wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:22 PM BST

PDB ID	:	5ADX
EMDB ID:	:	EMD-2856
Title	:	CryoEM structure of dynactin complex at 4.0 angstrom resolution
Authors	:	Zhang, K.; Urnavicius, L.; Diamant, A.G.; Motz, C.; Schlage, M.A.; Yu, M.; Patel, N.A.; Robinson, C.V.; Carter, A.P.
Deposited on	:	2015-08-24
Resolution	:	4.00 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
A user guide is available at
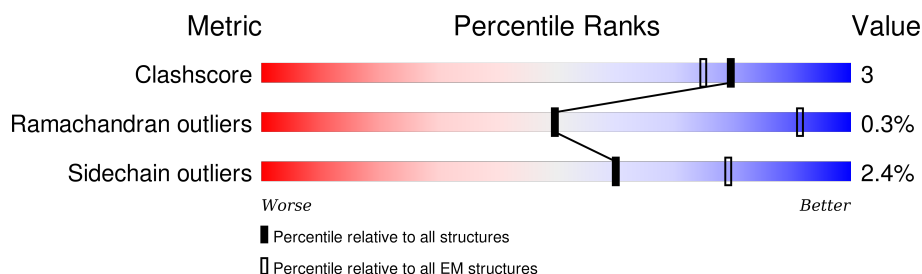http://wwpdb.org/validation/2016/EMValidationReportHelp

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 4.00 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		2.4%

Worse .... *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures
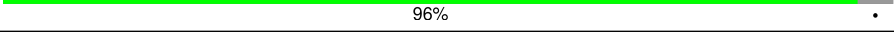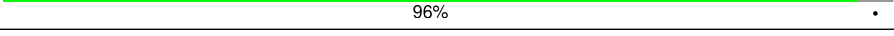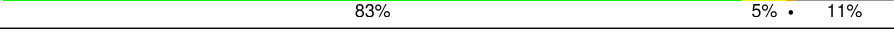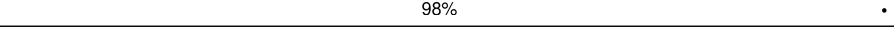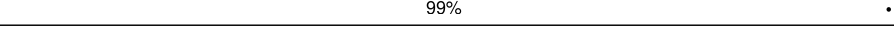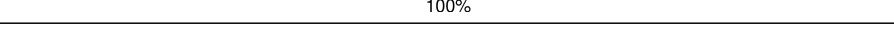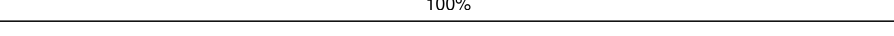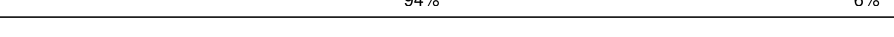
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	370	96%
1	B	370	98%
1	C	370	96%
1	D	370	97%
1	E	370	98%
1	F	370	98%
1	G	370	95% 5%
1	I	370	94% 6%
2	H	370	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	417	85% · 12%
4	K	275	78% 21% ·
5	L	270	82% 17% ·
6	M	824	67% · 31%
7	N	818	71% · 26%
8	O	88	67% 7% 26%
8	P	88	64% 10% 26%
9	Q	91	96% ·
9	R	91	96% ·
10	U	190	83% 5% · 11%
11	V	165	98%
12	Y	243	99% ·
13	Z	419	100%
13	z	419	100%
14	a	48	85% 13% ·
15	b	71	83% 17%
16	c	31	94% 6%
17	d	20	90% 5% 5%

2   Entry composition ⓘ

There are 17 unique types of molecules in this entry. The entry contains 49392 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 RELATED PROTEIN 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
1	B	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
1	C	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
1	D	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
1	E	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
1	F	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
1	G	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		
1	I	370	Total	C	N	O	S	0	0
			2957	1893	509	545	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	GLU	ASP	CONFLICT	UNP F2Z5G5
B	97	GLU	ASP	CONFLICT	UNP F2Z5G5
C	97	GLU	ASP	CONFLICT	UNP F2Z5G5
D	97	GLU	ASP	CONFLICT	UNP F2Z5G5
E	97	GLU	ASP	CONFLICT	UNP F2Z5G5
F	97	GLU	ASP	CONFLICT	UNP F2Z5G5
G	97	GLU	ASP	CONFLICT	UNP F2Z5G5
I	97	GLU	ASP	CONFLICT	UNP F2Z5G5

- Molecule 2 is a protein called ACTIN, CYTOPLASMIC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	370	Total	C	N	O	S	0	0
			2885	1827	486	550	22		

- Molecule 3 is a protein called ACTIN RELATED PROTEIN 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	369	Total 2879	C 1857	N 486	O 520	S 16	0	0

- Molecule 4 is a protein called CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	275	Total 2242	C 1415	N 393	O 429	S 5	0	0

- Molecule 5 is a protein called F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	270	Total 2137	C 1333	N 373	O 420	S 11	0	0

- Molecule 6 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	571	Total 2855	C 1713	N 571	O 571	0	0

- Molecule 7 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	602	Total 3010	C 1806	N 602	O 602	0	0

- Molecule 8 is a protein called DYNACTIN SUBUNIT 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	65	Total 323	C 193	N 65	O 65	0	0
8	P	65	Total 323	C 193	N 65	O 65	0	0

- Molecule 9 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	87	Total 435	C 261	N 87	O 87	0	0
9	R	87	Total 435	C 261	N 87	O 87	0	0

- Molecule 10 is a protein called DYNACTIN 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	169	Total 831	C 493	N 169	O 169	0	0

- Molecule 11 is a protein called DYNACTIN SUBUNIT 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	V	165	Total 812	C 482	N 165	O 165	0	0

- Molecule 12 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	243	Total 1215	C 729	N 243	O 243	0	0

- Molecule 13 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Z	419	Total 2095	C 1257	N 419	O 419	0	0
13	z	419	Total 2095	C 1257	N 419	O 419	0	0

- Molecule 14 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	48	Total 341	C 216	N 58	O 66	S 1	0	0

- Molecule 15 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	71	Total 517	C 324	N 93	O 99	S 1	0	0

• Molecule 16 is a protein called DYNACTIN SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	c	31	Total	C	N	O	S	0	0
			179	112	34	32	1		

• Molecule 17 is a protein called DYNACTIN SUBUNIT 2.

| Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	20	Total	C	N	O	S	0	0
			127	80	23	23	1		

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 RELATED PROTEIN 1
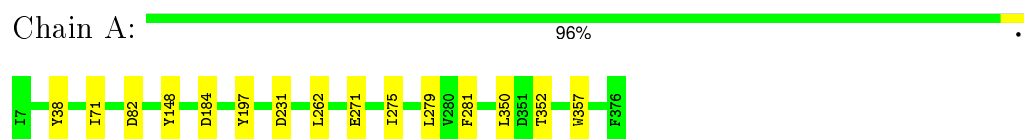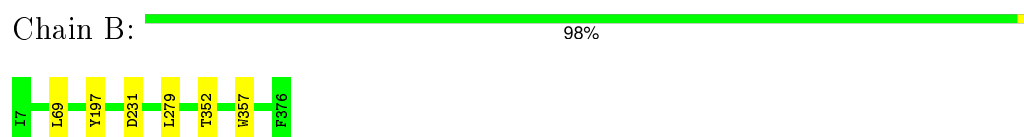
Chain A:

- Molecule 1: ACTIN RELATED PROTEIN 1

Chain B:

- Molecule 1: ACTIN RELATED PROTEIN 1

Chain C:

- Molecule 1: ACTIN RELATED PROTEIN 1
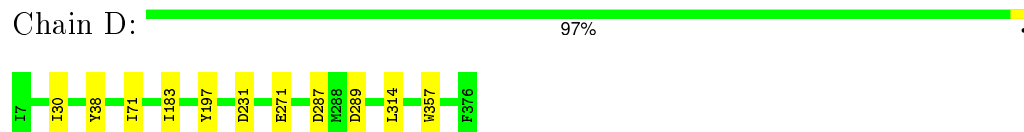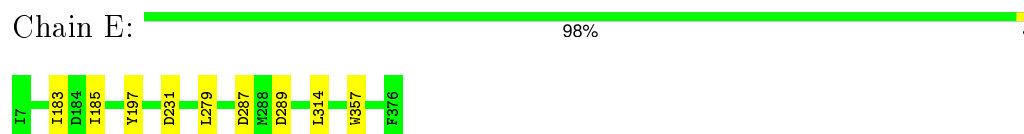
Chain D:

- Molecule 1: ACTIN RELATED PROTEIN 1

Chain E:

- Molecule 1: ACTIN RELATED PROTEIN 1

Chain F:

- Molecule 1: ACTIN RELATED PROTEIN 1

Chain G:

95% 5%

I7 R121 R182 I183 D184 I185 Y197 D231 L261 L262 E271 S272 E273 G274 I275 V278 D287 L315 I330 W357 I371 T375 F376

- Molecule 1: ACTIN RELATED PROTEIN 1

Chain I:

94% 6%
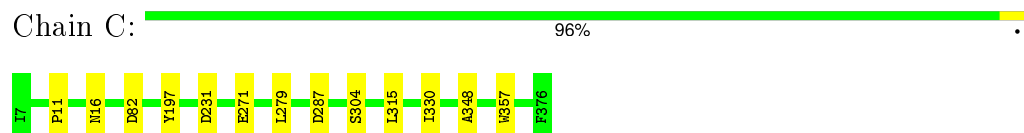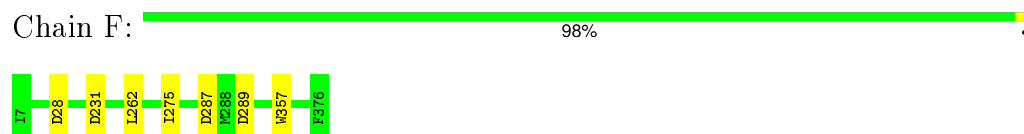
I7 R41 P42 K43 H44 V45 R46 V47 M48 E53 G54 D55 I56 F57 I58 R72 I183 D184 I185 D189 V190 D231 L261 I268 L279 D287 W357 F376
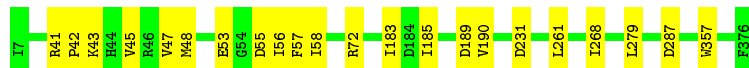
- Molecule 2: ACTIN, CYTOPLASMIC 1

Chain H:

99%

A6 V43 Q49 P70 I85 F375

- Molecule 3: ACTIN RELATED PROTEIN 11

Chain J:

85% 12%

MET PRO LEU TYR GLU GLY LEU GLY SER GLY GLY E12 E93 L128 I133 A136 P156 G188 ALA ALA LYS GLU Q193 F231 N232 ILE ASP GLY ASN THR GLU R239 D274 N275 E276 E277 E328 L364 Q365 W387 L390 ASN ASN PRO PRO LEU GLU MET

VAL PHE ASP VAL GLY LYS SER GLN PRO PRO LEU MET LYS ARG ALA PHE SER THR GLU LYS
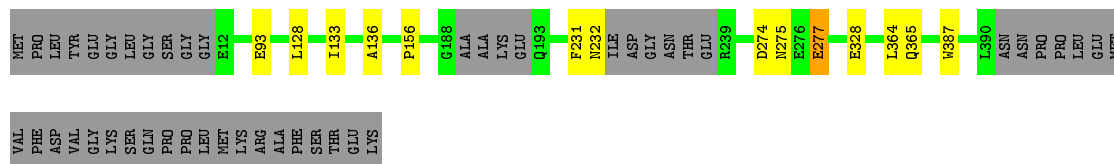
- Molecule 4: CAPPING PROTEIN (ACTIN FILAMENT) MUSCLE Z-LINE, ALPHA 1

Chain K:

78% 21%

R7 P26 G27 E28 V32 V36 R37 L38 L39 L40 L46 P64 I67 Y70 Q73 V74 L75 H79 K93 V113 D114 L117 K118 R121 E122 S123 C124 L128 R129 A130 Y131 Y136 C141 T142 A145 T153 I154 I155 Q162 N167

F168 W169 N170 G171 R172 W177 T180 I181 L192 H197 Y198 Y199 E200 H209 T224 I229 N237 I243 T249 D252 K256 A257 L258 R259 R266 I269 K278 K281
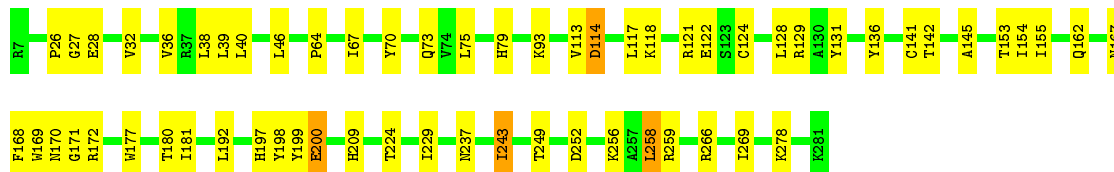
- Molecule 5: F-ACTIN CAPPING PROTEIN BETA SUBUNIT VARIANT II

Chain L:

82% 17%
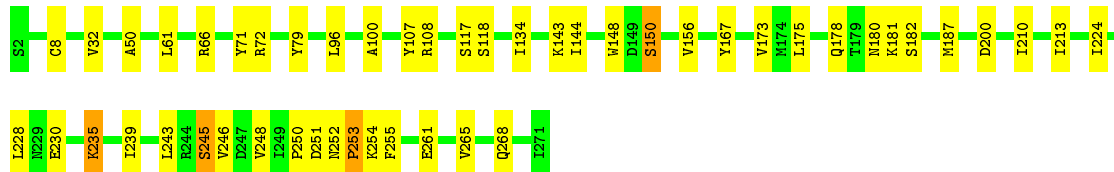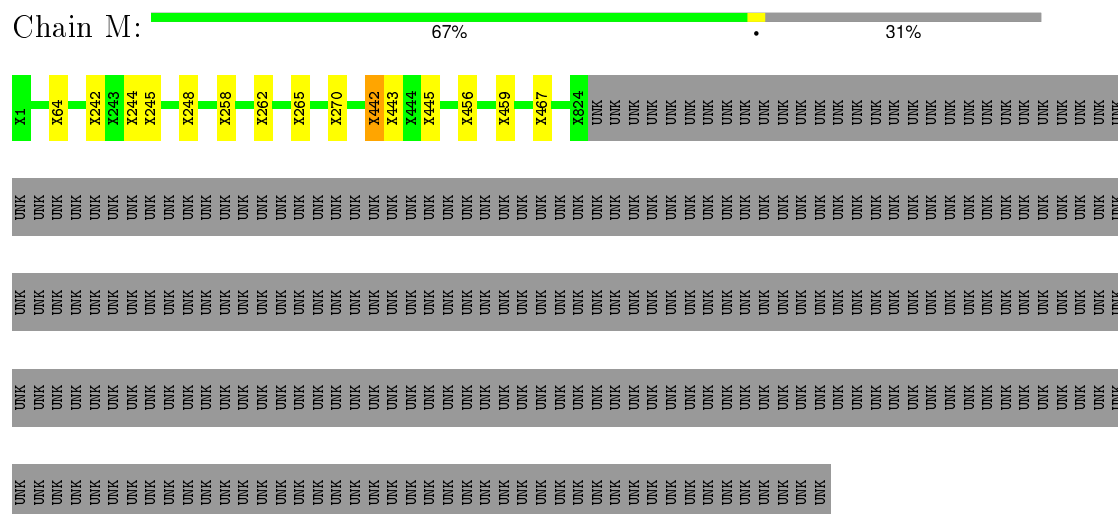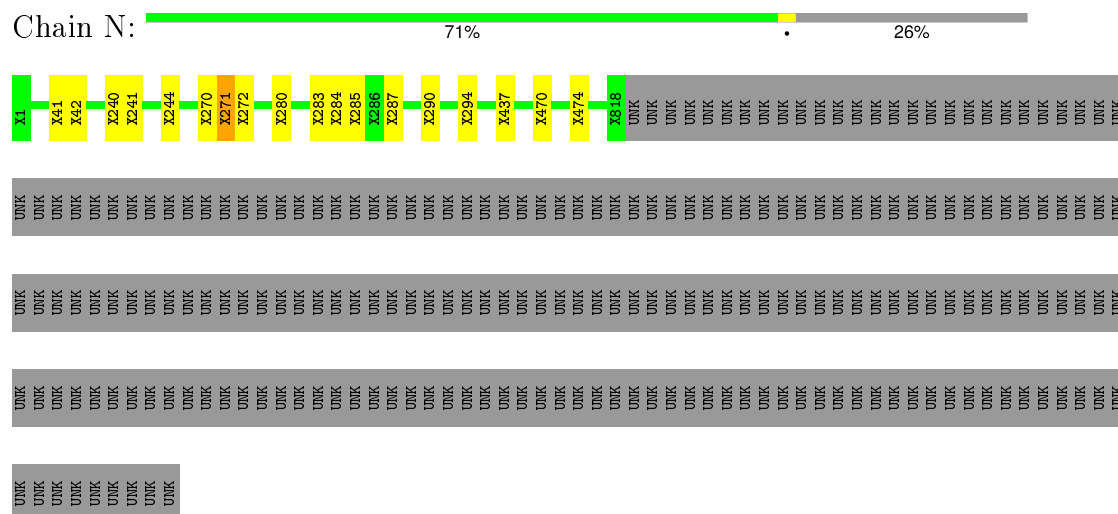
S2 C8 V32 A50 L61 R66 Y71 R72 Y79 L96 A100 Y107 R108 S117 S118 I134 K143 I144 W148 D149 S150 V156 Y167 V173 M174 L175 Q178 T179 N180 K181 S182 M187 D200 I210 I213 I224

L228 N229 E230 K235 I239 L243 R244 S245 V246 D247 V248 I249 P250 D251 N252 P253 K254 F255 E261 V265 Q268 I271

- Molecule 6: DYNACTIN SUBUNIT 2

Chain M:

• Molecule 7: DYNACTIN SUBUNIT 2

Chain N:

• Molecule 8: DYNACTIN SUBUNIT 3

Chain O:

• Molecule 8: DYNACTIN SUBUNIT 3

Chain P:

• Molecule 9: DYNACTIN SUBUNIT 2

Chain Q:

X1 X91 UNK UNK UNK

• Molecule 9: DYNACTIN SUBUNIT 2

Chain R:

96%

X1 X91 UNK UNK UNK

• Molecule 10: DYNACTIN 5

Chain U:

83%　　　　　5%　·　11%

MET ALA GLU LYS THR GLN LYS SER VAL LYS ILE ALA P13 P67 D68 P72 E75 ASP SER GLU PRO K76 I114 I120 N136 P153 Q154 P155 Q156 T157 L158 S181 THR PRO VAL LYS ASN
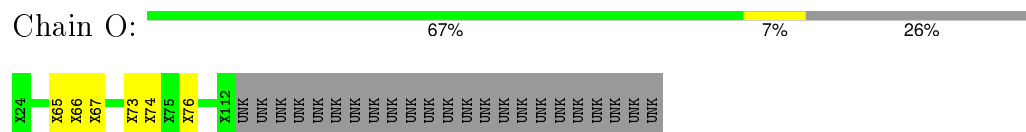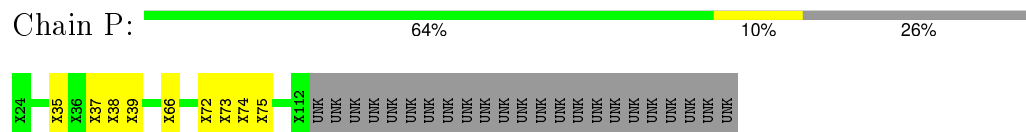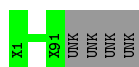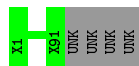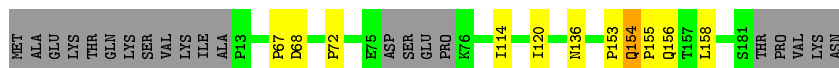
• Molecule 11: DYNACTIN SUBUNIT 6

Chain V:

98%

S18 I41 P72 A101 V182

• Molecule 12: DYNACTIN SUBUNIT 2

Chain Y:

99%

X14 X449 X452 X708

• Molecule 13: DYNACTIN SUBUNIT 2

Chain Z:

100%

X146 X1023 X1052
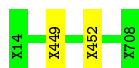
• Molecule 13: DYNACTIN SUBUNIT 2

Chain z:

100%

There are no outlier residues recorded for this chain.

• Molecule 14: DYNACTIN SUBUNIT 2

Chain a:

85%　　　　　　　13%　·

M1 Y6 L9 P10 E39 S42 N51 P52 N53 V64

• Molecule 15: DYNACTIN SUBUNIT 2

Chain b:

83%　　　　　　17%

M1 Y6 L9 R14 I37 E38 E39 S42 N51 P52 N53 D61 K67 G68 L69 T78 E87

• Molecule 16: DYNACTIN SUBUNIT 2

Chain c:

94%　　　　　　6%

M1 Y6 L9 X50

• Molecule 17: DYNACTIN SUBUNIT 2

Chain d:

90%　　　　5%　5%

M1 A2 D3 L9 Y20
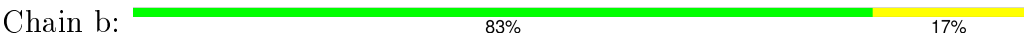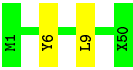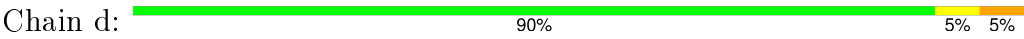
4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	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	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II	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	0.37	0/3026	0.51	0/4086
1	B	0.37	0/3026	0.51	0/4086
1	C	0.37	0/3026	0.52	0/4086
1	D	0.37	0/3026	0.52	0/4086
1	E	0.37	0/3026	0.53	0/4086
1	F	0.37	0/3026	0.51	0/4086
1	G	0.37	0/3026	0.52	0/4086
1	I	0.38	0/3026	0.52	0/4086
10	U	0.28	0/830	0.50	0/1152
11	V	0.30	0/811	0.48	0/1126
14	a	0.52	1/347 (0.3%)	0.67	1/473 (0.2%)
15	b	0.41	0/525	0.66	0/708
16	c	0.45	0/127	0.71	0/175
17	d	0.46	0/130	0.73	0/179
2	H	0.37	0/2948	0.51	0/3991
3	J	0.37	0/2939	0.53	0/3987
4	K	0.39	0/2294	0.63	1/3106 (0.0%)
5	L	0.37	0/2173	0.60	1/2935 (0.0%)
All	All	0.37	1/37332 (0.0%)	0.53	3/50520 (0.0%)

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	G	0	1
6	M	0	1
7	N	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	10	PRO	N-CD	5.05	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	253	PRO	CA-N-CD	-8.89	99.05	111.50
14	a	9	LEU	C-N-CD	5.78	140.54	128.40
4	K	114	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	375	THR	Peptide
6	M	442	UNK	Peptide
7	N	270	UNK	Peptide
7	N	271	UNK	Peptide

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	A	2957	0	2952	7	0
1	B	2957	0	2952	7	0
1	C	2957	0	2952	2	0
1	D	2957	0	2952	1	0
1	E	2957	0	2952	1	0
1	F	2957	0	2952	1	0
1	G	2957	0	2952	15	0
1	I	2957	0	2952	25	0
2	H	2885	0	2856	2	0
3	J	2879	0	2969	18	0
4	K	2242	0	2169	69	0
5	L	2137	0	2122	74	0
6	M	2855	0	585	12	0
7	N	3010	0	619	13	0
8	O	323	0	76	3	0
8	P	323	0	77	10	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Q	435	0	93	0	0
9	R	435	0	93	0	0
10	U	831	0	374	6	0
11	V	812	0	344	1	0
12	Y	1215	0	286	2	0
13	Z	2095	0	429	1	0
13	z	2095	0	427	0	0
14	a	341	0	310	0	0
15	b	517	0	490	0	0
16	c	179	0	116	0	0
17	d	127	0	103	0	0
All	All	49392	0	38154	229	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 3.

The worst 5 of 229 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:L:251:ASP:CG	5:L:255:PHE:HE2	1.36	1.28
5:L:251:ASP:O	5:L:255:PHE:CD2	1.94	1.20
1:G:183:ILE:HD11	1:G:278:VAL:CG2	1.72	1.19
5:L:253:PRO:HD2	5:L:254:LYS:H	1.08	1.17
4:K:162:GLN:HG3	5:L:243:LEU:CD2	1.77	1.13

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	368/370 (100%)	350 (95%)	18 (5%)	0	100 100

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	368/370 (100%)	348 (95%)	20 (5%)	0	100	100
1	C	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
1	D	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
1	E	368/370 (100%)	346 (94%)	22 (6%)	0	100	100
1	F	368/370 (100%)	341 (93%)	27 (7%)	0	100	100
1	G	368/370 (100%)	344 (94%)	24 (6%)	0	100	100
1	I	368/370 (100%)	347 (94%)	21 (6%)	0	100	100
2	H	368/370 (100%)	350 (95%)	18 (5%)	0	100	100
3	J	363/417 (87%)	331 (91%)	31 (8%)	1 (0%)	46	82
4	K	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
5	L	268/270 (99%)	257 (96%)	11 (4%)	0	100	100
10	U	167/190 (88%)	145 (87%)	16 (10%)	6 (4%)	4	41
11	V	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	30	73
14	a	44/48 (92%)	40 (91%)	3 (7%)	1 (2%)	8	51
15	b	67/71 (94%)	58 (87%)	8 (12%)	1 (2%)	13	58
16	c	18/31 (58%)	16 (89%)	1 (6%)	1 (6%)	2	29
17	d	18/20 (90%)	15 (83%)	1 (6%)	2 (11%)	0	10
All	All	4693/4817 (97%)	4386 (94%)	294 (6%)	13 (0%)	50	82

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	U	67	PRO
10	U	72	PRO
10	U	154	GLN
14	a	9	LEU
15	b	9	LEU

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	318/318 (100%)	312 (98%)	6 (2%)	65	86
1	B	318/318 (100%)	314 (99%)	4 (1%)	76	90
1	C	318/318 (100%)	309 (97%)	9 (3%)	51	79
1	D	318/318 (100%)	309 (97%)	9 (3%)	51	79
1	E	318/318 (100%)	310 (98%)	8 (2%)	55	82
1	F	318/318 (100%)	313 (98%)	5 (2%)	70	88
1	G	318/318 (100%)	311 (98%)	7 (2%)	60	84
1	I	318/318 (100%)	310 (98%)	8 (2%)	55	82
2	H	313/313 (100%)	312 (100%)	1 (0%)	94	97
3	J	322/363 (89%)	318 (99%)	4 (1%)	78	90
4	K	245/245 (100%)	239 (98%)	6 (2%)	57	82
5	L	242/242 (100%)	236 (98%)	6 (2%)	55	82
14	a	31/41 (76%)	26 (84%)	5 (16%)	3	22
15	b	49/60 (82%)	38 (78%)	11 (22%)	1	10
16	c	7/16 (44%)	6 (86%)	1 (14%)	4	28
17	d	8/16 (50%)	7 (88%)	1 (12%)	6	32
All	All	3761/3840 (98%)	3670 (98%)	91 (2%)	60	82

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	183	ILE
1	I	53	GLU
15	b	53	ASN
1	G	197	TYR
1	G	287	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	61	GLN
4	K	73	GLN
5	L	209	HIS
4	K	41	ASN
4	K	197	HIS

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.