382 (96%)	354 (96%)	12 (3%)	1 (0%)	44	81
1	D	361/382 (94%)	347 (96%)	11 (3%)	3 (1%)	22	67
All	All	1456/1528 (95%)	1402 (96%)	46 (3%)	8 (0%)	37	74

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	SER
1	C	364	SER
1	B	278	ASN
1	D	278	ASN
1	B	257	PRO

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 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	315/325 (97%)	308 (98%)	7 (2%)	57	79
1	B	311/325 (96%)	302 (97%)	9 (3%)	48	73
1	C	315/325 (97%)	308 (98%)	7 (2%)	57	79
1	D	311/325 (96%)	302 (97%)	9 (3%)	48	73
All	All	1252/1300 (96%)	1220 (97%)	32 (3%)	55	75

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297	TYR
1	C	66	LEU
1	D	269	GLU
1	C	24	VAL
1	C	177	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	HIS
1	D	207	HIS

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.