



wwPDB NMR Structure Validation Summary Report ⓘ

Aug 10, 2023 – 07:37 PM EDT

PDB ID : 7U8K
BMRB ID : 30877
Title : Magic Angle Spinning NMR Structure of Human Cofilin-2 Assembled on Actin Filaments
Authors : Kraus, J.; Russell, R.; Kudryashova, E.; Xu, C.; Katyal, N.; Kudryashov, D.; Perilla, J.R.; Polenova, T.
Deposited on : 2022-03-08

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : **FAILED**
NmrClust : **FAILED**
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : **FAILED**
PANAV : **FAILED**
wwPDB-ShiftChecker : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance

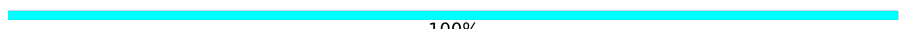
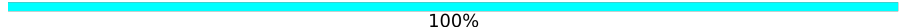
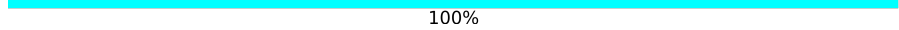
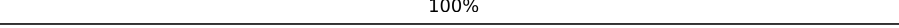
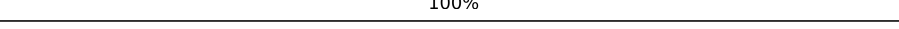
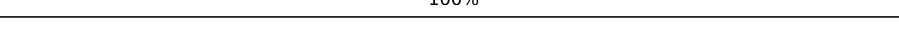


The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment was not calculated.

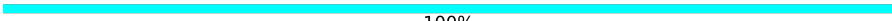
There are no overall percentile quality scores available for this entry.

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	377	 100%
1	B	377	 100%
1	C	377	 100%
1	D	377	 100%
1	E	377	 100%
1	F	377	 100%
1	G	377	 100%
1	H	377	 100%
1	I	377	 100%
1	J	377	 100%
2	K	168	 100%
2	L	168	 100%
2	M	168	 100%
2	N	168	 100%
2	O	168	 100%
2	P	168	 100%
2	Q	168	 100%

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Mol	Chain	Length	Quality of chain
2	R	168	 100%

2 Ensemble composition and analysis

This entry contains 4 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 79778 atoms, of which 39858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms						Trace
1	A	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	B	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	C	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	D	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	E	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	F	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	G	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	H	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	I	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	
1	J	377	Total	C	H	N	O	S	1
			5833	1856	2897	494	565	21	

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P68135
A	376	NH2	-	amidation	UNP P68135
B	0	ACE	-	acetylation	UNP P68135
B	376	NH2	-	amidation	UNP P68135
C	0	ACE	-	acetylation	UNP P68135
C	376	NH2	-	amidation	UNP P68135
D	0	ACE	-	acetylation	UNP P68135
D	376	NH2	-	amidation	UNP P68135
E	0	ACE	-	acetylation	UNP P68135
E	376	NH2	-	amidation	UNP P68135
F	0	ACE	-	acetylation	UNP P68135
F	376	NH2	-	amidation	UNP P68135
G	0	ACE	-	acetylation	UNP P68135

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Chain	Residue	Modelled	Actual	Comment	Reference
G	376	NH2	-	amidation	UNP P68135
H	0	ACE	-	acetylation	UNP P68135
H	376	NH2	-	amidation	UNP P68135
I	0	ACE	-	acetylation	UNP P68135
I	376	NH2	-	amidation	UNP P68135
J	0	ACE	-	acetylation	UNP P68135
J	376	NH2	-	amidation	UNP P68135

- Molecule 2 is a protein called Cofilin-2.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	K	168	2681	842	1361	218	255	5	1
2	L	168	2681	842	1361	218	255	5	1
2	M	168	2681	842	1361	218	255	5	1
2	N	168	2681	842	1361	218	255	5	1
2	O	168	2681	842	1361	218	255	5	1
2	P	168	2681	842	1361	218	255	5	1
2	Q	168	2681	842	1361	218	255	5	1
2	R	168	2681	842	1361	218	255	5	1

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	ACE	-	acetylation	UNP Q9Y281
K	167	NH2	-	amidation	UNP Q9Y281
L	0	ACE	-	acetylation	UNP Q9Y281
L	167	NH2	-	amidation	UNP Q9Y281
M	0	ACE	-	acetylation	UNP Q9Y281
M	167	NH2	-	amidation	UNP Q9Y281
N	0	ACE	-	acetylation	UNP Q9Y281
N	167	NH2	-	amidation	UNP Q9Y281
O	0	ACE	-	acetylation	UNP Q9Y281
O	167	NH2	-	amidation	UNP Q9Y281
P	0	ACE	-	acetylation	UNP Q9Y281

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Chain	Residue	Modelled	Actual	Comment	Reference
P	167	NH2	-	amidation	UNP Q9Y281
Q	0	ACE	-	acetylation	UNP Q9Y281
Q	167	NH2	-	amidation	UNP Q9Y281
R	0	ACE	-	acetylation	UNP Q9Y281
R	167	NH2	-	amidation	UNP Q9Y281

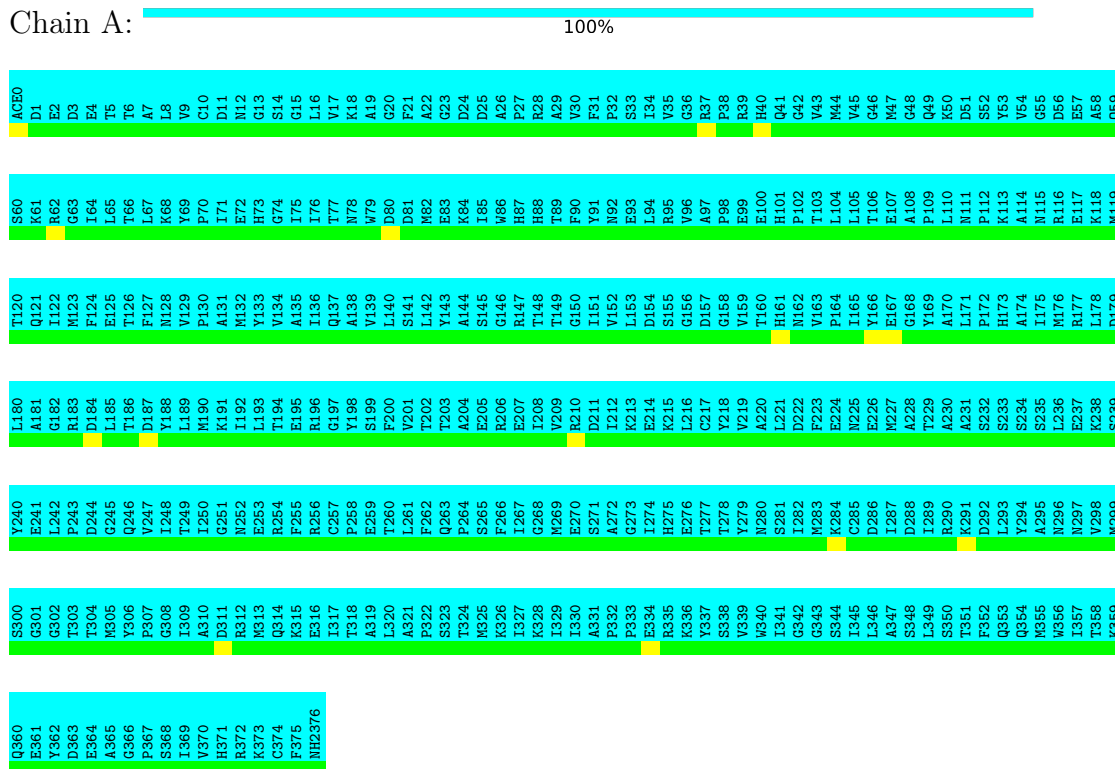
4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

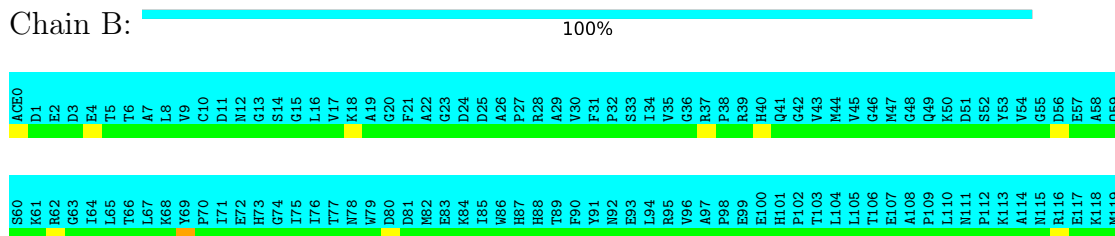
- Molecule 1: Actin, alpha skeletal muscle

Chain A:



- Molecule 1: Actin, alpha skeletal muscle

Chain B:



T120	L180	Y240	S300	Q360
Q121	A181	E241	G301	E361
I122	G182	L242	G302	Y362
M123	R183	P243	T303	D363
F124	L184	D244	T304	E364
E125	L185	G245	M305	A365
T126	L186	Q246	Y306	G366
F127	D187	V247	P307	P367
M128	Y188	L248	G308	S368
L129	L189	T249	I309	I369
M130	M190	C10	A310	V370
A131	K191	G251	D311	H371
M132	K192	N252	R312	R372
Y133	L193	E253	M313	K373
L134	T194	R254	Q314	C374
A135	E195	F255	K315	F375
A136	E196	R256	E316	NH2376
L136	R197	C257	I317	
Q137	Y198	P258	T318	
A138	S199	E259	A319	
Y139	F200	T260	L320	
L140	V201	L261	A321	
L141	T202	F262	P322	
L142	T203	Q263	S323	
L143	T203	Q263	S323	
A144	A204	P264	T324	
S145	E205	S265	M325	
S146	R206	F266	K326	
L147	E207	L267	I327	
L148	I208	G268	K328	
T149	I209	N269	I329	
G150	R210	E270	I330	
I151	D211	S271	A331	
I152	L212	A272	P332	
L153	K213	G273	S333	
L154	E214	L274	E334	
S155	K215	H275	R335	
G156	L216	E276	K336	
D157	C217	T277	Y337	
G158	Y218	T278	S338	
V159	V219	Y279	V339	
T160	A220	N280	W340	
H161	L221	S281	I341	
H162	D222	I282	P102	
V163	F223	M283	G42	
P164	E224	K284	V43	
I165	N225	C285	L104	
Y166	E226	D286	L105	
E167	M227	L287	T106	
G168	A228	D288	E107	
Y169	T229	I289	M47	
A170	A230	R290	A108	
L171	A231	K291	P109	
P172	S232	D292	L110	
H173	S233	L293	M111	
A174	S234	Y294	P112	
L175	S235	A295	S52	
M176	L236	N296	K113	
L177	E237	M297	V53	
K178	K238	V298	A114	
D179	S239	M299	G55	
			M115	
			A116	
			B56	
			E57	
			K118	
			A58	
			M119	

• Molecule 1: Actin, alpha skeletal muscle

Chain C:

100%

ACE0	S60	T120	L180	Y240	S300	Q360
D1	K61	Q121	A181	E241	G301	E361
E2	R62	I122	G182	L242	G302	Y362
D3	G63	M123	R183	P243	T303	D363
E4	I64	F124	L184	D244	T304	E364
T5	L65	E125	L185	G245	M305	A365
T6	T66	T126	L186	Q246	Y306	G366
A7	L67	F127	D187	V247	P307	P367
L8	K68	M128	Y188	L248	G308	S368
V9	Y69	I129	L189	T249	I309	I369
C10	P70	M130	M190	C10	A310	V370
D11	I71	A131	K191	G251	D311	H371
M12	I72	M132	K192	N252	R312	R372
G13	H73	Y133	L193	E253	M313	K373
S14	G74	V134	T194	R254	Q314	C374
I15	I75	A135	E195	F255	K315	F375
I16	I76	L136	E196	R256	E316	NH2376
V17	T77	Q137	G197	C257	I317	
K18	N78	T138	T318	P258	T318	
A19	W79	A139	A319	E259	A319	
G20	D80	L140	L320	T260	L320	
F21	D81	V201	A321	L261	A321	
A22	M82	T202	P322	F262	P322	
G23	E83	Y143	S323	Q263	S323	
D24	K84	D24	T324	P264	T324	
D25	I85	D25	M325	S265	M325	
A26	W86	A26	K326	F266	K326	
R28	H87	P27	I327	L267	I327	
A29	H88	I208	K328	G268	K328	
V30	T89	I209	I329	N269	I329	
F31	F90	R210	I330	E270	I330	
N92	Y91	D211	A331	S271	A331	
S93	M92	L212	P332	A272	P332	
L94	E93	K213	S333	G273	S333	
V95	R95	E214	E334	L274	E334	
G96	V96	K215	R335	H275	R335	
C97	A97	L216	K336	E276	K336	
F98	P98	C217	Y337	T277	Y337	
R99	E99	Y218	S338	T278	S338	
H40	E100	V219	V339	Y279	V339	
O41	H101	A220	W340	N280	W340	
G42	P102	S281	I341	S281	I341	
V43	G42	I282	P102	I282	P102	
M44	V43	M283	G42	M283	G42	
L104	L104	K284	V43	K284	V43	
L105	L105	N225	L104	N225	L105	
G46	G46	D286	L106	D286	L106	
M47	E107	L287	T106	E107	M47	
G48	A108	D288	E107	M47	A108	
O49	P109	I289	A108	I289	P109	
K50	L110	R290	P109	R290	K50	
D51	M111	K291	L110	K291	D51	
S52	P112	D292	M111	D292	S52	
Y53	K113	L293	P112	L293	Y53	
V54	A114	Y294	K113	Y294	V54	
G55	M115	A295	A114	A295	G55	
B56	A116	N296	M115	N296	B56	
E57	E117	M297	A116	M297	E57	
K118	L118	V298	E117	V298	K118	
A58	M119	M299	L118	M299	A58	
O59			M119		O59	

• Molecule 1: Actin, alpha skeletal muscle

Chain D:

100%

ACE0	S60	T120	L180	Y240	S300	Q360
D1	K61	Q121	A181	E241	G301	E361
E2	R62	I122	G182	L242	G302	Y362
D3	G63	M123	R183	P243	T303	D363
E4	I64	F124	L184	D244	T304	E364
T5	L65	E125	L185	G245	M305	A365
T6	T66	T126	L186	Q246	Y306	G366
A7	L67	F127	D187	V247	P307	P367
L8	K68	M128	Y188	L248	G308	S368
V9	Y69	I129	L189	T249	I309	I369
C10	P70	M130	M190	C10	A310	V370
D11	I71	A131	K191	G251	D311	H371
M12	I72	M132	K192	N252	R312	R372
G13	H73	Y133	L193	E253	M313	K373
S14	G74	V134	T194	R254	Q314	C374
I15	I75	A135	E195	F255	K315	F375
I16	I76	L136	E196	R256	E316	NH2376
V17	T77	Q137	G197	C257	I317	
K18	N78	T138	T318	P258	T318	
A19	W79	A139	A319	E259	A319	
G20	D80	L140	L320	T260	L320	
F21	D81	V201	A321	L261	A321	
A22	M82	T202	P322	F262	P322	
G23	E83	Y143	S323	Q263	S323	
D24	K84	D24	T324	P264	T324	
D25	I85	D25	M325	S265	M325	
A26	W86	A26	K326	F266	K326	
R28	H87	P27	I327	L267	I327	
A29	H88	I208	K328	G268	K328	
V30	T89	I209	I329	N269	I329	
F31	F90	R210	I330	E270	I330	
N92	Y91	D211	A331	S271	A331	
S93	M92	L212	P332	A272	P332	
L94	E93	K213	S333	G273	S333	
V95	R95	E214	E334	L274	E334	
G96	V96	K215	R335	H275	R335	
C97	A97	L216	K336	E276	K336	
F98	P98	C217	Y337	T277	Y337	
R99	E99	Y218	S338	T278	S338	
H40	E100	V219	V339	Y279	V339	
O41	H101	A220	W340	N280	W340	
G42	P102	S281	I341	S281	I341	
V43	G42	I282	P102	I282	P102	
M44	V43	M283	G42	M283	G42	
L104	L104	K284	V43	K284	V43	
L105	L105	N225	L104	N225	L105	
G46	G46	D286	L106	D286	L106	
M47	E107	L287	T106	E107	M47	
G48	A108	D288	E107	M47	A108	
O49	P109	I289	A108	I289	P109	
K50	L110	R290	P109	R290	K50	
D51	M111	K291	L110	K291	D51	
S52	P112	D292	M111	D292	S52	
Y53	K113	L293	P112	L293	Y53	
V54	A114	Y294	K113	Y294	V54	
G55	M115	A295	A114	A295	G55	
B56	A116	N296	M115	N296	B56	
E57	E117	M297	A116	M297	E57	
K118	L118	V298	E117	V298	K118	
A58	M119	M299	L118	M299	A58	
O59			M119		O59	

T120	L180	Y240	S300	Q360
Q121	A181	E241	G301	E361
I122	G182	L242	G302	Y362
M123	R183	P243	T303	D363
F124	R184	D244	T304	E364
E125	L185	G245	M305	A365
T126	L186	Q246	Y306	G366
F127	D187	V247	P307	P367
M128	Y188	L248	G308	S368
L129	L189	T249	I309	I369
P130	M190	L250	A310	V370
A131	K191	G251	D311	H371
M132	K192	W252	R312	R372
Y133	L193	E253	M313	K373
V134	T194	R254	Q314	C374
A135	E195	F255	K315	F375
R196	R196	R256	E316	NH2376
G197	G197	C257	I317	
Q137	Y198	P258	T318	
L138	S199	E259	A319	
V139	F200	T260	L320	
L140	V201	L261	A321	
L141	T202	F262	P322	
L142	T203	Q263	S323	
L143	T203	Q263	S323	
A144	A204	P264	T324	
S145	E205	S265	M325	
S146	R206	F266	K326	
R147	E207	L267	I327	
L148	I208	G268	K328	
V149	I209	M269	I329	
R210	R210	E270	I330	
D211	D211	S271	A331	
L152	L212	A272	P332	
L153	K213	G273	S333	
D154	E214	L274	E334	
S155	K215	H275	R335	
G156	L216	E276	K336	
D157	C217	T277	Y337	
G158	Y218	T278	S338	
V159	V219	Y279	V339	
T160	A220	N280	W340	
H161	L221	S281	I341	
D222	L222	L282	P102	
V163	F223	M283	G343	
P164	E224	K284	S344	
I165	N225	C285	I345	
Y166	E226	D286	L346	
E167	M227	L287	A347	
G168	A228	D288	S348	
Y169	T229	I289	L349	
A170	A230	K290	S350	
L171	A231	K291	T351	
P172	S232	D292	F352	
H173	S233	L293	Q353	
A174	S234	Y294	Q354	
L175	S235	A295	M355	
M176	L236	N296	W356	
R177	E237	N297	I357	
L178	K238	V298	T358	
D179	S239	M299	K359	

• Molecule 1: Actin, alpha skeletal muscle

Chain E:

100%

ACE0	S60	T120	L180	Y240	S300	Q360
D1	K61	Q121	A181	E241	G301	E361
E2	R62	I122	G182	L242	G302	Y362
D3	G63	M123	R183	P243	T303	D363
E4	I64	F124	R184	D244	T304	E364
T5	L65	T125	L185	G245	M305	A365
T6	T66	T126	L186	Q246	Y306	G366
A7	L67	F127	D187	V247	P307	P367
L8	K68	M128	Y188	L248	G308	S368
V9	Y69	I129	L189	T249	I309	I369
C10	P70	P130	M190	L250	A310	V370
D11	I71	I131	K191	G251	D311	H371
M12	I72	M132	K192	W252	R312	R372
G13	H73	Y133	L193	E253	M313	K373
S14	G74	V134	T194	R254	Q314	C374
I15	I75	A135	E195	F255	K315	F375
L16	I76	L136	R196	R256	E316	NH2376
V17	T77	Q137	G197	C257	I317	
K18	W78	M138	T198	P258	T318	
A19	W79	I139	S199	E259	A319	
G20	D80	L140	F200	T260	L320	
D81	F21	S141	V201	L261	A321	
A22	M82	L142	T202	F262	P322	
G23	E83	Y143	T203	Q263	S323	
D24	K84	D24	A204	P264	T324	
D25	I85	D25	M325	S265	M325	
A26	W86	A26	K326	F266	K326	
R28	H87	R28	I327	L267	I327	
A29	H88	R28	K328	G268	K328	
V30	T89	T89	I329	M269	I329	
F31	F90	V30	I330	E270	I330	
N92	Y91	D11	A331	S271	A331	
S93	M92	L152	P332	A272	P332	
L94	E93	L153	S333	G273	S333	
V95	R95	D154	E334	L274	E334	
G96	K96	S155	R335	H275	R335	
C97	V96	L216	K336	E276	K336	
F98	A97	D157	Y337	T277	Y337	
E99	P98	G158	S338	T278	S338	
H40	E99	Y219	V339	Y279	V339	
O41	E100	T160	W340	N280	W340	
P102	H101	L221	I341	S281	I341	
G103	P102	D222	P102	L282	P102	
M44	T103	F223	G343	M283	G343	
L104	L104	E224	S344	K284	S344	
V45	L105	N225	I345	C285	I345	
G46	T106	E226	L346	D286	L346	
M47	E107	E167	A347	L287	A347	
G48	A108	D228	S348	D288	S348	
O49	P109	T229	L349	I289	L349	
K50	L110	K290	S350	K290	S350	
D51	M111	R291	T351	K291	T351	
S52	P112	D292	F352	D292	F352	
Y53	K113	L293	Q353	L293	Q353	
V54	A114	Y294	Q354	Y294	Q354	
G55	M115	A295	M355	A295	M355	
D56	R116	N296	W356	N296	W356	
E57	I117	N297	I357	N297	I357	
A58	K118	V298	T358	V298	T358	
O59	M119	M299	K359	M299	K359	

• Molecule 1: Actin, alpha skeletal muscle

Chain F:

100%

ACE0	S60	T120	L180	Y240	S300	Q360
D1	K61	Q121	A181	E241	G301	E361
E2	R62	I122	G182	L242	G302	Y362
D3	G63	M123	R183	P243	T303	D363
E4	I64	F124	R184	D244	T304	E364
T5	L65	T125	L185	G245	M305	A365
T6	T66	T126	L186	Q246	Y306	G366
A7	L67	F127	D187	V247	P307	P367
L8	K68	M128	Y188	L248	G308	S368
V9	Y69	I129	L189	T249	I309	I369
C10	P70	P130	M190	L250	A310	V370
D11	I71	I131	K191	G251	D311	H371
M12	I72	M132	K192	W252	R312	R372
G13	H73	Y133	L193	E253	M313	K373
S14	G74	V134	T194	R254	Q314	C374
I15	I75	A135	E195	F255	K315	F375
L16	I76	L136	R196	R256	E316	NH2376
V17	T77	Q137	G197	C257	I317	
K18	W78	M138	T198	P258	T318	
A19	W79	I139	S199	E259	A319	
G20	D80	L140	F200	T260	L320	
D81	F21	S141	V201	L261	A321	
A22	M82	L142	T202	F262	P322	
G23	E83	Y143	T203	Q263	S323	
D24	K84	D24	A204	P264	T324	
D25	I85	D25	M325	S265	M325	
A26	W86	A26	K326	F266	K326	
R28	H87	R28	I327	L267	I327	
A29	H88	R28	K328	G268	K328	
V30	T89	T89	I329	M269	I329	
F31	F90	V30	I330	E270	I330	
N92	Y91	D11	A331	S271	A331	
S93	M92	L152	P332	A272	P332	
L94	E93	L153	S333	G273	S333	
V95	R95	D154	E334	L274	E334	
G96	K96	S155	R335	H275	R335	
C97	V96	L216	K336	E276	K336	
F98	A97	D157	Y337	T277	Y337	
E99	P98	G158	S338	T278	S338	
H40	E99	Y219	V339	Y279	V339	
O41	E100	T160	W340	N280	W340	
P102	H101	L221	I341	S281	I341	
G103	P102	D222	P102	L282	P102	
M44	T103	F223	G343	M283	G343	
L104	L104	E224	S344	K284	S344	
V45	L105	N225	I345	C285	I345	
G46	T106	E226	L346	D286	L346	
M47	E107	E167	A347	L287	A347	
G48	A108	D228	S348	D288	S348	
O49	P109	T229	L349	I289	L349	
K50	L110	K290	S350	K290	S350	
D51	M111	R291	T351	K291	T351	
S52	P112	D292	F352	D292	F352	
Y53	K113	L293	Q353	L293	Q353	
V54	A114	Y294	Q354	Y294	Q354	
G55	M115	A295	M355	A295	M355	
D56	R116	N296	W356	N296	W356	
E57	I117	N297	I357	N297	I357	
A58	K118	V298	T358	V298	T358	
O59	M119	M299	K359	M299	K359	

T120	L180	Y240	S300	Q360
Q121	A181	E241	G301	E361
I122	G182	L242	G302	Y362
M123	R183	P243	T303	D363
F124	R184	D244	T304	E364
E125	L185	G245	M305	L185
T126	L186	Q246	Y306	A365
F127	D187	V247	P307	G366
M128	Y188	L248	G308	P367
V129	L189	T249	I309	S368
P130	M190	L250	I309	S368
A131	K191	G251	A310	I369
I132	K191	P252	P70	V370
Y133	L192	W252	D311	H371
V134	L194	E253	R312	R372
A135	T194	R254	M313	K373
E136	E195	R254	Q314	C374
G137	R196	R256	E316	F375
Q137	G197	C257	I317	NH2376
A138	Y198	P258	T318	
V139	S199	E259	A319	
L140	F200	T260	L320	
L141	V201	L261	A321	
L142	T202	F262	P322	
Y143	T203	Q263	S323	
A144	A204	P264	T324	
S145	E205	S265	M325	
G146	R206	F266	K326	
R147	E207	L267	I327	
L148	I208	G268	K328	
T149	V209	M269	I329	
G150	R210	E270	I330	
I151	D211	S271	A331	
I152	L212	A272	P332	
L153	K213	G273	P333	
D154	E214	L274	E334	
S155	K215	H275	R335	
G156	L216	E276	K336	
D157	C217	T277	Y337	
G158	Y218	T278	S338	
V159	V219	Y279	V339	
H160	A220	N280	W340	
H161	L221	S281	I341	
D222	L222	D282	P102	
F223	D223	M283	G42	
P163	F224	K284	T103	
P164	E224	K284	M44	
I165	M225	C285	L104	
Y166	E226	D286	V45	
E167	M227	L287	T106	
G168	A228	D288	G46	
Y169	T229	I289	M47	
A170	A230	L289	P109	
L171	A231	K290	L110	
P172	S232	K291	M111	
H173	S233	D292	P112	
A174	S234	L293	S52	
I175	S235	Y294	K113	
M176	L236	A295	V54	
R177	E237	N296	A114	
K238	K238	M297	M115	
S239	S239	V298	R116	
			E57	
			K118	
			A58	
			M119	

• Molecule 1: Actin, alpha skeletal muscle

Chain G:

100%

ACE0	S60	T120	L180	Y240	S300	Q360
D1	K61	Q121	A181	E241	G301	E361
E2	R62	I122	G182	L242	G302	Y362
D3	G63	M123	R183	P243	T303	D363
E4	I64	F124	L184	D244	T304	E364
T5	L65	E125	L185	G245	M305	L185
T6	T66	T126	L186	Q246	Y306	A365
A7	L67	F127	D187	V247	P307	G366
L8	K68	M128	Y188	L248	G308	P367
V9	Y69	V129	L189	T249	I309	S368
C10	P70	P130	M190	L250	I309	S368
D11	I71	A131	K191	G251	A310	I369
M12	I71	P70	K191	P252	P70	V370
G13	E72	M132	L192	W252	D311	H371
S14	H73	Y133	L193	E253	R312	R372
G15	G74	V134	L194	R254	M313	K373
I16	I75	A135	E195	R254	Q314	C374
L17	I76	L136	E195	R256	E316	F375
V17	I77	L136	I196	R256	I317	NH2376
K18	N78	D24	G197	C257	T318	
A19	W79	D25	T177	E259	A319	
G20	D80	D25	K18	P258	L320	
F21	L81	A26	N78	E259	A319	
A22	F21	A26	W79	E259	L320	
G23	M82	A22	D80	T260	A321	
E83	M82	A22	F21	L261	F201	
D24	E83	G23	M82	F262	D81	
D25	K84	E83	E83	Q263	A22	
A26	I85	D25	I85	P264	G23	
R26	W86	A26	I86	S265	D24	
P27	H87	P27	W86	F266	D25	
H88	H88	H87	H87	F266	A26	
V29	I88	I88	H88	L267	R26	
F30	F90	F30	I88	E207	I87	
F31	Y91	F31	F90	E207	F31	
N92	N92	N92	F90	E270	Y91	
S93	S93	S93	F90	S271	F31	
L94	L94	L94	F90	A272	N92	
V95	R95	R95	F90	G273	E93	
G96	V96	V96	F90	L274	S93	
R97	A97	A97	F90	H275	L94	
F98	P98	P98	F90	E276	R95	
E99	E99	E99	F90	T277	V96	
H40	H40	H40	F90	T278	A97	
O41	H101	O41	F90	Y279	P98	
G42	P102	G42	F90	Y279	E99	
G43	T103	G43	F90	N280	R39	
S344	L104	S344	F90	A220	H40	
L105	T106	L105	F90	L221	E100	
G46	E107	G46	F90	H101	H101	
M47	M47	M47	F90	L221	O41	
G48	P109	G48	F90	D222	G42	
O49	K50	O49	F90	F223	G42	
D51	M111	D51	F90	E224	V43	
S52	P112	S52	F90	K284	M44	
Y53	K113	Y53	F90	N225	L104	
V54	A114	V54	F90	M225	V45	
M115	N115	M115	F90	E226	T106	
G55	R116	G55	F90	L287	E107	
D56	E117	D56	F90	D288	M47	
E57	K118	E57	F90	A228	G48	
A58	A58	A58	F90	T229	P109	
M119	M119	M119	F90	L290	O49	
			F90	K290	K50	
			F90	R291	M111	
			F90	D292	D51	
			F90	L293	P112	
			F90	Y294	S52	
			F90	A295	K113	
			F90	N296	V54	
			F90	M297	A114	
			F90	V298	M115	
			F90		R116	
			F90		E57	
			F90		K118	
			F90		A58	
			F90		M119	

• Molecule 1: Actin, alpha skeletal muscle

Chain H:

100%

ACE0	S60	T120	L180	Y240	S300	Q360
D1	K61	Q121	A181	E241	G301	E361
E2	R62	I122	G182	L242	G302	Y362
D3	G63	M123	R183	P243	T303	D363
E4	I64	F124	L184	D244	T304	E364
T5	L65	E125	L185	G245	M305	L185
T6	T66	T126	L186	Q246	Y306	A365
A7	L67	F127	D187	V247	P307	G366
L8	K68	M128	Y188	L248	G308	P367
V9	Y69	V129	L189	T249	I309	S368
C10	P70	P130	M190	L250	I309	S368
D11	I71	A131	K191	G251	A310	I369
M12	I71	P70	K191	P252	P70	V370
G13	E72	M132	L192	W252	D311	H371
S14	H73	Y133	L193	E253	R312	R372
G15	G74	V134	L194	R254	M313	K373
I16	I75	A135	E195	R254	Q314	C374
L17	I76	L136	E195	R256	E316	F375
V17	I77	L136	I196	R256	I317	NH2376
K18	N78	D24	G197	C257	T318	
A19	W79	D25	T177	E259	A319	
G20	D80	D25	K18	P258	L320	
F21	L81	A26	N78	E259	A319	
A22	F21	A26	W79	E259	L320	
G23	M82	A22	D80	T260	A321	
E83	M82	A22	F21	L261	F201	
D24	E83	G23	M82	F262	D81	
D25	K84	E83	E83	Q263	A22	
A26	I85	D25	I85	P264	G23	
R26	W86	A26	I86	S265	D24	
P27	H87	P27	W86	F266	D25	
H88	H88	H87	H87	F266	A26	
V29	I88	I88	H88	L267	R26	
F30	F90	F30	I88	E207	I87	
F31	Y91	F31	F90	E207	F31	
N92	N92	N92	F90	E270	Y91	
S93	S93	S93	F90	S271	F31	
L94	L94	L94	F90	A272	N92	
V95	R95	R95	F90	G273	E93	
G96	V96	V96	F90	L274	S93	
R97	A97	A97	F90	H275	L94	
F98	P98	P98	F90	E276	R95	
E99	E99	E99	F90	T277	V96	
H40	H40	H40	F90	T278	A97	
O41	H101	O41	F90	Y279	P98	
G42	P102	G42	F90	Y279	E99	
G43	T103	G43	F90	N280	R39	
S344	L104	S344	F90	A220	H40	
L105	T106	L105	F90	L221	E100	
G46	E107	G46	F90	H101	H101	
M47	M47	M47	F90	L221	O41	
G48	P109	G48	F90	D222	G42	
O49	K50	O49	F90	F223	G42	
D51	M111	D51	F90	E224	V43	
S52	P112	S52	F90	K284	M44	
Y53	K113	Y53	F90	N225	L104	
V54	A114	V54	F90	M225	V45	
M115	N115	M115	F90	E226	T106	
G55	R116	G55	F90	L287	E107	
D56	E117	D56	F90	D288	M47	
E57	K118	E57	F90	A228	G48	
A58	A58	A58	F90	T229	P109	
M119	M119	M119	F90	L290	O49	
			F90	K290	K50	
			F90	R291	M111	
			F90	D292	D51	
			F90	L293	P112	
			F90	Y294	S52	
			F90	A295	K113	
			F90	N296	V54	
			F90	M297	A114	
			F90	V298	M115	
			F90		R116	
			F90		E57	
			F90		K118	
			F90		A58	
			F90		M119	

T120	T180	Y240	S300	Q360
Q121	A181	E241	G301	E361
I122	G182	L242	G302	Y362
M123	R183	P243	T303	D363
F124	D184	D244	T304	E364
E125	L185	G245	M305	A365
T126	T186	Q246	Y306	G366
F127	D187	V247	P307	P367
M128	Y188	L248	G308	S368
I129	L189	T249	I309	I369
P130	M190	L250	P130	V370
A131	K191	G251	D311	H371
M132	K192	N252	R312	R372
Y133	L193	E253	M313	K373
V134	T194	R254	Q314	C374
A135	E195	F255	K315	F375
R136	R196	R256	E316	NH2376
Q137	G197	C257	I317	
I138	Y198	P258	T318	
V139	S199	E259	A319	
L140	F200	T260	L320	
V201	L261	L261	A321	
L142	T202	F262	P322	
Y143	T203	Q263	S323	
A144	A204	P264	T324	
S145	E205	S265	M325	
R206	R206	F266	K326	
R147	E207	L267	I327	
T148	I208	G268	K328	
V209	T149	N269	I329	
T149	R210	E270	I330	
G150	D211	S271	A331	
I151	L212	A272	P332	
V152	K213	G273	S333	
L153	E214	I274	E334	
D154	K215	H275	R335	
S155	L216	E276	K336	
G156	C217	T277	Y337	
D157	Y218	T278	S338	
G158	V219	Y279	V339	
L160	A220	N280	W340	
H161	L221	S281	I341	
H162	D222	I282	P102	
V163	F223	M283	G343	
P164	E224	K284	S344	
I165	N225	C285	I345	
Y166	E226	D286	L346	
E167	M227	L287	A347	
G168	A228	D288	S348	
Y169	T229	I289	L349	
A170	A230	R290	S350	
L171	A231	K291	T351	
P172	D232	D292	P352	
H173	S233	L293	Q353	
A174	S234	Y294	M354	
I175	S235	A295	M355	
M176	L236	N296	W356	
R177	E237	N297	I357	
L178	K238	V298	T358	
D179	S239	M299	K359	

- Molecule 1: Actin, alpha skeletal muscle

Chain I:

100%

ACE0	S60	T120	Y240	S300	Q360
D1	K61	Q121	E241	G301	E361
E2	R62	I122	L242	G302	Y362
D3	G63	M123	P243	T303	D363
E4	I64	F124	D244	T304	E364
T5	L65	E125	G245	M305	A365
T6	T66	T126	Q246	Y306	G366
A7	L67	F127	V247	P307	P367
L8	K68	M128	L248	G308	S368
V9	Y69	I129	T249	I309	I369
C10	P70	M130	L250	P130	V370
D11	I71	A131	G251	D311	H371
M12	K72	M132	N252	R312	R372
G13	H73	Y133	E253	M313	K373
S14	G74	V134	R254	Q314	C374
I15	I75	A135	F255	K315	F375
I16	I76	L136	R256	E316	NH2376
V17	T77	Q137	C257	I317	
K18	N78	T138	P258	T318	
A19	W79	V139	E259	A319	
G20	D80	L140	T260	L320	
F21	M81	S141	L261	A321	
A22	M82	T142	F262	P322	
G23	E83	Y143	Q263	S323	
D24	K84	D24	P264	T324	
D25	I85	D25	S265	M325	
A26	W86	A26	F266	K326	
R28	H87	P27	L267	I327	
V29	H88	Q268	G268	K328	
F30	T89	N269	N269	I329	
F31	F90	E270	E270	I330	
N92	Y91	S271	S271	A331	
S93	M92	A272	A272	P332	
I94	E93	G273	G273	S333	
V95	L94	I274	I274	E334	
G96	R95	H275	H275	R335	
G96	V96	E276	E276	K336	
R97	A97	T277	T277	Y337	
F98	P98	T278	T278	S338	
R99	E99	Y279	Y279	V339	
H40	E100	N280	N280	W340	
Q41	H101	S281	S281	I341	
G42	P102	I282	I282	P102	
V43	T103	D222	D222	G343	
M44	L104	F223	F223	S344	
V45	L105	N225	N225	I345	
G46	T106	E226	E226	L346	
M47	E107	M227	M227	A347	
G48	A108	D288	D288	S348	
Q49	P109	I289	I289	L349	
K50	L110	R290	R290	S350	
D51	M111	K291	K291	T351	
S52	P112	D292	D292	P352	
Y53	K113	L293	L293	Q353	
V54	A114	Y294	Y294	M354	
G55	N115	A295	A295	M355	
D56	R116	N296	N296	W356	
E57	I117	N297	N297	I357	
A58	K118	V298	V298	T358	
O59	M119	M299	M299	K359	

- Molecule 1: Actin, alpha skeletal muscle

Chain J:

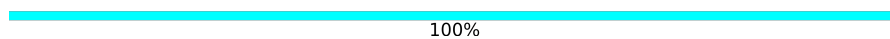
100%

ACE0	S60	T120	Y240	S300	Q360
D1	K61	Q121	E241	G301	E361
E2	R62	I122	L242	G302	Y362
D3	G63	M123	P243	T303	D363
E4	I64	F124	D244	T304	E364
T5	L65	E125	G245	M305	A365
T6	T66	T126	Q246	Y306	G366
A7	L67	F127	V247	P307	P367
L8	K68	M128	L248	G308	S368
V9	Y69	I129	T249	I309	I369
C10	P70	M130	L250	P130	V370
D11	I71	A131	G251	D311	H371
M12	K72	M132	N252	R312	R372
G13	H73	Y133	E253	M313	K373
S14	G74	V134	R254	Q314	C374
I15	I75	A135	F255	K315	F375
I16	I76	L136	R256	E316	NH2376
V17	T77	Q137	C257	I317	
K18	N78	T138	P258	T318	
A19	W79	V139	E259	A319	
G20	D80	L140	T260	L320	
F21	M81	S141	L261	A321	
A22	M82	T142	F262	P322	
G23	E83	Y143	Q263	S323	
D24	K84	D24	P264	T324	
D25	I85	D25	S265	M325	
A26	W86	A26	F266	K326	
R28	H87	P27	L267	I327	
V29	H88	Q268	G268	K328	
F30	T89	N269	N269	I329	
F31	F90	E270	E270	I330	
N92	Y91	S271	S271	A331	
S93	M92	A272	A272	P332	
I94	E93	G273	G273	S333	
L94	L94	I274	I274	E334	
V95	R95	H275	H275	R335	
G96	V96	E276	E276	K336	
R97	A97	T277	T277	Y337	
F98	P98	T278	T278	S338	
R99	E99	Y279	Y279	V339	
H40	E100	N280	N280	W340	
Q41	H101	S281	S281	I341	
G42	P102	I282	I282	P102	
V43	T103	D222	D222	G343	
M44	L104	F223	F223	S344	
V45	L105	N225	N225	I345	
G46	T106	E226	E226	L346	
M47	E107	M227	M227	A347	
G48	A108	D288	D288	S348	
Q49	P109	I289	I289	L349	
K50	L110	R290	R290	S350	
D51	M111	K291	K291	T351	
S52	P112	D292	D292	P352	
Y53	K113	L293	L293	Q353	
V54	A114	Y294	Y294	M354	
G55	N115	A295	A295	M355	
D56	R116	N296	N296	W356	
E57	I117	N297	N297	I357	
A58	K118	V298	V298	T358	
O59	M119	M299	M299	K359	

T120	L180	Y240	S300	Q360
Q121	A181	E241	G301	E361
I122	G182	L242	G302	Y362
M123	R183	P243	T303	D363
F124	D184	D244	T304	E364
E125	L185	G245	M305	A365
T126	T186	Q246	Y306	G366
F127	D187	V247	P307	P367
L128	Y188	I248	G308	S368
M129	L189	T249	I309	I369
P130	M190	L250	A310	V370
A131	K191	G251	D311	H371
I132	L192	N252	R312	H372
Y133	L193	E253	M313	K373
V134	T194	R254	Q314	Q374
A135	E195	F255	K315	F375
I136	R196	R256	E316	NH2376
Q137	G197	C257	I317	
A138	Y198	P258	T318	
Y139	S199	E259	A319	
F200	F200	T260	L320	
S141	V201	L261	R21	
L142	T202	F262	P322	
Y143	T203	Q263	S323	
A144	A204	P264	S234	
S145	E205	S265	M325	
G146	R206	F266	K326	
R147	E207	L267	I327	
I148	I208	G268	K328	
T149	V209	N269	I29	
G150	R210	E270	K330	
I151	D211	S271	A331	
V152	L212	G272	P332	
L153	K213	G273	E333	
E154	E214	L274	K334	
S155	K215	H275	R335	
G156	L216	E276	K336	
D157	C217	T277	Y337	
G158	Y218	T278	S338	
V159	V219	Y279	V339	
H160	A220	N280	W340	
H161	L221	S281	I341	
D162	L222	L282	G342	
V163	F223	M283	G343	
P164	E224	K284	S344	
I165	N225	C285	L345	
Y166	E226	D286	L346	
E167	M227	L287	A347	
G168	A228	D288	S348	
Y169	T229	L289	L349	
A170	A230	K290	S350	
L171	A231	R291	T351	
P172	S232	D292	F352	
H173	S233	L293	Q353	
A174	S234	Y294	Q354	
S175	S235	A295	M355	
M176	L236	N296	W356	
R177	E237	N297	I357	
L178	K238	V298	T358	
D179	S239	M299	K359	

• Molecule 2: Cofilin-2

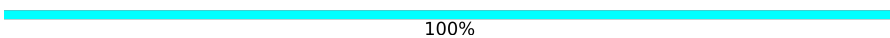
Chain K:



ACE0	T60	S120
M1	G61	K121
A2	D62	D122
S3	T63	A123
G4	V64	I124
V5	E65	K125
T6	D66	K126
V7	P67	K127
N8	F68	F128
D9	T69	T129
E10	S70	G130
V11	F71	I131
I12	W72	K132
K13	K73	H133
V14	L74	E134
F15	L75	W135
M16	P76	Q136
D17	L77	V137
M18	W78	M138
K19	D79	G139
V20	C80	L140
R21	R81	D141
K22	Y82	D142
S23	A83	I143
S24	L84	K144
T25	Y85	D145
Q26	D86	R146
E27	A87	S147
E28	T88	T148
I29	Y89	L149
K30	E90	G150
K31	T91	E151
R32	K92	K152
K33	E93	L153
K34	S94	G154
A35	K95	G155
V36	K96	N156
L37	E97	V157
F38	D98	V158
C39	L99	V159
L40	M100	S160
S41	F101	L161
D42	I102	E162
D43	F103	G163
K44	W104	K164
R45	A105	P165
Q46	P106	L166
I47	E107	E107
I48	S108	I48
V49	A109	V49
E50	F110	F110
E51	L111	L111
A52	K112	K112
K53	S113	K53
Q54	K114	K114
I55	M115	M115
L56	I116	I116
V57	Y117	Y117
G58	A118	A118
D59	S119	S119

• Molecule 2: Cofilin-2

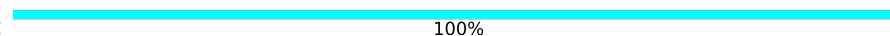
Chain L:



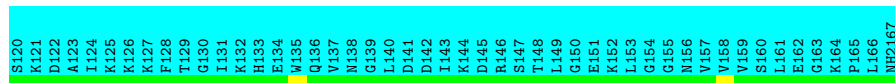
ACE0	T60	S120
M1	G61	K121
A2	D62	D122
S3	T63	A123
G4	V64	I124
V5	E65	K125
T6	D66	K126
V7	P67	K127
N8	F68	F128
D9	T69	T129
E10	S70	G130
V11	F71	I131
I12	W72	K132
K13	K73	H133
V14	L74	E134
F15	L75	W135
M16	P76	Q136
D17	L77	V137
M18	W78	M138
K19	D79	G139
V20	C80	L140
R21	R81	D141
K22	Y82	D142
S23	A83	I143
S24	L84	K144
T25	Y85	D145
Q26	D86	R146
E27	A87	S147
E28	T88	T148
I29	Y89	L149
K30	E90	G150
K31	T91	E151
R32	K92	K152
K33	E93	L153
K34	S94	G154
A35	K95	G155
V36	K96	N156
L37	E97	V157
F38	D98	V158
C39	L99	V159
L40	M100	S160
S41	F101	L161
D42	I102	E162
D43	F103	G163
K44	W104	K164
R45	A105	P165
Q46	P106	L166
I47	E107	E107
I48	S108	I48
V49	A109	V49
E50	F110	F110
E51	L111	L111
A52	K112	K112
K53	S113	K53
Q54	K114	K114
I55	M115	M115
L56	I116	I116
V57	Y117	Y117
G58	A118	A118
D59	S119	S119

• Molecule 2: Cofilin-2

Chain M:

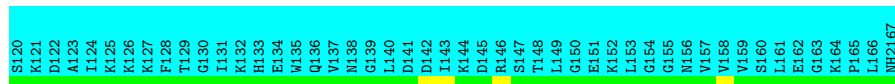
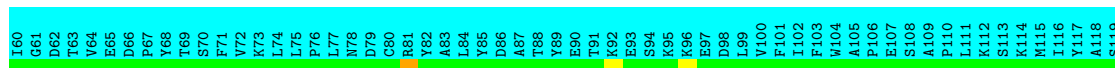
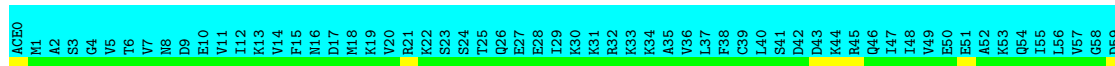


ACE0	I60	S120
M1	G61	K121
A2	D62	D122
S3	T63	A123
G4	V64	I124
V5	E65	K125
T6	D66	K126
V7	P67	K127
N8	F68	F128
D9	T69	T129
E10	S70	G130
V11	F71	I131
I12	W72	K132
K13	K73	H133
V14	L74	E134
F15	L75	W135
M16	P76	Q136
D17	L77	V137
M18	W78	M138
K19	D79	G139
V20	C80	L140
R21	R81	D141
K22	Y82	D142
S23	A83	I143
S24	L84	K144
T25	Y85	D145
Q26	D86	R146
E27	A87	S147
E28	T88	T148
I29	Y89	L149
K30	E90	G150
K31	T91	E151
R32	K92	K152
K33	E93	L153
K34	S94	G154
A35	K95	G155
V36	K96	N156
L37	E97	V157
F38	D98	V158
C39	L99	V159
L40	M100	S160
S41	F101	L161
D42	I102	E162
D43	F103	G163
K44	W104	K164
R45	A105	P165
Q46	P106	L166
I47	E107	E107
I48	S108	I48
V49	A109	V49
E50	F110	F110
E51	L111	L111
A52	K112	K112
K53	S113	K53
Q54	K114	K114
I55	M115	M115
L56	I116	I116
V57	Y117	Y117
G58	A118	A118
D59	S119	S119



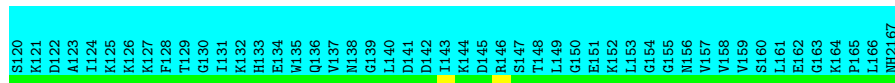
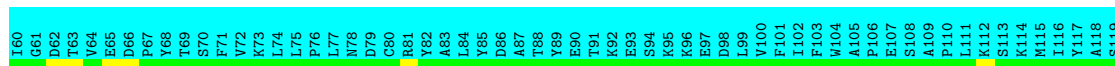
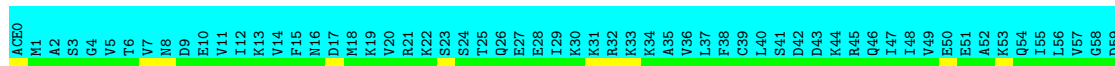
• Molecule 2: Cofilin-2

Chain N: 100%



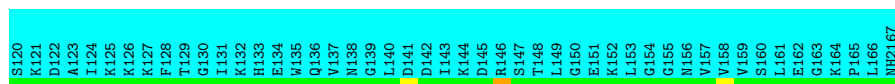
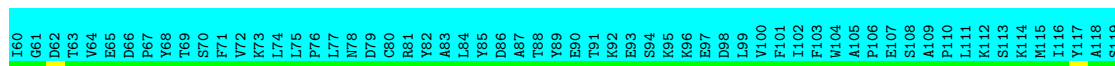
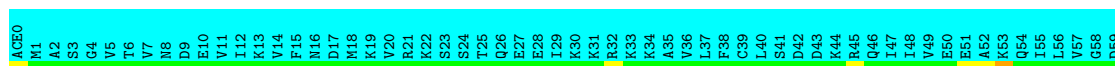
• Molecule 2: Cofilin-2

Chain O: 100%



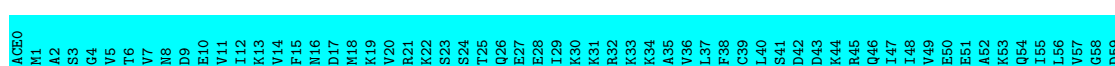
• Molecule 2: Cofilin-2

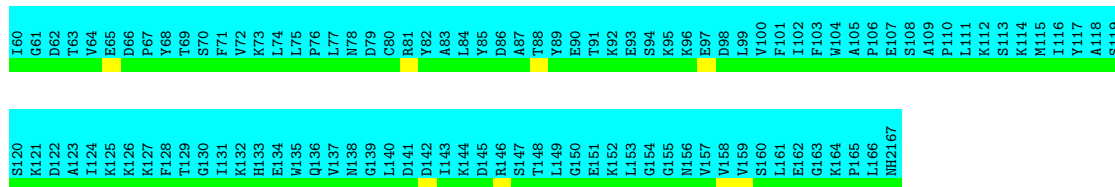
Chain P: 100%



• Molecule 2: Cofilin-2

Chain Q: 100%

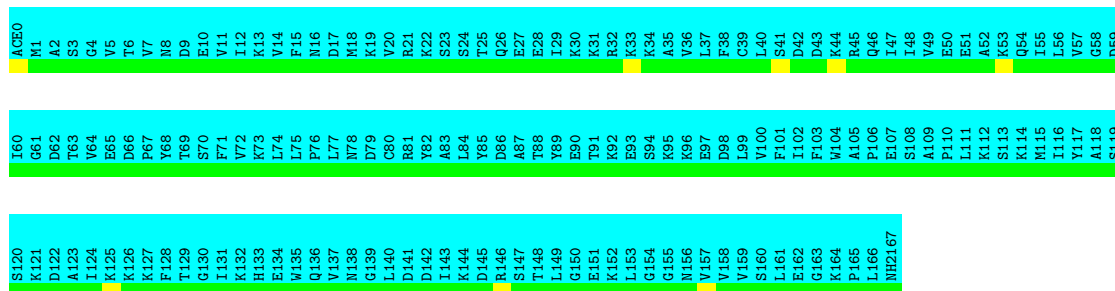




- Molecule 2: Cofilin-2

Chain R:

100%



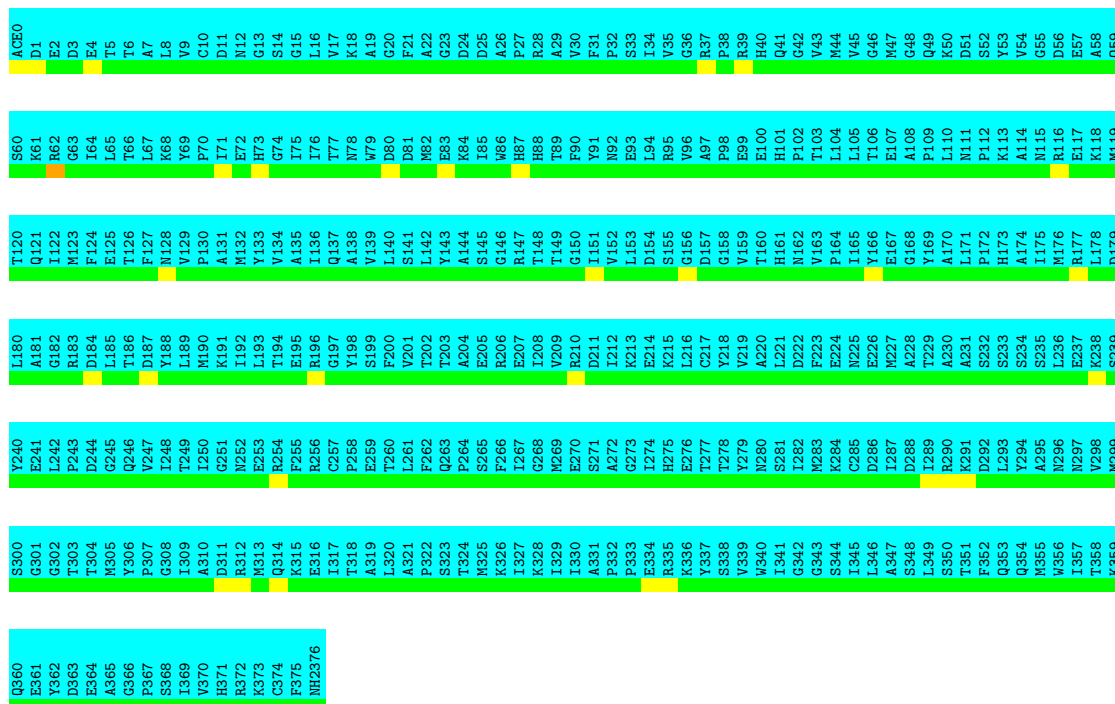
4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Actin, alpha skeletal muscle

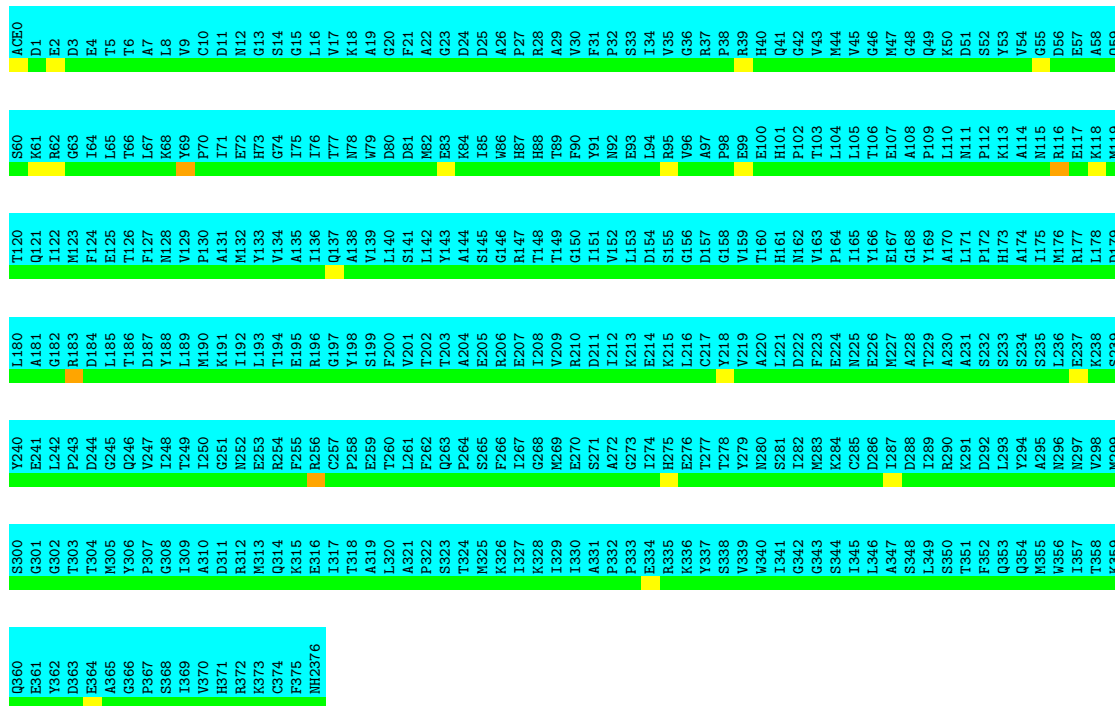
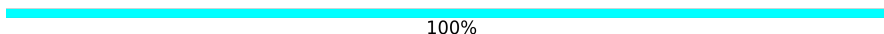
Chain A:

100%



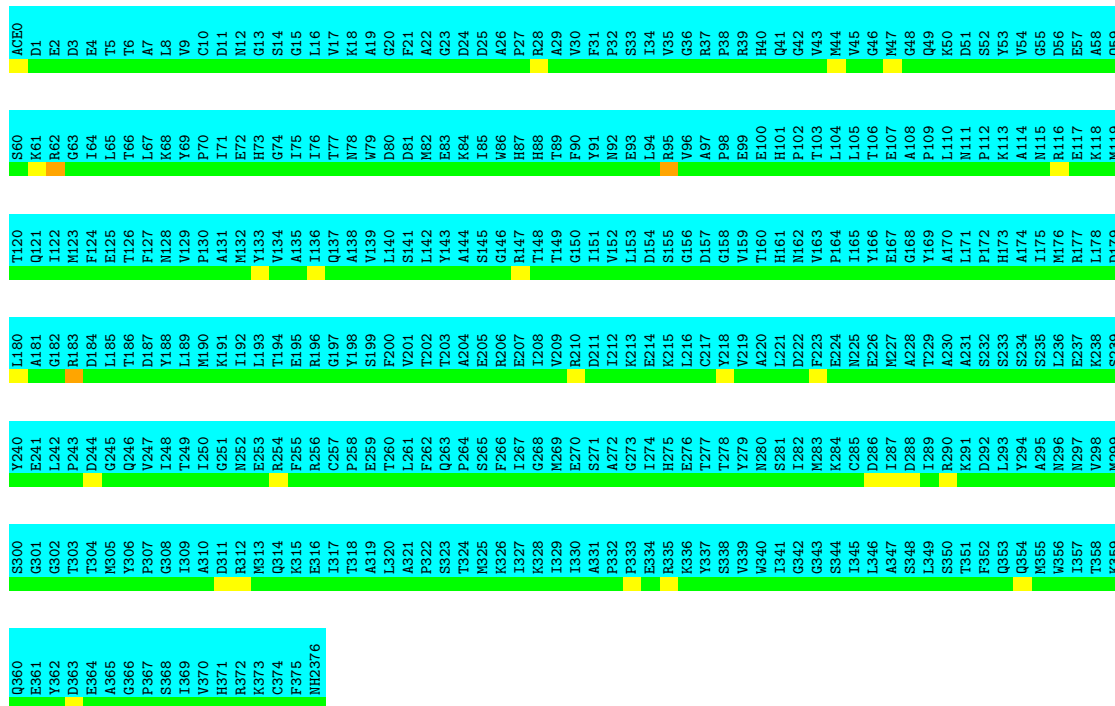
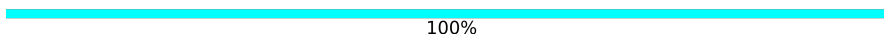
• Molecule 1: Actin, alpha skeletal muscle

Chain B:



• Molecule 1: Actin, alpha skeletal muscle

Chain C:



• Molecule 1: Actin, alpha skeletal muscle

Chain D:

100%

ACE0	D1	S60	L180	Y240	S300	Q360
E2	R61	E241	A181	E241	G301	E361
D3	R62	L242	G182	L242	G302	Y362
E4	G63	P243	R183	P243	T303	D363
T5	G64	D244	D184	D244	T304	E364
T6	L65	G245	L185	G245	M305	A365
A7	T66	Q246	M186	Q246	Y306	C366
L8	L67	V247	T187	V247	F307	P367
V9	K68	L248	Y188	L248	G308	S368
C10	P70	T249	L189	T249	I309	I369
D11	F71	I250	M190	I250	A310	V370
N12	I72	G251	K191	G251	D311	H371
G13	E73	M32	L192	M32	N312	R372
S14	H74	Y133	L193	E253	H313	K373
G15	G74	V134	T194	R254	Q314	C374
L16	I75	F255	I195	F255	K315	F375
V17	I76	R256	R196	R256	E316	NH2376
K18	T77	C257	G197	C257	I317	
A19	N78	P258	Y198	P258	T318	
G20	W79	E259	S199	E259	A319	
D21	D80	T260	L320	T260	L320	
A22	M82	L261	V201	L261	A321	
G23	E83	F262	T202	F262	P322	
D24	K84	Q263	T203	Q263	S323	
D25	L85	S265	A204	S265	T324	
A26	W86	F266	E205	F266	H325	
P27	H87	R207	R206	R207	K326	
R28	H88	G268	I208	G268	I327	
A29	T89	M269	V209	M269	K328	
V30	F90	E270	R210	E270	I329	
F31	Y91	S271	D211	S271	L330	
P32	N92	A272	L212	A272	A331	
S33	E93	G273	K213	G273	F333	
L34	L94	I274	E214	I274	E334	
V35	R95	H275	K215	H275	R335	
G36	V96	E276	L216	E276	K336	
R37	A97	T277	C217	T277	Y337	
P38	P98	T278	T218	T278	S338	
R39	E99	Y279	V219	Y279	V339	
H40	E100	N280	A220	N280	W340	
Q41	H101	I281	L221	I281	I341	
G42	H102	D222	D222	D222	G342	
V43	T103	M283	F223	M283	C343	
M44	L104	K284	E224	K284	S344	
G46	L105	C285	M225	C285	I345	
V47	T106	D286	E226	D286	L346	
M47	E107	I287	M227	I287	A347	
G48	A108	A228	A228	A228	S348	
Q49	P109	I289	T229	I289	L349	
K50	L110	R290	A230	R290	S350	
D51	M111	K291	T291	K291	T351	
S52	P112	D292	S232	D292	F352	
Y53	K113	L293	S233	L293	Q353	
V54	A114	Y294	S234	Y294	O354	
G55	I115	A295	M235	A295	K355	
D56	R116	N296	L236	N296	H356	
E57	L117	N297	E237	N297	I357	
A58	K118	V298	K238	V298	T358	
Q59	M119	M299	K359	M299	K359	

- Molecule 1: Actin, alpha skeletal muscle

Chain E:

100%

ACE0	D1	S60	L180	Y240	S300	Q360
E2	R61	E241	A181	E241	G301	E361
D3	G63	L242	G182	L242	G302	Y362
E4	G64	P243	R183	P243	T303	D363
T5	L65	D244	D184	D244	T304	E364
T6	L66	G245	L185	G245	M305	A365
A7	T66	Q246	M186	Q246	Y306	C366
L8	L67	V247	T187	V247	F307	P367
V9	K68	L248	Y188	L248	G308	S368
C10	P70	T249	L189	T249	I309	I369
D11	F71	I250	M190	I250	A310	V370
N12	I72	G251	K191	G251	D311	H371
G13	E73	M32	L192	M32	N312	R372
S14	H74	Y133	L193	E253	H313	K373
G15	G74	V134	T194	R254	Q314	C374
L16	I75	F255	I195	F255	K315	F375
V17	I76	R256	R196	R256	E316	NH2376
K18	T77	C257	G197	C257	I317	
A19	N78	P258	Y198	P258	T318	
G20	W79	E259	S199	E259	A319	
D21	D80	T260	L320	T260	L320	
A22	M82	L261	V201	L261	A321	
G23	E83	F262	T202	F262	P322	
D24	K84	Q263	T203	Q263	S323	
D25	L85	S265	A204	S265	T324	
A26	W86	F266	E205	F266	H325	
P27	H87	R207	R206	R207	K326	
R28	H88	G268	I208	G268	I327	
A29	T89	M269	V209	M269	K328	
V30	F90	E270	R210	E270	I329	
F31	Y91	S271	D211	S271	L330	
P32	N92	A272	L212	A272	A331	
S33	E93	G273	K213	G273	F333	
L34	L94	I274	E214	I274	E334	
V35	R95	H275	K215	H275	R335	
G36	V96	E276	L216	E276	K336	
R37	A97	T277	C217	T277	Y337	
P38	P98	T278	T218	T278	S338	
R39	E99	Y279	V219	Y279	V339	
H40	E100	N280	A220	N280	W340	
Q41	H101	I281	L221	I281	I341	
G42	H102	D222	D222	D222	G342	
V43	T103	M283	F223	M283	C343	
M44	L104	K284	E224	K284	S344	
G46	L105	C285	M225	C285	I345	
V47	T106	D286	E226	D286	L346	
M47	E107	I287	M227	I287	A347	
G48	A108	A228	A228	A228	S348	
Q49	P109	I289	T229	I289	L349	
K50	L110	R290	A230	R290	S350	
D51	M111	K291	T291	K291	T351	
S52	P112	D292	S232	D292	F352	
Y53	K113	L293	S233	L293	Q353	
V54	A114	Y294	S234	Y294	O354	
G55	I115	A295	M235	A295	K355	
D56	R116	N296	L236	N296	H356	
E57	L117	N297	E237	N297	I357	
A58	K118	V298	K238	V298	T358	
Q59	M119	M299	K359	M299	K359	

- Molecule 1: Actin, alpha skeletal muscle

Chain F:

100%

ACE0	D1	S60	T120	L180	Y240	S300	Q360
D1	A61	Q121	A181	E241	G301	Q361	E361
E2	R62	I122	G182	L242	G302	Y362	Y362
D3	G63	M123	R183	P243	T303	D363	D363
E4	P64	F124	D184	D244	T304	E364	E364
T5	L65	E125	L185	G245	M305	A365	A365
T6	T66	T126	T186	Q246	Y306	Y366	Y366
A7	L67	F127	D187	V247	F307	P367	P367
L8	K68	M128	L188	L248	G308	S368	S368
V9	V69	L129	L189	T249	I309	I369	I369
C10	P70	P130	M190	I250	A310	V370	V370
D11	I71	A131	K191	G251	D311	H371	H371
N12	E72	M132	K192	N252	R312	R372	R372
G13	H73	Y133	L193	E253	H313	K373	K373
G15	G74	V134	T194	R254	Q314	C374	C374
L16	I75	A135	I195	F255	K315	F375	F375
V17	I76	I136	R196	R256	E316	E376	E376
K18	T77	Q137	G197	C257	I317	T377	T377
A19	N78	A138	Y198	P258	T318	T378	T378
G20	W79	V139	S199	E259	A319	NH2376	NH2376
D21	D80	L140	F200	T260	L320		
F21	D81	S141	V201	L261	A321		
A22	M82	L142	T202	F262	P322		
G23	E83	Y143	T203	Q263	S323		
D24	K84	A144	A204	P264	T324		
D25	L85	S145	E205	S265	H325		
A26	W86	G146	R206	F266	K326		
P27	H87	L147	E207	L267	I327		
R28	H88	T148	M208	G268	K328		
A29	T89	T149	V209	M269	I329		
V30	F90	G150	E270	E270	L330		
F31	Y91	I151	S271	S271	A331		
P32	N92	V152	I212	A272	F332		
S33	E93	L153	K213	G273	P333		
L34	L94	D154	E214	I274	E334		
V35	R95	S155	K215	H275	R335		
G36	V96	G156	L216	E276	K336		
R37	A97	D157	C217	T277	Y337		
P38	P98	G158	Y218	T278	S338		
R39	E99	V159	V219	Y279	V339		
H40	E100	T160	A220	N280	W340		
Q41	H101	H161	L221	S281	I341		
G42	P102	M162	D222	I282	G342		
V43	T103	V163	F223	M283	C343		
M44	L104	P164	E224	K284	S344		
G46	L105	I165	M225	C285	I345		
M47	T106	E166	E226	I286	A347		
G48	E107	G168	M227	I288	S348		
Q49	A108	A169	A228	I289	L349		
K50	P109	L170	T229	R290	S350		
D51	M110	L171	A230	K291	T351		
S52	L111	P172	S232	D292	F352		
Y53	K113	H173	S233	L293	Q353		
V54	A114	A174	S234	Y294	Q354		
G55	M115	I175	S235	A295	K355		
D56	R116	M176	L236	N296	H356		
E57	L117	R177	E237	N297	I357		
A58	K118	L178	K238	V298	T358		
Q59	M119	D179	S239	M299	K359		

- Molecule 1: Actin, alpha skeletal muscle

Chain G:

100%

ACE0	D1	S60	T120	L180	Y240	S300	Q360
D1	A61	Q121	A181	E241	G301	Q361	E361
E2	R62	I122	G182	L242	G302	Y362	Y362
D3	G63	M123	R183	P243	T303	D363	D363
E4	P64	F124	D184	D244	T304	E364	E364
T5	L65	E125	L185	G245	M305	A365	A365
T6	T66	T126	T186	Q246	Y306	Y366	Y366
A7	L67	F127	D187	V247	F307	P367	P367
L8	K68	M128	L188	L248	G308	S368	S368
V9	V69	L129	L189	T249	I309	I369	I369
C10	P70	P130	M190	I250	A310	V370	V370
D11	I71	A131	K191	G251	D311	H371	H371
N12	E72	M132	K192	N252	R312	R372	R372
G13	H73	Y133	L193	E253	H313	K373	K373
G15	G74	V134	T194	R254	Q314	C374	C374
L16	I75	A135	I195	F255	K315	F375	F375
V17	I76	I136	R196	R256	E316	E376	E376
K18	T77	Q137	G197	C257	I317	T377	T377
A19	N78	A138	Y198	P258	T318	T378	T378
G20	W79	V139	S199	E259	A319	NH2376	NH2376
D21	D80	L140	F200	T260	L320		
F21	D81	S141	V201	L261	A321		
A22	M82	L142	T202	F262	P322		
G23	E83	Y143	T203	Q263	S323		
D24	K84	A144	A204	P264	T324		
D25	L85	S145	E205	S265	H325		
A26	W86	G146	R206	F266	K326		
P27	H87	L147	E207	L267	I327		
R28	H88	T148	M208	G268	K328		
A29	T89	T149	V209	M269	I329		
V30	F90	G150	E270	E270	L330		
F31	Y91	I151	S271	S271	A331		
P32	N92	V152	I212	A272	F332		
S33	E93	L153	K213	G273	P333		
L34	L94	D154	E214	I274	E334		
V35	R95	S155	K215	H275	R335		
G36	V96	G156	L216	E276	K336		
R37	A97	D157	C217	T277	Y337		
P38	P98	G158	Y218	T278	S338		
R39	E99	V159	V219	Y279	V339		
H40	E100	T160	A220	N280	W340		
Q41	H101	H161	L221	S281	I341		
G42	P102	M162	D222	I282	G342		
V43	T103	V163	F223	M283	C343		
M44	L104	P164	E224	K284	S344		
G46	L105	I165	M225	C285	I345		
M47	T106	E166	E226	I286	A347		
G48	E107	G168	M227	I288	S348		
Q49	A108	A169	A228	I289	L349		
K50	P109	L170	T229	R290	S350		
D51	M111	L171	A231	K291	T351		
S52	L112	P172	S232	D292	F352		
Y53	K113	H173	S233	L293	Q353		
V54	A114	A174	S234	Y294	Q354		
G55	M115	I175	S235	A295	K355		
D56	R116	M176	L236	N296	H356		
E57	L117	R177	E237	N297	I357		
A58	K118	L178	K238	V298	T358		
Q59	M119	D179	S239	M299	K359		

- Molecule 1: Actin, alpha skeletal muscle

Chain H:

100%

ACE0	D1	S60	T120	L180	Y240	S300	Q360
D1	A61	Q121	A181	G301	E241	G301	E361
E2	A62	I122	G182	G302	L242	G302	Y362
D3	G63	M123	R183	T303	P243	T303	D363
E4	A64	F124	D184	D304	D244	T304	E364
T5	L65	E125	L185	M305	G245	M305	A365
T6	T66	T126	T186	Y306	Q246	Y306	C366
A7	L67	F127	D187	F307	L247	F307	P367
L8	K68	M128	L188	G308	I248	G308	S368
V9	P69	V129	L189	I309	T249	I309	I369
C10	P70	P130	M190	A310	I250	A310	V370
D11	I71	A131	K191	D311	G251	D311	H371
M12	E72	M132	L192	R312	N252	R312	R372
G13	H73	Y133	L193	H313	E253	H313	K373
S14	G74	V134	I194	K314	R254	K314	C374
G15	I75	A135	E195	Q315	F255	Q315	F375
L16	I76	I136	R196	E316	R256	E316	NH2376
V17	T77	Q137	G197	I317	C257	I317	
K18	N78	A138	Y198	T318	P258	T318	
A19	W79	V139	S199	A319	E259	A319	
G20	D80	L140	F200	L320	T260	L320	
F21	D81	S141	W201	A321	L261	A321	
A22	M82	L142	T202	P322	F262	P322	
G23	E83	Y143	T203	S323	Q263	S323	
D24	K84	A144	A204	T324	P264	T324	
D25	L85	S145	E205	H325	S265	H325	
A26	W86	G146	R206	K326	F266	K326	
P27	H87	R147	E207	I327	L267	I327	
R28	H88	T148	I208	K328	G268	K328	
A29	T89	T149	V209	I329	M269	I329	
V30	F90	G150	R210	L330	E270	L330	
F31	Y91	I151	D211	A331	S271	A331	
P32	N92	V152	L212	F332	A272	F332	
S33	E93	L153	K213	P333	G273	P333	
I34	L94	D154	E214	E334	I274	E334	
V35	R95	S155	R215	R335	H275	R335	
G36	V96	G156	L216	K336	E276	K336	
R37	A97	D157	C217	Y337	T277	Y337	
P38	P98	G158	T218	S338	T278	S338	
R39	E99	V159	V219	V339	Y279	V339	
H40	E100	H160	A220	W340	N280	W340	
Q41	H101	H161	L221	I341	S281	I341	
G42	H102	M162	D222	G342	I282	G342	
V43	T103	V163	F223	C343	M283	C343	
M44	L104	P164	E224	S344	K284	S344	
G46	L105	I165	N225	I345	C285	I345	
M47	T106	Y166	E226	L346	D286	L346	
G48	E107	E167	M227	A347	I287	A347	
O49	A108	G168	A228	S348	D288	S348	
K50	P109	Y169	T229	L349	I289	L349	
D51	L110	A170	A230	S350	R290	S350	
S52	L111	K291	A231	T351	K291	T351	
H53	P112	P172	S232	F352	D292	F352	
V54	K113	H173	S233	Q353	L293	Q353	
G55	A114	A174	S234	O354	Y294	O354	
D56	M115	I175	A235	H355	A295	H355	
E57	R116	M176	L236	H356	N296	H356	
A58	L118	L178	E237	I357	N297	I357	
Q59	M119	D179	S239	K359	M299	K359	

- Molecule 1: Actin, alpha skeletal muscle

Chain I:

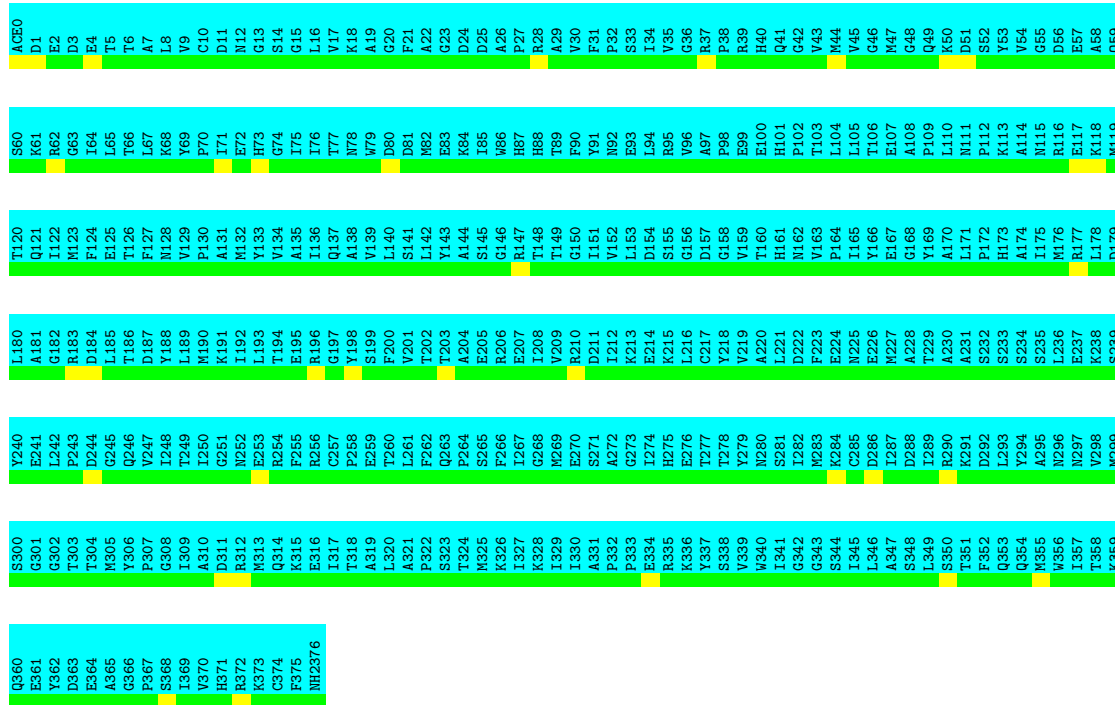
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ACE0	D1	S60	T120	L180	Y240	S300	Q360
D1	A61	Q121	A181	G301	E241	G301	E361
E2	A62	I122	G182	G302	L242	G302	Y362
D3	G63	M123	R183	T303	P243	T303	D363
E4	A64	F124	D184	D304	D244	T304	E364
T5	L65	E125	L185	M305	G245	M305	A365
T6	T66	T126	T186	Y306	Q246	Y306	C366
A7	L67	F127	D187	F307	L247	F307	P367
L8	K68	M128	L188	G308	I248	G308	S368
V9	P69	V129	L189	I309	T249	I309	I369
C10	P70	P130	M190	A310	I250	A310	V370
D11	I71	A131	K191	D311	G251	D311	H371
M12	E72	M132	L192	R312	N252	R312	R372
G13	H73	Y133	L193	H313	E253	H313	K373
S14	G74	V134	I194	K314	R254	K314	C374
G15	I75	A135	E195	Q315	F255	Q315	F375
L16	I76	I136	R196	E316	R256	E316	NH2376
V17	T77	Q137	G197	I317	C257	I317	
K18	N78	A138	Y198	T318	P258	T318	
A19	W79	V139	S199	A319	E259	A319	
G20	D80	L140	F200	L320	T260	L320	
F21	D81	S141	W201	A321	L261	A321	
A22	M82	L142	T202	P322	F262	P322	
G23	E83	Y143	T203	S323	Q263	S323	
D24	K84	A144	A204	T324	P264	T324	
D25	L85	S145	E205	H325	S265	H325	
A26	W86	G146	R206	K326	F266	K326	
P27	H87	R147	E207	I327	L267	I327	
R28	H88	T148	I208	K328	G268	K328	
A29	T89	T149	V209	I329	M269	I329	
V30	F90	G150	R210	L330	E270	L330	
F31	Y91	I151	D211	A331	S271	A331	
P32	N92	V152	L212	F332	A272	F332	
S33	E93	L153	K213	P333	G273	P333	
I34	L94	D154	E214	E334	I274	E334	
V35	R95	S155	R215	R335	H275	R335	
G36	V96	G156	L216	K336	E276	K336	
R37	A97	D157	C217	Y337	T277	Y337	
P38	P98	G158	T218	S338	T278	S338	
R39	E99	V159	V219	V339	Y279	V339	
H40	E100	H160	A220	W340	N280	W340	
Q41	H101	H161	L221	I341	S281	I341	
G42	H102	M162	D222	G342	I282	G342	
V43	T103	V163	F223	C343	M283	C343	
M44	L104	P164	E224	S344	K284	S344	
G46	L105	I165	N225	I345	C285	I345	
M47	T106	Y166	E226	L346	D286	L346	
G48	E107	E167	M227	A347	I287	A347	
O49	A108	G168	A228	S348	D288	S348	
K50	P109	Y169	T229	L349	I289	L349	
D51	L110	A170	A230	S350	R290	S350	
S52	L111	K291	A231	T351	K291	T351	
H53	P112	P172	S232	F352	D292	F352	
V54	K113	H173	S233	Q353	L293	Q353	
G55	A114	A174	S234	O354	Y294	O354	
D56	M115	I175	A235	H355	A295	H355	
E57	R116	M176	L236	H356	N296	H356	
A58	L118	L178	E237	I357	N297	I357	
Q59	M119	D179	S239	K359	M299	K359	

- Molecule 1: Actin, alpha skeletal muscle

Chain J:

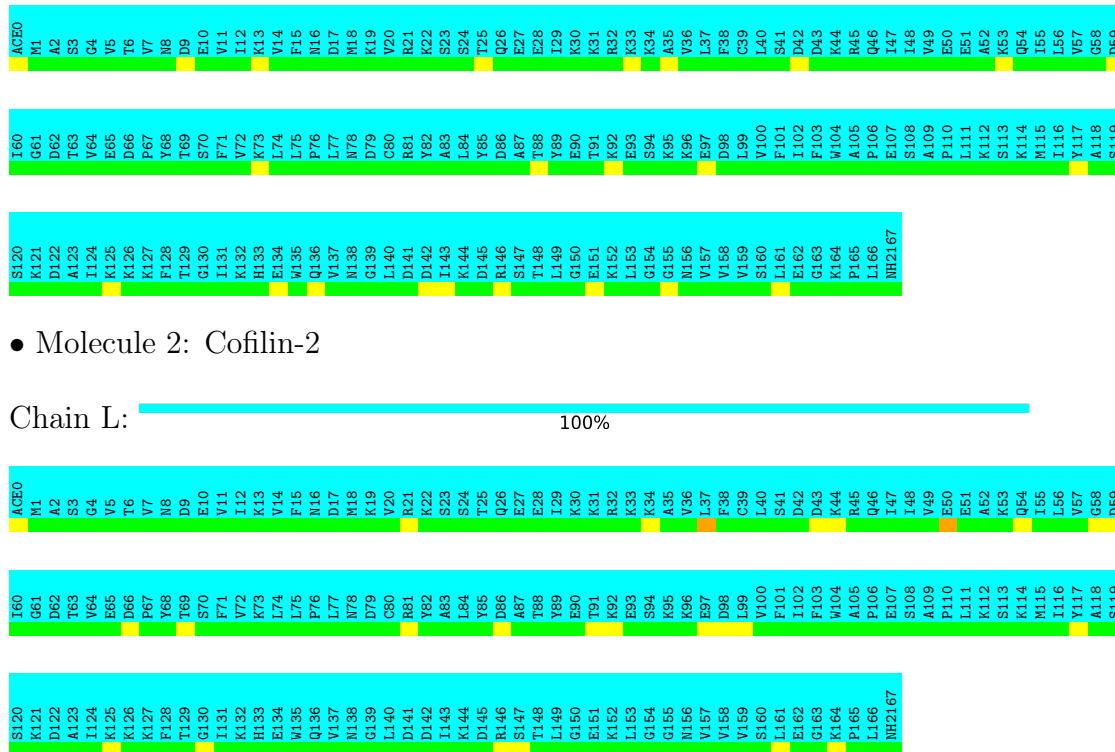
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• Molecule 2: Cofilin-2

Chain K:

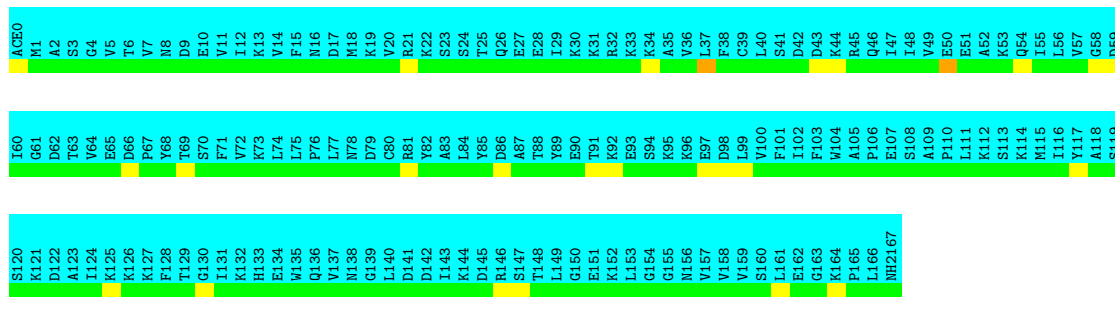
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• Molecule 2: Cofilin-2

Chain L:

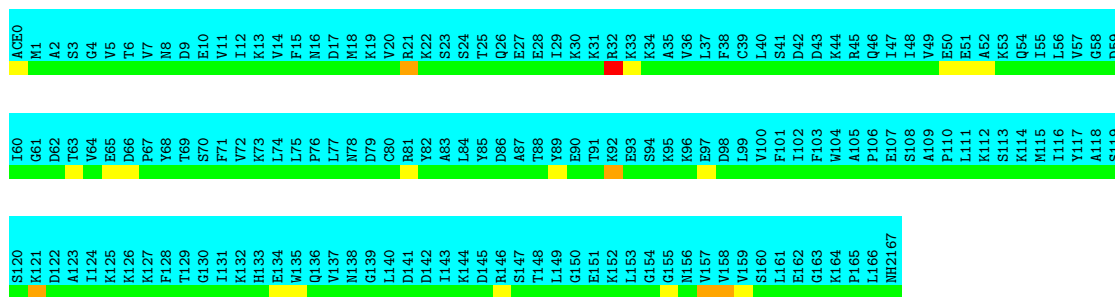
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• Molecule 2: Cofilin-2

Chain M:

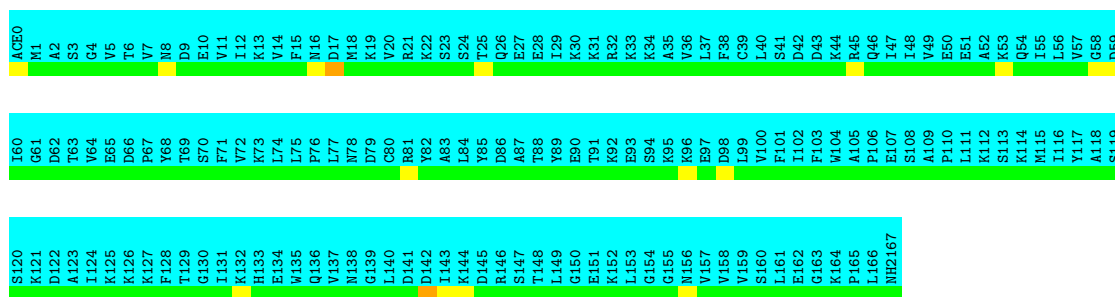
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• Molecule 2: Cofilin-2

Chain N:

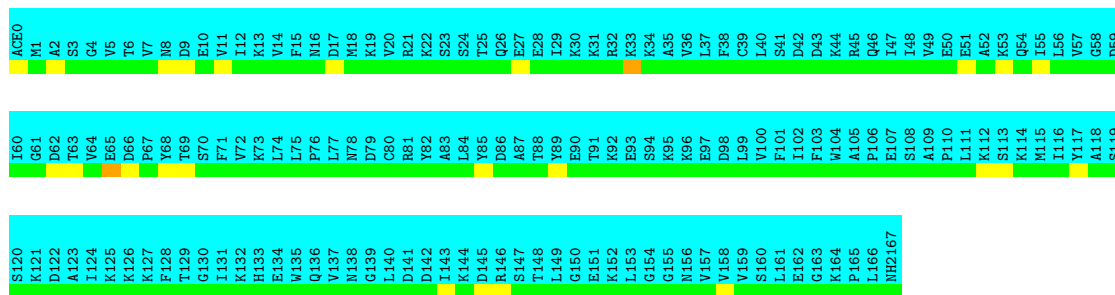
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• Molecule 2: Cofilin-2

Chain O:

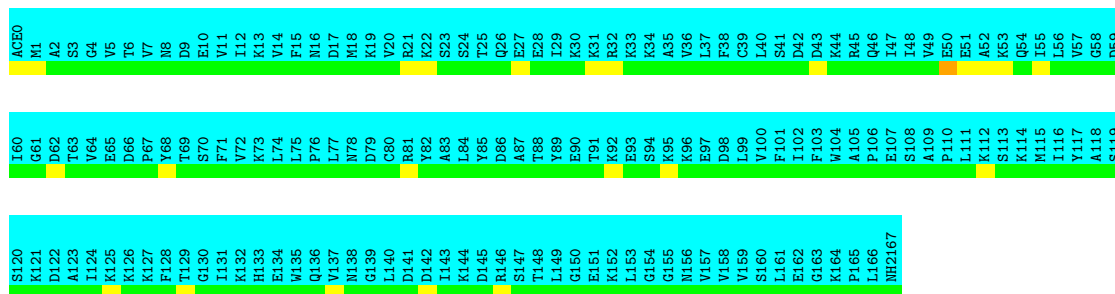
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• Molecule 2: Cofilin-2

Chain P:

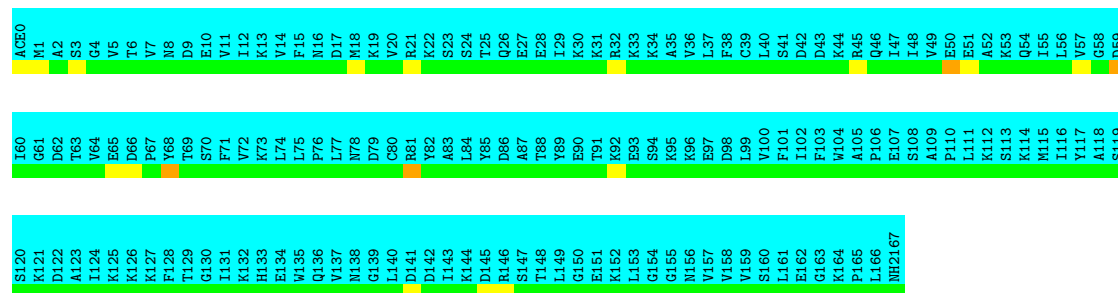
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- Molecule 2: Cofilin-2

Chain Q:

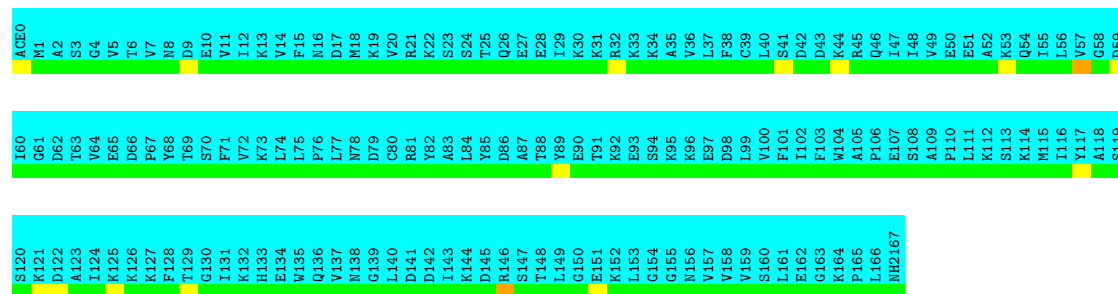
100%



- Molecule 2: Cofilin-2

Chain R:

100%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 4 calculated structures, 4 were deposited, based on the following criterion: *all calculated structures submitted*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
TALOS-N	structure calculation	
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	
NAMD	refinement	

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	C	0	0	0	0±0
1	G	0	0	0	0±0
1	H	0	0	0	0±0
1	I	0	0	0	0±0
1	J	0	0	0	0±0
1	A	0	0	0	0±0
1	D	0	0	0	0±0
1	E	0	0	0	0±0
1	F	0	0	0	0±0
1	B	0	0	0	0±0
2	K	0	0	0	0±0
2	M	0	0	0	0±0
2	O	0	0	0	0±0
2	P	0	0	0	0±0
2	Q	0	0	0	0±0
2	L	0	0	0	0±0
2	N	0	0	0	0±0
2	R	0	0	0	0±0
All	All	0	0	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 -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 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 NMR 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	0	-	-	-	-
1	B	0	-	-	-	-
1	C	0	-	-	-	-
1	D	0	-	-	-	-
1	E	0	-	-	-	-
1	F	0	-	-	-	-
1	G	0	-	-	-	-
1	H	0	-	-	-	-
1	I	0	-	-	-	-
1	J	0	-	-	-	-
2	K	0	-	-	-	-
2	L	0	-	-	-	-
2	M	0	-	-	-	-
2	N	0	-	-	-	-
2	O	0	-	-	-	-
2	P	0	-	-	-	-
2	Q	0	-	-	-	-
2	R	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 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 NMR 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	0	-	-	-
1	B	0	-	-	-
1	C	0	-	-	-
1	D	0	-	-	-
1	E	0	-	-	-
1	F	0	-	-	-
1	G	0	-	-	-
1	H	0	-	-	-
1	I	0	-	-	-
1	J	0	-	-	-
2	K	0	-	-	-
2	L	0	-	-	-
2	M	0	-	-	-
2	N	0	-	-	-
2	O	0	-	-	-
2	P	0	-	-	-
2	Q	0	-	-	-
2	R	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.