



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3B63
EMDB ID: : EMD-1088
Title : Actin filament model in the extended form of acromosomal bundle in the Limulus sperm
Authors : Cong, Y.; Topf, M.; Sali, A.; Matsudaira, P.; Dougherty, M.; Chiu, W.; Schmid, M.F.
Deposited on : 2007-10-26
Resolution : 9.50 Å (reported)
Based on PDB ID : 1T44,1HLU,1ATN,1YAG,1YVN,1MDU,1HIV,1NWK,1ESV

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

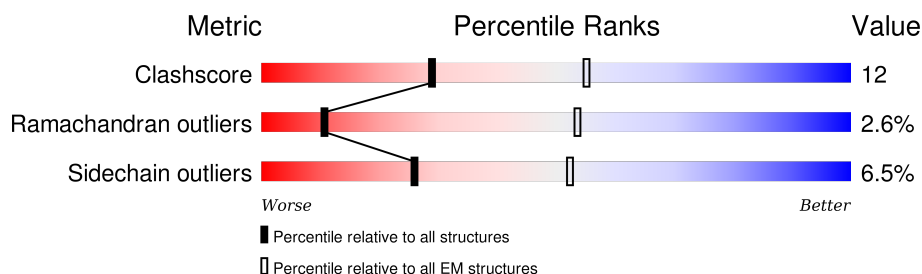
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	365	
1	G	365	
2	B	364	
3	C	365	
3	I	365	
4	D	357	
5	E	365	
5	H	365	
5	J	365	

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Mol	Chain	Length	Quality of chain
5	K	365	<div><div></div><div>63%</div><div>33%</div><div></div><div>• •</div></div>
5	N	365	<div><div></div><div>58%</div><div>36%</div><div>5%</div><div>•</div></div>
6	F	357	<div><div></div><div>57%</div><div>37%</div><div>5%</div><div>•</div></div>
7	L	365	<div><div></div><div>60%</div><div>35%</div><div></div><div>• •</div></div>
7	M	365	<div><div></div><div>64%</div><div>32%</div><div></div><div>•</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39685 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 Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	365	Total	C	N	O	S	0	0
			2843	1800	480	545	18		
1	G	365	Total	C	N	O	S	0	0
			2843	1800	480	545	18		

- Molecule 2 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	364	Total	C	N	O	S	0	0
			2835	1796	474	545	20		

- Molecule 3 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	365	Total	C	N	O	S	0	0
			2842	1801	479	544	18		
3	I	365	Total	C	N	O	S	0	0
			2842	1801	479	544	18		

- Molecule 4 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	357	Total	C	N	O	S	0	0
			2791	1768	467	536	20		

- Molecule 5 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	H	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	K	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	N	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		

- Molecule 6 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	357	Total	C	N	O	S	0	0
			2788	1767	467	534	20		

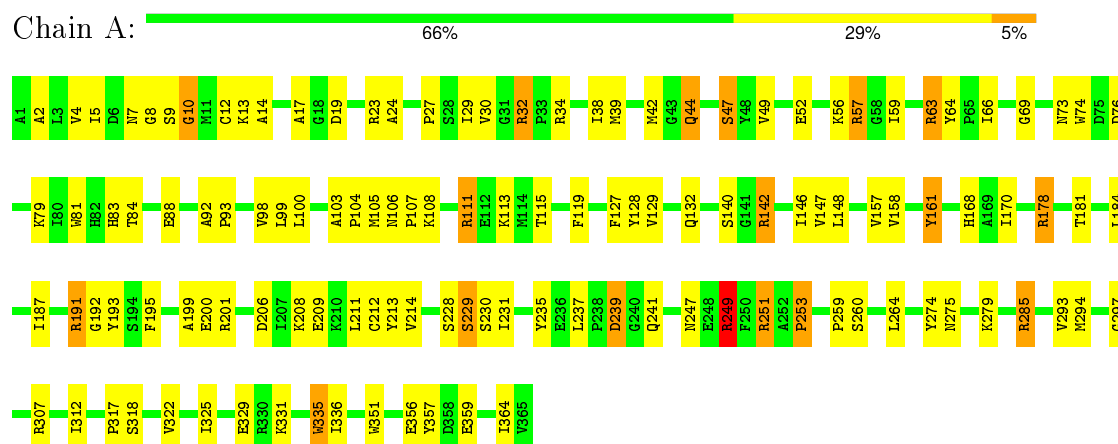
- Molecule 7 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	365	Total	C	N	O	S	0	0
			2838	1797	475	545	21		
7	M	365	Total	C	N	O	S	0	0
			2838	1797	475	545	21		

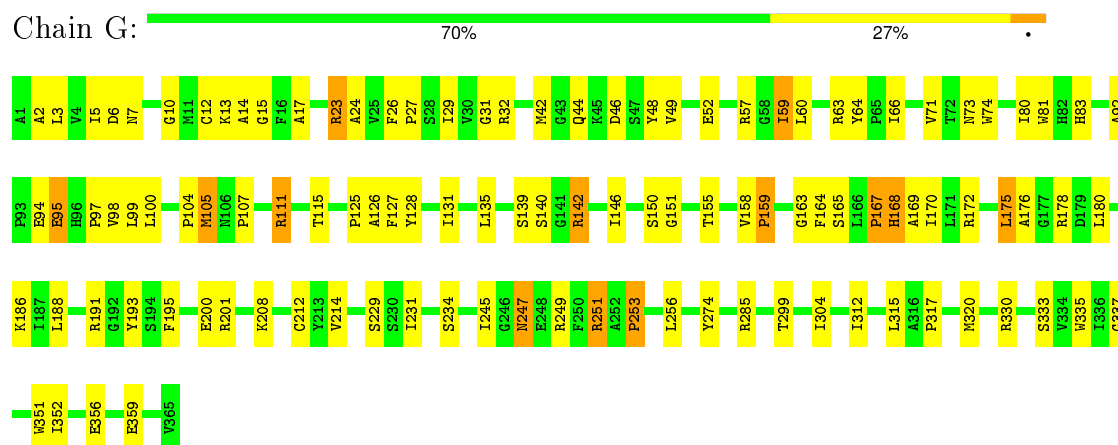
3 Residue-property plots

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.

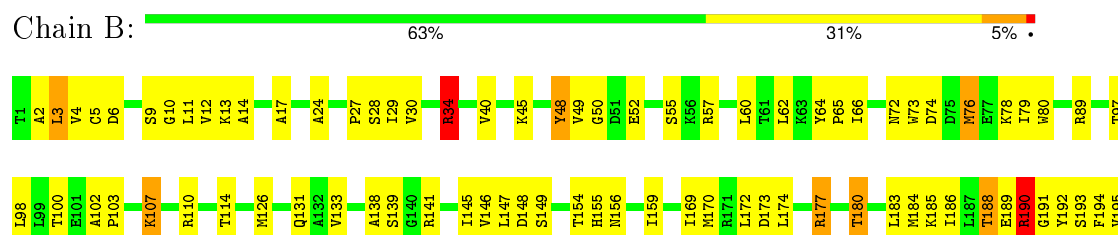
• Molecule 1: Actin

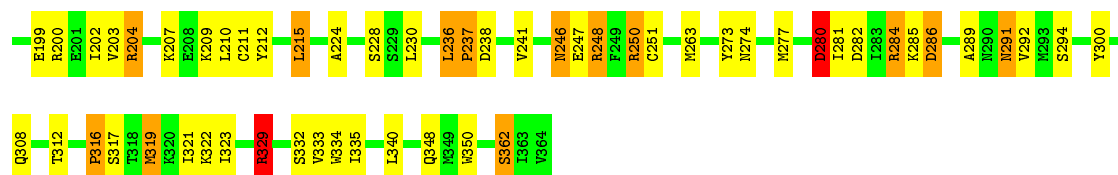


• Molecule 1: Actin



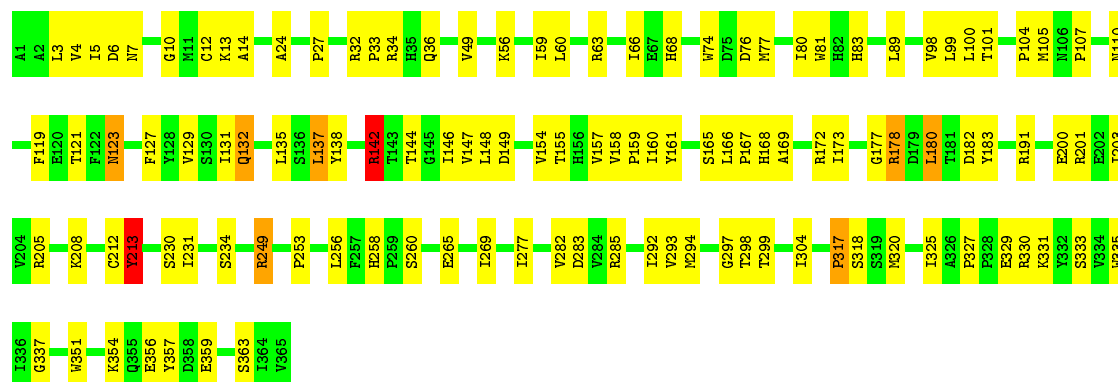
• Molecule 2: Actin





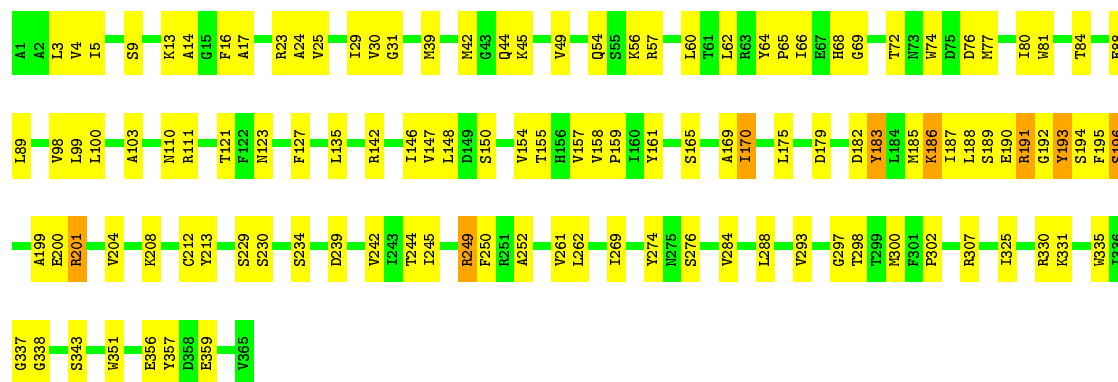
• Molecule 3: Actin

Chain C: 68% 30%



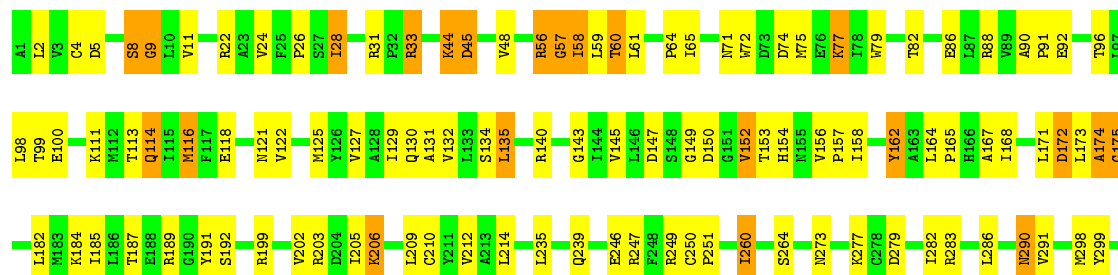
• Molecule 3: Actin

Chain I: 67% 30%



• Molecule 4: Actin

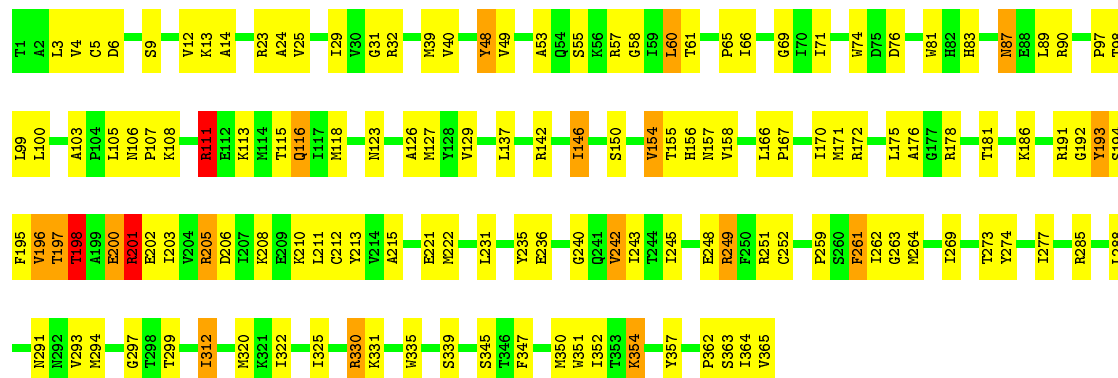
Chain D: 63% 31% 6%





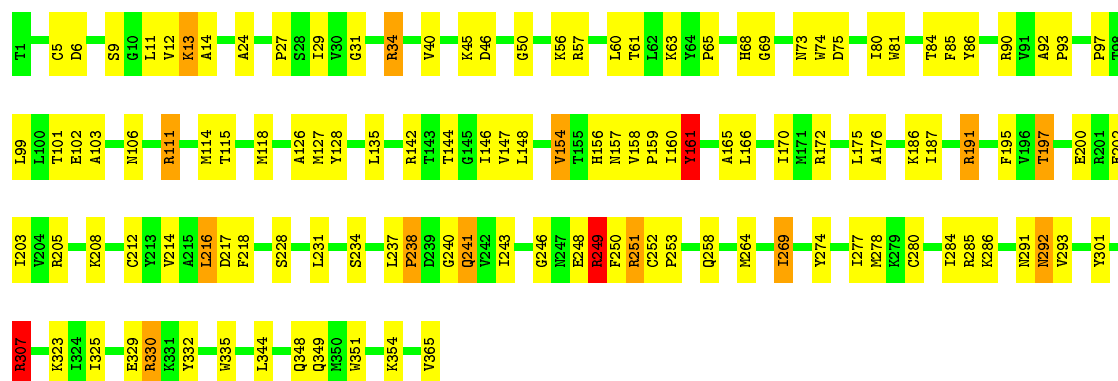
• Molecule 5: Actin

Chain E: 62% 33% 5% •



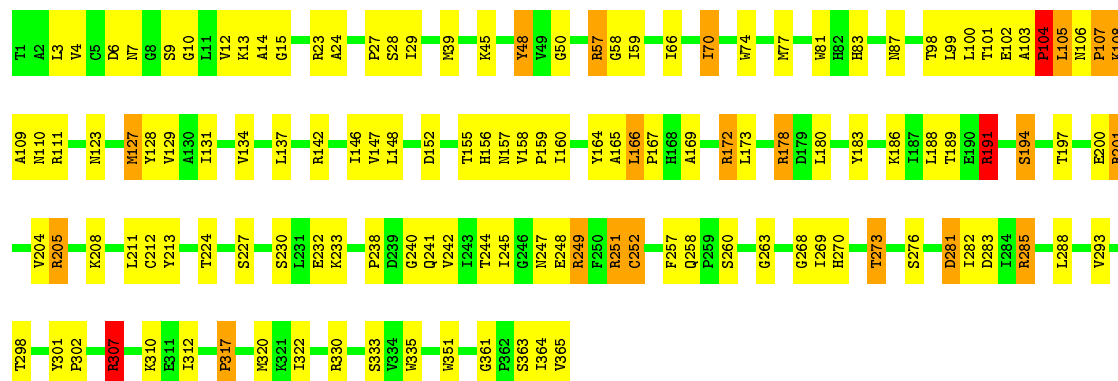
• Molecule 5: Actin

Chain H: 66% 30% • •



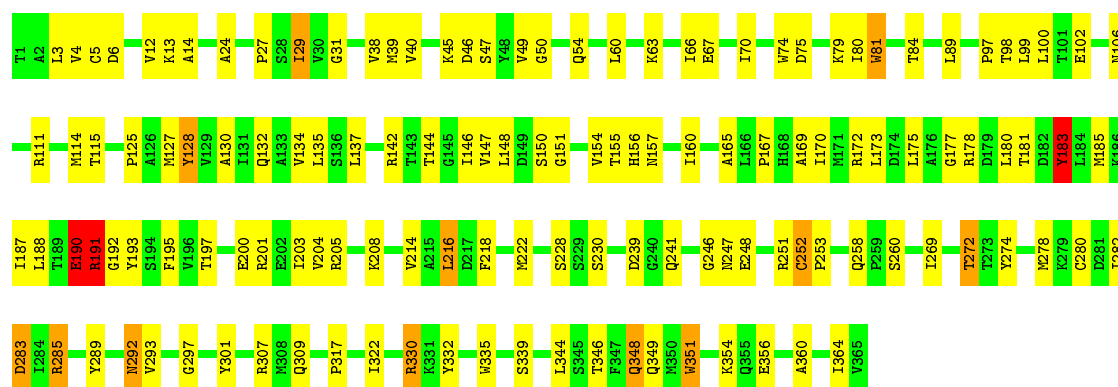
• Molecule 5: Actin

Chain J: 64% 30% 5% •



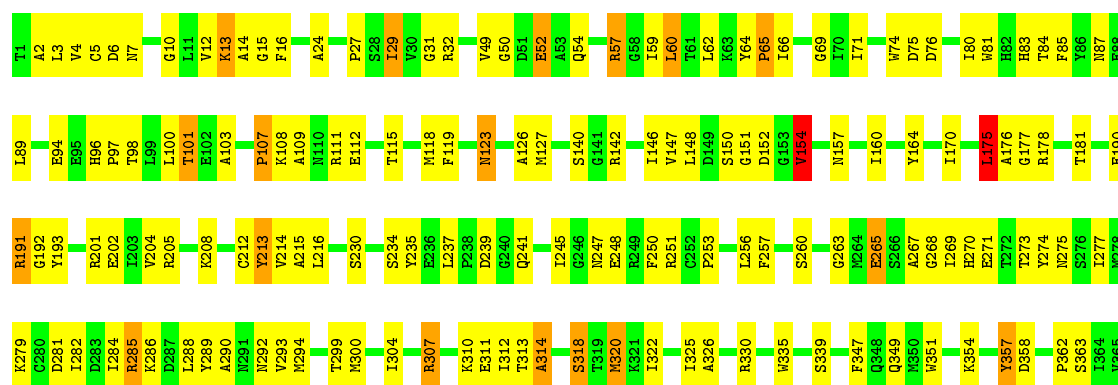
• Molecule 5: Actin

Chain K:  63% 33% ..



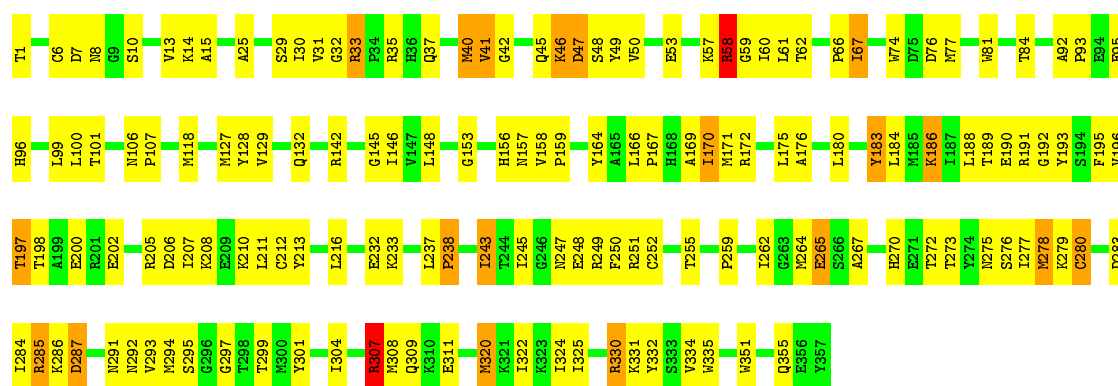
• Molecule 5: Actin

Chain N:  58% 36% 5% ..



• Molecule 6: Actin

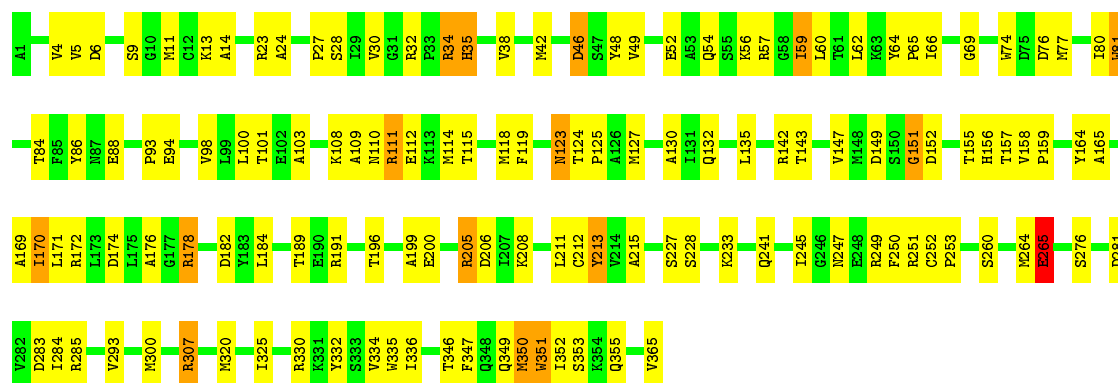
Chain F:  57% 37% 5% ..



• Molecule 7: Actin

Chain L:  60% 35% ..





4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 4000EX	Depositor
Voltage (kV)	400	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO163 FILM	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	0.64	0/2904	1.31	30/3931 (0.8%)
1	G	0.64	0/2904	1.25	25/3931 (0.6%)
2	B	0.64	0/2895	1.37	29/3923 (0.7%)
3	C	0.64	0/2903	1.29	26/3930 (0.7%)
3	I	0.64	0/2903	1.28	26/3930 (0.7%)
4	D	0.64	0/2850	1.29	18/3860 (0.5%)
5	E	0.64	0/2906	1.31	27/3938 (0.7%)
5	H	0.63	0/2906	1.32	26/3938 (0.7%)
5	J	0.65	0/2906	1.35	32/3938 (0.8%)
5	K	0.64	0/2906	1.34	29/3938 (0.7%)
5	N	0.65	0/2906	1.29	24/3938 (0.6%)
6	F	0.63	0/2847	1.32	19/3857 (0.5%)
7	L	0.64	0/2899	1.34	22/3927 (0.6%)
7	M	0.64	0/2899	1.28	18/3927 (0.5%)
All	All	0.64	0/40534	1.31	351/54906 (0.6%)

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	G	0	7
2	B	0	9
3	C	0	6
3	I	0	9
4	D	0	5
5	E	0	8
5	H	0	7
5	J	0	6
5	K	0	9
5	N	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	7
7	L	0	5
7	M	0	6
All	All	0	104

There are no bond length outliers.

The worst 5 of 351 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	204	ARG	NE-CZ-NH2	-13.13	113.74	120.30
2	B	204	ARG	NE-CZ-NH1	10.70	125.65	120.30
6	F	58	ARG	NE-CZ-NH2	-10.32	115.14	120.30
5	N	32	ARG	NE-CZ-NH2	-10.25	115.18	120.30
5	K	191	ARG	NE-CZ-NH1	10.18	125.39	120.30

There are no chirality outliers.

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	142	ARG	Sidechain
1	A	161	TYR	Sidechain
1	A	57	ARG	Sidechain
1	A	64	TYR	Sidechain

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	2843	0	2818	55	0
1	G	2843	0	2818	57	0
2	B	2835	0	2813	80	0
3	C	2842	0	2821	69	0
3	I	2842	0	2821	81	0
4	D	2791	0	2766	75	0
5	E	2845	0	2820	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	2845	0	2820	66	0
5	J	2845	0	2820	80	0
5	K	2845	0	2820	69	0
5	N	2845	0	2820	85	0
6	F	2788	0	2770	108	0
7	L	2838	0	2812	78	0
7	M	2838	0	2812	66	0
All	All	39685	0	39351	972	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 12.

The worst 5 of 972 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)
5:E:198:THR:HA	6:F:265:GLU:HG3	1.51	0.91
5:E:248:GLU:HA	5:E:251:ARG:HB3	1.54	0.88
7:L:159:PRO:HG3	7:L:169:ALA:HB3	1.56	0.86
1:G:317:PRO:HG2	1:G:320:MET:HB2	1.58	0.85
7:L:259:PRO:HG2	7:L:266:SER:HB2	1.58	0.84

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	363/365 (100%)	319 (88%)	36 (10%)	8 (2%)	8 49
1	G	363/365 (100%)	333 (92%)	25 (7%)	5 (1%)	14 58
2	B	362/364 (100%)	317 (88%)	33 (9%)	12 (3%)	5 40
3	C	363/365 (100%)	328 (90%)	33 (9%)	2 (1%)	30 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	363/365 (100%)	328 (90%)	30 (8%)	5 (1%)	14	58
4	D	355/357 (99%)	307 (86%)	36 (10%)	12 (3%)	5	40
5	E	363/365 (100%)	314 (86%)	36 (10%)	13 (4%)	4	38
5	H	363/365 (100%)	319 (88%)	36 (10%)	8 (2%)	8	49
5	J	363/365 (100%)	309 (85%)	44 (12%)	10 (3%)	6	44
5	K	363/365 (100%)	315 (87%)	38 (10%)	10 (3%)	6	44
5	N	363/365 (100%)	322 (89%)	32 (9%)	9 (2%)	7	46
6	F	355/357 (99%)	295 (83%)	47 (13%)	13 (4%)	4	38
7	L	363/365 (100%)	305 (84%)	48 (13%)	10 (3%)	6	44
7	M	363/365 (100%)	307 (85%)	42 (12%)	14 (4%)	4	36
All	All	5065/5093 (100%)	4418 (87%)	516 (10%)	131 (3%)	11	45

5 of 131 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	VAL
2	B	280	ASP
2	B	329	ARG
2	B	362	SER
3	C	265	GLU

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	310/310 (100%)	291 (94%)	19 (6%)	23	60
1	G	310/310 (100%)	293 (94%)	17 (6%)	27	63
2	B	307/307 (100%)	284 (92%)	23 (8%)	17	53
3	C	310/310 (100%)	297 (96%)	13 (4%)	36	70
3	I	310/310 (100%)	305 (98%)	5 (2%)	70	88
4	D	302/302 (100%)	283 (94%)	19 (6%)	22	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	308/308 (100%)	290 (94%)	18 (6%)	25	61
5	H	308/308 (100%)	287 (93%)	21 (7%)	20	57
5	J	308/308 (100%)	283 (92%)	25 (8%)	15	50
5	K	308/308 (100%)	286 (93%)	22 (7%)	18	55
5	N	308/308 (100%)	284 (92%)	24 (8%)	16	51
6	F	302/302 (100%)	282 (93%)	20 (7%)	21	57
7	L	308/308 (100%)	280 (91%)	28 (9%)	12	43
7	M	308/308 (100%)	284 (92%)	24 (8%)	16	51
All	All	4307/4307 (100%)	4029 (94%)	278 (6%)	26	58

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	234	SER
5	J	29	ILE
5	N	49	VAL
5	H	9	SER
5	H	278	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	309	GLN
1	G	275	ASN
5	N	87	ASN
1	G	7	ASN
1	G	73	ASN

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 [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.