



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:50 PM BST

PDB ID : 3J82  
EMDB ID: : EMD-6102  
Title : Electron cryo-microscopy of DNCR-1 in complex with F-actin  
Authors : Hanc, P.; Fujii, T.; Yamada, Y.; Huotari, J.; Schulz, O.; Ahrens, S.; Kjaer, S.;  
Way, M.; Namba, K.; Reis e Sousa, C.  
Deposited on : 2014-09-25  
Resolution : 7.70 Å(reported)

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
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

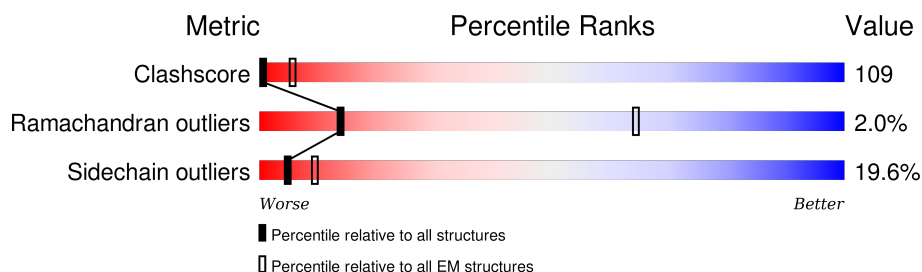
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.70 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  $\geq 3$ , 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	131	
2	B	374	
2	C	374	
2	D	374	

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
2	HIC	C	73	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9884 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 C-type lectin domain family 9 member A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	131	Total	C	N	O	S	0	0
			1050	672	171	197	10		

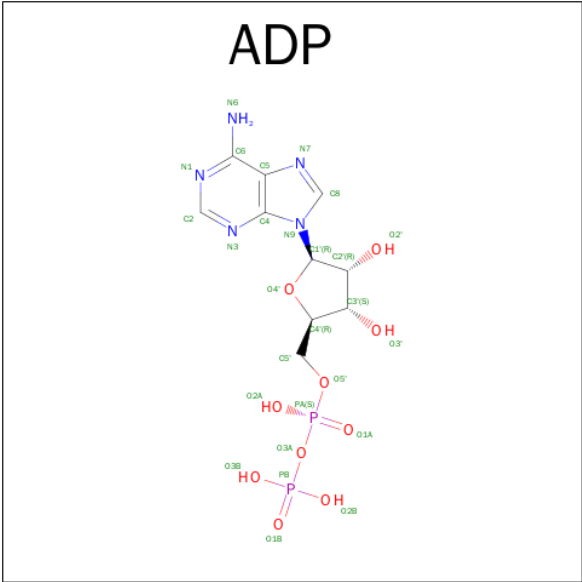
- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	374	Total	C	N	O	S	0	0
			2917	1846	490	559	22		
2	C	374	Total	C	N	O	S	0	0
			2917	1846	490	559	22		
2	D	374	Total	C	N	O	S	0	0
			2918	1846	490	560	22		

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

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

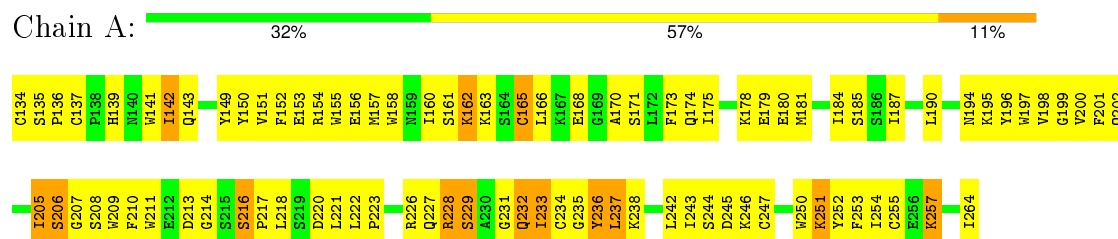


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

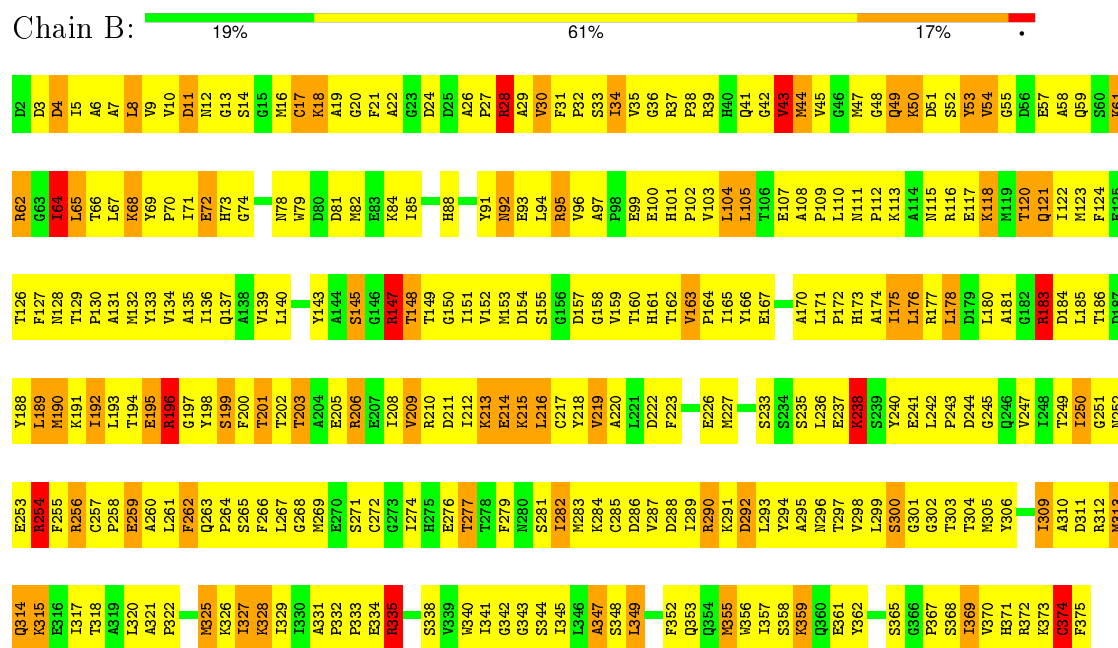
### 3 Residue-property plots

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. 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.

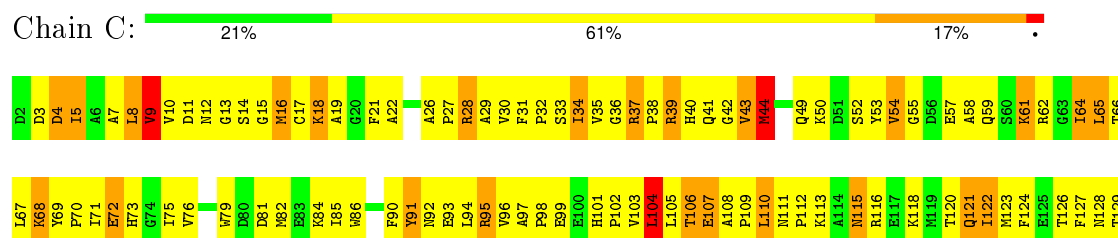
- Molecule 1: C-type lectin domain family 9 member A



- Molecule 2: Actin, cytoplasmic 1



- Molecule 2: Actin, cytoplasmic 1





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	73608	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each Particle	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	60000	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.91	0/1080	1.11	1/1451 (0.1%)
2	B	0.99	0/2967	1.24	11/4017 (0.3%)
2	C	0.99	0/2967	1.23	9/4017 (0.2%)
2	D	0.98	0/2968	1.20	9/4017 (0.2%)
All	All	0.98	0/9982	1.21	30/13502 (0.2%)

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	1
2	B	0	11
2	C	0	6
2	D	0	3
All	All	0	21

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	THR	CA-CB-CG2	-11.90	95.74	112.40
2	C	106	THR	CA-CB-CG2	-8.51	100.49	112.40
2	B	183	ARG	NE-CZ-NH2	-8.40	116.10	120.30
2	D	375	PHE	CB-CG-CD2	-8.10	115.13	120.80
2	B	28	ARG	NE-CZ-NH1	7.84	124.22	120.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	236	TYR	Peptide
2	B	147	ARG	Sidechain
2	B	61	LYS	Peptide
2	B	62	ARG	Sidechain
2	B	64	ILE	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	1050	0	1002	227	0
2	B	2917	0	2880	682	0
2	C	2917	0	2880	606	0
2	D	2918	0	2880	684	0
3	A	1	0	0	0	0
4	B	27	0	12	7	0
4	C	27	0	12	7	0
4	D	27	0	12	8	0
All	All	9884	0	9678	2141	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 109.

The worst 5 of 2141 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:C:73:HIC:HD2	2:C:183:ARG:NH1	1.50	1.26
2:D:300:SER:HA	2:D:335:ARG:HD3	1.25	1.18
2:B:61:LYS:HD2	2:B:64:ILE:HG21	1.26	1.17
2:D:178:LEU:HD12	2:D:180:LEU:H	1.12	1.14
2:C:189:LEU:HD12	2:C:209:VAL:HG22	1.28	1.14

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 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	129/131 (98%)	117 (91%)	7 (5%)	5 (4%)	4	36
2	B	371/374 (99%)	347 (94%)	16 (4%)	8 (2%)	8	49
2	C	371/374 (99%)	343 (92%)	22 (6%)	6 (2%)	12	56
2	D	371/374 (99%)	342 (92%)	23 (6%)	6 (2%)	12	56
All	All	1242/1253 (99%)	1149 (92%)	68 (6%)	25 (2%)	14	51

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	43	VAL
2	B	72	GLU
2	B	244	ASP
2	B	374	CYS
2	C	43	VAL

### 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	115/115 (100%)	105 (91%)	10 (9%)	13	45
2	B	316/316 (100%)	244 (77%)	72 (23%)	1	8
2	C	316/316 (100%)	248 (78%)	68 (22%)	1	9
2	D	316/316 (100%)	258 (82%)	58 (18%)	2	14
All	All	1063/1063 (100%)	855 (80%)	208 (20%)	5	12

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	95	ARG
2	C	190	MET
2	D	282	ILE
2	C	107	GLU
2	C	148	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	115	ASN
2	C	314	GLN
2	D	252	ASN
2	C	121	GLN
2	C	353	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
2	HIC	B	73	2	6,11,12	1.28	1 (16%)	6,14,16	0.86	0
2	HIC	C	73	2	6,11,12	1.26	1 (16%)	6,14,16	0.86	1 (16%)
2	HIC	D	73	2	6,11,12	1.27	1 (16%)	6,14,16	0.94	1 (16%)

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
2	HIC	B	73	2	-	0/4/6/8	0/1/1/1
2	HIC	C	73	2	-	0/4/6/8	0/1/1/1
2	HIC	D	73	2	-	0/4/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	HIC	CD2-NE2	-2.84	1.34	1.38
2	D	73	HIC	CD2-NE2	-2.81	1.34	1.38
2	C	73	HIC	CD2-NE2	-2.78	1.34	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	73	HIC	O-C-CA	-2.21	119.78	125.72
2	C	73	HIC	O-C-CA	-2.00	120.36	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	73	HIC	3	0
2	C	73	HIC	7	0
2	D	73	HIC	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	ADP	B	401	-	24,29,29	0.99	1 (4%)	23,45,45	1.76	1 (4%)
4	ADP	C	401	-	24,29,29	0.99	1 (4%)	23,45,45	1.77	2 (8%)
4	ADP	D	401	-	24,29,29	1.00	1 (4%)	23,45,45	1.76	1 (4%)

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	ADP	B	401	-	-	0/12/32/32	0/3/3/3
4	ADP	C	401	-	-	0/12/32/32	0/3/3/3
4	ADP	D	401	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	ADP	C5-C4	3.12	1.47	1.40
4	B	401	ADP	C5-C4	3.12	1.47	1.40
4	C	401	ADP	C5-C4	3.12	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	ADP	N3-C2-N1	-6.61	123.68	128.87
4	D	401	ADP	N3-C2-N1	-6.53	123.74	128.87
4	B	401	ADP	N3-C2-N1	-6.52	123.75	128.87
4	C	401	ADP	C4'-O4'-C1'	2.01	111.77	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	ADP	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	ADP	7	0
4	D	401	ADP	8	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.