



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 29, 2026 – 10:31 AM UTC

PDB ID : 7U8K / pdb_00007u8k
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

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

1 Overall quality at a glance ⓘ

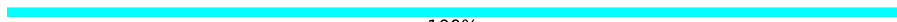
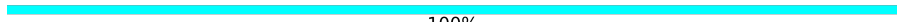
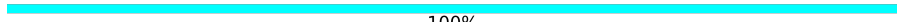
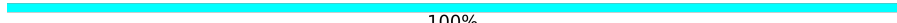
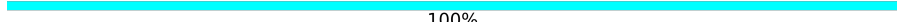
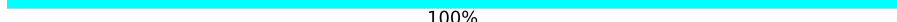
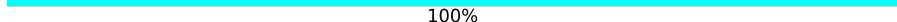
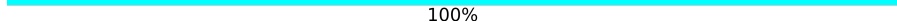
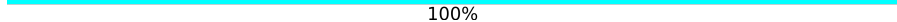
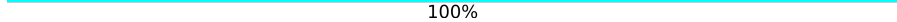
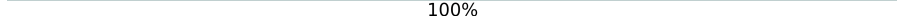
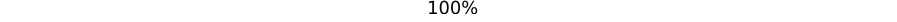
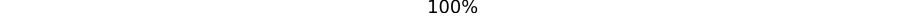
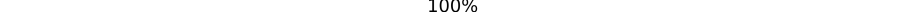
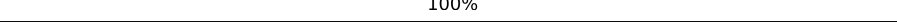
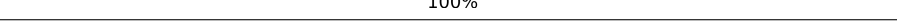
The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment was not calculated.

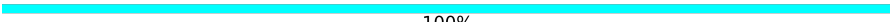
There are no overall percentile quality scores available for this entry.

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

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

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

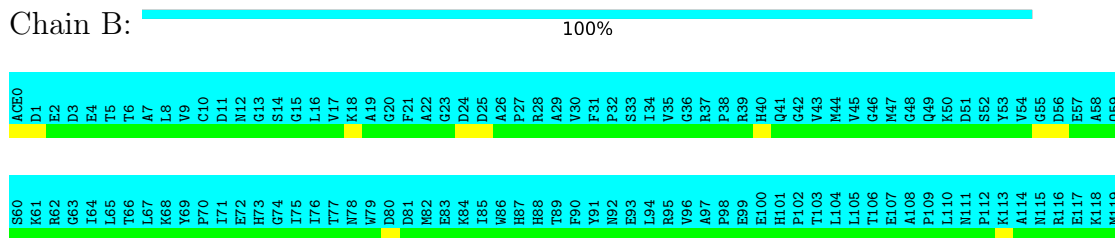
4.1 Average score per residue in the NMR ensemble

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



- Molecule 1: Actin, alpha skeletal muscle



T120	Q121	A181	L180	Y240	S300	Q360
I122	G182	E2	E361	E241	G301	E361
R123	G183	R62	Y362	L242	G302	Y362
F124	R184	T03	D363	P243	T303	D363
G125	L185	I64	E364	D244	T304	E364
T126	L186	T5	A365	G245	M305	A365
F127	D187	T6	G366	Q246	Y306	G366
L128	D188	A7	P367	V247	P307	P367
L129	L189	K8	S368	K248	G308	S368
P130	M190	Y9	I369	T249	I309	I369
A131	K191	C10	V370	L250	A310	V370
I132	L192	D11	H371	G251	D311	H371
Y133	L193	M12	R372	W252	R312	R372
V134	T194	G13	K373	E253	M313	K373
A135	E195	S14	C374	R254	Q314	C374
R136	E196	G15	F375	F255	K315	F375
Q137	R197	L16	NH2376	R256	E316	E316
A138	Y198	V17		C257	I317	I317
V139	S199	K18		P258	T318	T318
F200	F200	A19		E259	A319	A319
L140	L140	G20		L260	L320	L320
V201	S141	F21		L261	A321	A321
T202	T202	M82		F262	P322	P322
L142	T202	M82		G263	S323	S323
Y143	T203	E83		Q264	T324	T324
A204	A204	K84		P265	M325	M325
S145	E205	I85		S266	K326	K326
R206	R206	H87		F267	K328	K328
G146	E207	H88		G268	I329	I329
R147	E207	T89		V269	F330	F330
L148	I208	F90		E270	A331	A331
T149	V209	Y91		S271	P332	P332
R210	R210	N92		A272	S333	S333
G150	G150	E93		G273	E334	E334
I151	I151	L94		I274	K335	K335
V152	V152	V35		H275	K336	K336
K215	S155	G36		E276	Y337	Y337
L216	L216	R37		T277	S338	S338
D157	D157	P98		T278	V339	V339
G158	G158	E99		Y279	W340	W340
V219	V219	H101		N280	G342	G342
A220	A220	L221		S281	I341	I341
H161	H161	P102		L282	G343	G343
L221	L221	V43		W283	S344	S344
D222	D222	L104		K284	I345	I345
V163	V163	T106		C285	L346	L346
P164	P164	E107		D286	A347	A347
N225	N225	G168		D288	S348	S348
I165	I165	A228		T289	L349	L349
E166	E166	T229		K290	S350	S350
Y167	Y167	A230		R291	T351	T351
G168	G168	P172		D292	F352	F352
A170	A170	H173		L293	Q353	Q353
L171	L171	S233		L294	K354	K354
P172	P172	S234		A295	M355	M355
H173	H173	L236		N296	W356	W356
S233	S233	E237		N297	I357	I357
S234	S234	L178		V298	T358	T358
A175	A175	S239		M299	K359	K359
S235	S235					
L176	L176					
M176	M176					
R177	R177					
E237	E237					
L236	L236					
S237	S237					
L178	L178					
K238	K238					
S239	S239					

• Molecule 1: Actin, alpha skeletal muscle

Chain C:

100%

ACE0	D1	S60	L180	Y240	S300	Q360
E2	E2	K61	A181	E241	G301	E361
D3	D3	R62	I182	L242	G302	Y362
E4	E4	G63	R183	P243	T303	D363
T5	T5	I64	D184	D244	T304	E364
T6	T6	L65	L185	G245	M305	A365
A7	A7	T66	T186	Q246	Y306	G366
L8	L8	L67	D187	V247	P307	P367
Y9	Y9	K68	L188	K248	G308	S368
C10	C10	Y69	L189	T249	I309	I369
D11	D11	C10	M190	L250	A310	V370
M12	M12	D11	A131	G251	D311	H371
G13	G13	I71	I191	W252	R312	R372
S14	S14	E72	L192	E253	M313	K373
G15	G15	H73	L193	R254	Q314	C374
L16	L16	G74	T194	F255	K315	F375
V17	V17	I75	E195	R256	E316	E316
K18	K18	I76	E196	C257	I317	I317
A19	A19	T77	G197	P258	T318	T318
G20	G20	N78	Y198	E259	A319	A319
F21	F21	W79	S199	L260	L320	L320
A22	A22	D80	F200	L261	A321	A321
Q23	Q23	M82	V201	F262	P322	P322
E83	E83	M82	S141	G263	S323	S323
D24	D24	K84	L142	Q264	T324	T324
D25	D25	I85	Y143	P265	M325	M325
A26	A26	H86	E205	S266	K326	K326
P27	P27	H87	R206	F267	K328	K328
R28	R28	H88	E207	G268	I329	I329
T89	T89	T89	V209	V269	F330	F330
F90	F90	F90	E270	E270	A331	A331
F31	F31	Y91	S271	S271	P332	P332
P32	P32	N92	A272	A272	S333	S333
E93	E93	E93	G273	G273	E334	E334
I34	I34	L94	I274	I274	K335	K335
V35	V35	V35	H275	H275	K336	K336
G36	G36	V96	E276	E276	Y337	Y337
R37	R37	A87	T277	T277	S338	S338
P38	P38	P98	T278	T278	V339	V339
R39	R39	E99	Y279	Y279	W340	W340
H40	H40	E100	N280	N280	G342	G342
Q41	Q41	H101	S281	S281	I341	I341
G42	G42	P102	L282	L282	G343	G343
V43	V43	V43	W283	W283	S344	S344
M44	M44	L104	K284	K284	I345	I345
V45	V45	T106	C285	C285	L346	L346
G46	G46	E107	D286	D286	A347	A347
M47	M47	G168	D288	D288	S348	S348
G48	G48	A228	T289	T289	L349	L349
Q49	Q49	K290	R290	R290	S350	S350
K50	K50	D291	D291	D291	T351	T351
D51	D51	P172	S232	S232	F352	F352
S52	S52	H173	L293	L293	Q353	Q353
Y53	Y53	S233	L294	L294	K354	K354
V54	V54	A174	A295	A295	M355	M355
G55	G55	N115	N296	N296	W356	W356
D56	D56	R116	N297	N297	I357	I357
E57	E57	E117	V298	V298	T358	T358
A58	A58	K118	M299	M299	K359	K359
Q59	Q59	M119				

• Molecule 1: Actin, alpha skeletal muscle

Chain D:

100%

ACE0	D1	S60	L180	Y240	S300	Q360
E2	E2	K61	A181	E241	G301	E361
D3	D3	R62	I182	L242	G302	Y362
E4	E4	G63	R183	P243	T303	D363
T5	T5	I64	D184	D244	T304	E364
T6	T6	L65	L185	G245	M305	A365
A7	A7	T66	T186	Q246	Y306	G366
L8	L8	L67	D187	V247	P307	P367
Y9	Y9	K68	L188	K248	G308	S368
C10	C10	Y69	L189	T249	I309	I369
D11	D11	C10	M190	L250	A310	V370
M12	M12	D11	A131	G251	D311	H371
G13	G13	I71	I191	W252	R312	R372
S14	S14	E72	L192	E253	M313	K373
G15	G15	H73	L193	R254	Q314	C374
L16	L16	G74	T194	F255	K315	F375
V17	V17	I75	E195	R256	E316	E316
K18	K18	I76	E196	C257	I317	I317
A19	A19	T77	G197	P258	T318	T318
G20	G20	N78	Y198	E259	A319	A319
F21	F21	W79	S199	L260	L320	L320
A22	A22	D80	F200	L261	A321	A321
Q23	Q23	M82	V201	F262	P322	P322
E83	E83	M82	S141	G263	S323	S323
D24	D24	K84	L142	Q264	T324	T324
D25	D25	I85	Y143	P265	M325	M325
A26	A26	H86	E205	S266	K326	K326
P27	P27	H87	R206	F267	K328	K328
R28	R28	H88	E207	G268	I329	I329
T89	T89	T89	V209	V269	F330	F330
F90	F90	F90	E270	E270	A331	A331
F31	F31	Y91	S271	S271	P332	P332
P32	P32	N92	A272	A272	S333	S333
E93	E93	E93	G273	G273	E334	E334
I34	I34	L94	I274	I274	K335	K335
V35	V35	V35	H275	H275	K336	K336
G36	G36	V96	E276	E276	Y337	Y337
R37	R37	A87	T277	T277	S338	S338
P38	P38	P98	T278	T278	V339	V339
R39	R39	E99	Y279	Y279	W340	W340
H40	H40	E100	N280	N280	G342	G342
Q41	Q41	H101	S281	S281	I341	I341
G42	G42	P102	L282	L282	G343	G343
V43	V43	V43	W283	W283	S344	S344
M44	M44	L104	K284	K284	I345	I345
V45	V45	T106	C285	C285	L346	L346
G46	G46	E107	D286	D286	A347	A347
M47	M47	G168	D288	D288	S348	S348
G48	G48	A228	T289	T289	L349	L349
Q49	Q49	K290	R290	R290	S350	S350
K50	K50	D291	D291	D291	T351	T351
D51	D51	P172	S232	S232	F352	F352
S52	S52	H173	L293	L293	Q353	Q353
Y53	Y53	S233	L294	L294	K354	K354
V54	V54	A174	A295	A295	M355	M355
G55	G55	N115	N296	N296	W356	W356
D56	D56	R116	N297	N297	I357	I357
E57	E57	E117	V298	V298	T358	T358
A58	A58	K118	M299	M299	K359	K359
Q59	Q59	M119				

T120	Q121	A181	E240	S300	Q360
I122	G182	E241	G301	E361	E361
F123	R183	L242	G302	Y362	Y362
F124	R184	P243	T303	D363	D363
E125	L185	D244	T304	E364	E364
T126	L186	G245	M305	A365	A365
F127	D187	Q246	Y306	G366	G366
I128	Y188	V247	P307	S367	P367
L129	L189	L248	G308	S368	S368
P130	M190	T249	I309	I369	I369
A131	K191	G251	A310	V370	V370
I132	L192	N252	D311	H371	H371
Y133	L193	E253	M313	R372	R372
L134	T194	R254	Q314	K373	K373
A135	E195	F255	G315	C374	C374
I136	R196	R256	E316	F375	F375
Q137	G197	C257	I317	NH2376	NH2376
A138	Y198	P258	T318		
V139	S199	E259	A319		
L140	F200	L260	L320		
S141	V201	L261	D81		
L142	T202	F262	A22		
Y143	T203	Q263	E83		
A144	A204	P264	D24		
S145	E205	S265	D25		
R146	R206	F266	A26		
R147	E207	L267	H87		
L148	I208	G268	H88		
T149	V209	M269	T89		
R210	R210	E270	F30		
D211	D211	S271	F31		
V152	I212	A272	N92		
L153	K213	G273	E93		
D154	E214	I274	L94		
S155	K215	H275	V95		
G156	L216	E276	V96		
D157	C217	T277	A97		
G158	Y218	T278	P98		
V159	V219	Y279	E99		
T160	A220	N280	H40		
H161	L221	S281	H101		
N162	D222	I282	P102		
V163	F223	W283	V43		
P164	E224	K284	L104		
N165	N225	C285	V45		
E166	E226	D286	T106		
E167	M227	I287	E107		
G168	A228	D288	A108		
Y169	T229	I289	P109		
A170	A230	K290	L110		
L171	A231	R291	M111		
P172	S232	D292	P112		
H173	S233	L293	K113		
S234	S234	Y294	A114		
A175	S235	A295	N115		
L176	L236	N296	R116		
R177	E237	N297	E117		
L178	K238	V298	K118		
D179	S239	M299	M119		

• Molecule 1: Actin, alpha skeletal muscle

Chain E:

100%

ACE0	D1	S60	K61	T120	L180	Y240	S300	Q360
E2	E2	K62	L242	Q121	A181	E241	G301	E361
D3	D3	G63	L243	I122	G182	L242	G302	Y362
E4	E4	I64	I64	M123	R183	P243	T303	D363
T5	T5	L65	T66	E124	D184	G244	T304	E364
T6	T6	G66	T66	E125	L185	G245	M305	A365
A7	A7	L67	L67	T126	T186	Q246	Y306	G366
L8	L8	K68	K68	F127	D187	V247	P307	S367
V9	V9	Y69	Y69	M128	Y188	L248	G308	S368
C10	C10	P70	P70	T249	L189	T249	I309	I369
D11	D11	I71	I71	M190	M190	G250	A310	V370
M12	M12	E72	E72	P130	K191	G251	D311	H371
G13	G13	H73	H73	A131	L192	N252	R312	R372
S14	S14	G74	G74	Y133	L193	E253	M313	K373
G15	G15	I75	I75	V134	T194	R254	Q314	C374
L16	L16	I76	I76	A135	E195	F255	G315	F375
V17	V17	T77	T77	R196	R196	R256	E316	NH2376
K18	K18	N78	N78	Q137	G197	C257	I317	
A19	A19	W79	W79	T148	Y198	P258	T318	
G20	G20	D80	D80	A138	S199	E259	A319	
F21	F21	L81	L81	V139	F200	L260	L320	
A22	A22	M82	M82	I140	V201	L261	D81	
E23	E23	E83	E83	S141	T202	F262	A22	
D24	D24	K84	K84	L142	T203	Q263	E83	
D25	D25	I85	I85	Y143	A204	P264	D24	
A26	A26	W86	W86	A144	E205	S265	M255	
P27	P27	H87	H87	S145	R206	F266	K326	
R28	R28	H88	H88	G146	E207	L267	L327	
A29	A29	T89	T89	R147	I208	G268	K328	
V30	V30	F90	F90	T149	V209	M269	I329	
F31	F31	Y91	Y91	G150	R210	E270	I330	
P32	P32	N92	N92	D211	R210	S271	A331	
S33	S33	E93	E93	V152	D211	A272	P332	
I34	I34	L94	L94	L153	I152	G273	P333	
V35	V35	R95	R95	D154	K213	I274	E334	
G36	G36	V96	V96	S155	K215	H275	K335	
R37	R37	A97	A97	G156	L216	E276	K336	
P38	P38	P98	P98	D157	C217	T277	Y337	
R39	R39	E99	E99	G158	Y218	T278	S338	
H40	H40	E100	E100	V159	Y219	Y279	V339	
Q41	Q41	H101	H101	T160	V219	N280	W340	
G42	G42	P102	P102	L221	A220	S281	I341	
V43	V43	V43	V43	H161	L221	I282	G342	
M44	M44	L104	L104	N162	D222	I282	G343	
V45	V45	V45	V45	F223	F223	W283	G344	
G46	G46	T106	T106	E224	E224	K284	S344	
E107	E107	E107	E107	N225	N225	C285	I345	
G168	G168	A108	A108	E226	E226	D286	L346	
P109	P109	P109	P109	E167	E167	I287	A347	
K50	K50	L110	L110	M227	M227	D288	S348	
D51	D51	M111	M111	A228	A228	I289	L349	
S52	S52	P112	P112	T229	T229	K290	S350	
Y53	Y53	K113	K113	A230	A230	R291	T351	
A114	A114	A114	A114	L171	L171	D292	F352	
G55	G55	N115	N115	P172	P172	S232	P352	
D56	D56	R116	R116	H173	H173	S233	Q353	
E57	E57	E117	E117	S234	S234	A174	Q354	
A58	A58	K118	K118	L175	L175	A295	M355	
O59	O59	M119	M119	L236	L236	N296	W356	
				E237	E237	N297	I357	
				L178	L178	V298	T358	
				S239	S239	M299	K359	

• Molecule 1: Actin, alpha skeletal muscle

Chain F:

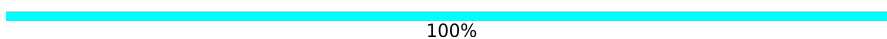
100%

ACE0	D1	S60	K61	T120	L180	Y240	S300	Q360
E2	E2	K62	L242	Q121	A181	E241	G301	E361
D3	D3	G63	L243	I122	G182	L242	G302	Y362
E4	E4	I64	I64	M123	R183	P243	T303	D363
T5	T5	L65	T66	E124	D184	G244	T304	E364
T6	T6	G66	T66	E125	L185	G245	M305	A365
A7	A7	L67	L67	T126	T186	Q246	Y306	G366
L8	L8	K68	K68	F127	D187	V247	P307	S367
V9	V9	Y69	Y69	M128	Y188	L248	G308	S368
C10	C10	P70	P70	T249	L189	T249	I309	I369
D11	D11	I71	I71	M190	M190	G250	A310	V370
M12	M12	E72	E72	P130	K191	G251	D311	H371
G13	G13	H73	H73	A131	L192	N252	R312	R372
S14	S14	G74	G74	Y133	L193	E253	M313	K373
G15	G15	I75	I75	V134	T194	R254	Q314	C374
L16	L16	I76	I76	A135	E195	F255	G315	F375
V17	V17	T77	T77	R196	R196	R256	E316	NH2376
K18	K18	N78	N78	Q137	G197	C257	I317	
A19	A19	W79	W79	T148	Y198	P258	T318	
G20	G20	D80	D80	A138	S199	E259	A319	
F21	F21	L81	L81	V139	F200	L260	L320	
A22	A22	M82	M82	I140	V201	L261	D81	
E23	E23	E83	E83	S141	T202	F262	A22	
D24	D24	K84	K84	L142	T203	Q263	E83	
D25	D25	I85	I85	Y143	A204	P264	D24	
A26	A26	W86	W86	A144	E205	S265	M255	
P27	P27	H87	H87	S145	R206	F266	K326	
R28	R28	H88	H88	G146	E207	L267	L327	
A29	A29	T89	T89	R147	I208	G268	K328	
V30	V30	F90	F90	T149	V209	M269	I329	
F31	F31	Y91	Y91	G150	R210	E270	I330	
P32	P32	N92	N92	D211	R210	S271	A331	
S33	S33	E93	E93	V152	D211	A272	P332	
I34	I34	L94	L94	L153	I152	G273	P333	
V35	V35	R95	R95	D154	K213	I274	E334	
G36	G36	V96	V96	S155	K215	H275	K335	
R37	R37	A97	A97	G156	L216	E276	K336	
P38	P38	P98	P98	D157	C217	T277	Y337	
R39	R39	E99	E99	G158	Y218	T278	S338	
H40	H40	E100	E100	V159	Y219	Y279	V339	
Q41	Q41	H101	H101	T160	V219	N280	W340	
G42	G42	P102	P102	L221	A220	S281	I341	
V43	V43	V43	V43	H161	L221	I282	G342	
M44	M44	L104	L104	N162	D222	I282	G343	
V45	V45	V45	V45	F223	F223	W283	G344	
G46	G46	T106	T106	E224	E224	K284	S344	
E107	E107	E107	E107	N225	N225	C285	I345	
G168	G168	A108	A108	E226	E226	D286	L346	
P109	P109	P109	P109	E167	E167	I287	A347	
K50	K50	L110	L110	M227	M227	D288	S348	
D51	D51	M111	M111	A228	A228	I289	L349	
S52	S52	P112	P112	T229	T229	K290	S350	
Y53	Y53	K113	K113	A230	A230	R291	T351	
A114	A114	A114	A114	L171	L171	D292	F352	
G55	G55	N115	N115	P172	P172	S232	P352	
D56	D56	R116	R116	H173	H173	S233	Q353	
E57	E57	E117	E117	S234	S234	A174	Q354	
A58	A58	K118	K118	L175	L175	A295	M355	
O59	O59	M119	M119	L236	L236	N296	W356	
				E237	E237	N297	I357	
				L178	L178	V298	T358	
				S239	S239	M299	K359	

Q360	S300	Y240	L180	T120
E361	G301	L241	A181	Q121
Y362	G302	L242	G182	I122
D363	T303	D243	D183	M123
E364	T304	P244	D184	F124
A365	M305	G245	D185	E125
G366	Y306	Q246	T186	T126
P367	P307	Y247	D187	F127
S368	G308	L248	Y188	M128
I369	I309	T249	L189	V129
V370	A310	L250	M190	P130
H371	D311	G251	K191	A131
R372	R312	N252	I192	M132
K373	M313	E253	L193	Y133
C374	Q314	R254	T194	V134
F375	K315	F255	E195	A135
NH2376	E316	R256	R196	I136
	I317	C257	G197	Q137
	T318	P258	Y198	A138
	A319	E259	S199	V139
	L320	T260	F200	L140
	A321	L261	V201	S141
	P322	F262	T202	L142
	S323	D263	T203	Y143
	T324	P264	A204	A144
	M325	S265	E205	G145
	K326	F266	R206	G146
	I327	L267	E207	R147
	K328	G268	T208	L148
	I329	M269	V209	T149
	I330	E270	R210	G150
	A331	S271	D211	I151
	P332	G272	L212	V152
	P333	G273	K213	L153
	E334	L274	E214	D154
	R335	H275	K215	S155
	K336	E276	L216	G156
	Y337	T277	C217	D157
	S338	T278	Y218	G158
	V339	Y279	V219	V159
	W340	N280	A220	T160
	I341	S281	L221	H161
	G342	L282	D222	M162
	G343	M283	F223	V163
	S344	K284	E224	P164
	I345	C285	N225	I165
	L346	D286	E226	Y166
	A347	L287	M227	E167
	S348	D288	A228	G168
	L349	R289	T229	V169
	S350	N290	A230	A170
	F351	K291	A231	L171
	F352	D292	S232	P172
	Q353	L293	S233	H173
	G354	Y294	S234	A174
	M355	A295	S235	I175
	W356	N296	L236	M176
	I357	N297	E237	R177
	T358	V298	C238	L178
	V359	W299	C239	A179

- Molecule 1: Actin, alpha skeletal muscle

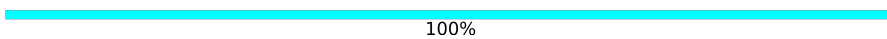
Chain G:



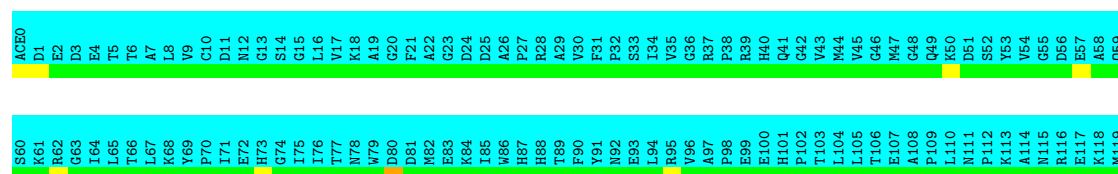
Q360	S300	Y240	L180	T120	S60	ACE0
E361	G301	E241	A181	Q121	R61	D1
Y362	G302	L242	G182	I122	H62	E2
D363	T303	D243	R183	M123	G63	D3
E364	T304	D244	D184	F124	H64	E4
A365	M305	G245	L185	E125	L65	T5
G366	Y306	Q246	T186	T126	T66	T6
P367	P307	Q247	T187	F127	L67	A7
S368	G308	T248	Y188	M128	R68	L8
I369	I309	T249	L189	V129	V69	V9
V370	A310	I250	M190	P130	P70	C10
H371	D311	G251	K191	A131	I71	D11
R372	R312	N252	I192	M132	E72	N12
K373	M313	E253	L193	Y133	H73	G13
C374	Q314	R254	T194	F134	G74	S14
F375	K315	P255	E195	A135	I75	G15
MH2376	E316	R256	R196	I136	I76	L16
	I317	C257	G197	Q137	T77	V17
	T318	P258	Y198	A138	N78	V17
	A319	E259	S199	V139	M79	K18
	L320	T260	F200	L140	D80	A19
	A321	L261	V201	S141	D81	F21
	P322	P262	T202	L142	M82	A22
	S323	Q263	T203	Y143	E83	G23
	T324	P264	A204	A144	K84	D24
	M325	S265	E205	S145	R85	D25
	K326	P266	R206	G146	M86	A26
	I327	T267	E207	R147	H87	P27
	K328	G268	T208	T148	H88	R28
	I329	M269	V209	T149	T89	A29
	I330	E270	R210	G150	F90	V30
	A331	S271	D211	L151	Y91	F31
	P332	A272	T212	V152	N92	P32
	P333	G273	K213	L153	E93	S33
	E334	I274	E214	D154	L94	I34
	R335	H275	K215	S155	R95	V35
	K336	E276	L216	G156	V96	G36
	Y337	T277	C217	D157	A97	R37
	S338	T278	Y218	G158	P98	P38
	V339	Y279	V219	V159	E99	R39
	M340	M280	A220	T160	E100	H40
	I341	S281	L221	H161	H101	Q41
	G342	T282	D222	M162	P102	G42
	G343	M283	F223	V163	T103	V43
	S344	K284	E224	P164	M104	M44
	I345	C285	N225	I165	L105	V45
	L346	D286	E226	V166	T106	G46
	A347	T287	M227	E167	E107	M47
	S348	D288	A228	G168	A108	G48
	L349	T289	T229	V169	P109	Q49
	S350	R290	A230	A170	L110	K50
	T351	K291	A231	L171	M111	D51
	F352	D292	S232	P172	P112	S52
	Q353	L293	S233	H173	K113	Y53
	K354	T294	S234	A174	A114	V54
	M355	A295	S235	L175	N115	G55
	V356	M296	L236	M176	R116	D56
	T357	N297	E237	R177	E117	M57
	V358	V298	K238	L178	K118	A58
	K359	M299	S239	D179	M119	O59

- Molecule 1: Actin, alpha skeletal muscle

Chain H:



S60	K61	R62	G63	I64	L65	T66	L67	K68	V69	P70	I71	E72	H73	G74	I75	T76	L77	H78	R79	D80	D81	M82	G83	E84	K85	R86	H87	H88	T89	F90	Y91	N92	E93	I94	R95	V96	A97	P98	E99	E100	H101	T102	T103	L104	L105	T106	E107	A108	P109	L110	N111	P112	K113	N114	N115	R116	E117	K118	N119
ACED	D1	E2	D3	E4	T5	T6	A7	L8	V9	C10	D11	M12	G13	S14	G15	L16	V17	K18	A19	G20	F21	A22	G23	D24	A25	A26	R27	R28	A29	V30	F31	P32	S33	T34	V35	G36	R37	P38	R39	H40	Q41	G42	V43	M44	V45	G46	M47	G48	Q49	K50	D51	S52	V53	G54	M55	D56	E57	A58	C59



T120	Q121	L180	Y240	S300	Q360
I122	A181	E241	G301	E361	E361
F124	R182	L242	G302	Y362	Y362
L125	R183	P243	T303	D363	D363
T126	D184	G244	G304	E364	E364
F127	L185	D245	M305	A365	A365
L128	T186	Q246	Y306	T366	T366
L129	D187	Y247	G307	P367	P367
P130	Y188	L248	G308	G368	G368
L131	L189	T249	I309	I369	I369
A132	M190	L250	A310	V370	V370
L133	K191	G251	D311	H371	H371
L134	L192	N252	R312	R372	R372
A135	L193	E253	M313	K373	K373
I136	T194	R254	Q314	C374	C374
Q137	E195	F255	E316	F375	F375
A138	R196	R256	N16	NH2376	NH2376
L139	G197	C257	I317		
L140	Y198	P258	T318		
S141	S199	E259	A319		
L142	F200	L260	L320		
Y143	V201	L261	R21		
A144	T202	F262	K22		
S145	T203	Q263	S323		
G146	A204	P264	S24		
R147	E205	S265	T25		
T148	R206	F266	Q26		
T149	E207	L267	E27		
G150	I208	G268	E28		
I151	T209	M269	I29		
V152	R210	E270	K30		
L153	D211	S271	K31		
D154	T212	G272	R32		
S155	K213	L273	K33		
G156	E214	K274	E34		
D157	L215	H275	A35		
G158	K216	E276	V36		
V159	C217	T277	L37		
H160	Y218	T278	F38		
H161	V219	Y279	C39		
V162	A220	N280	L40		
V163	L221	S281	S41		
P164	D222	L282	D42		
I165	F223	M283	D43		
E166	E224	K284	K44		
E167	N225	C285	R45		
G168	E226	D286	P106		
Y169	M227	L287	E107		
A170	A228	D288	S108		
P171	T229	L289	A109		
P172	A230	R290	F110		
H173	L171	K291	L111		
A174	S232	D292	K112		
I175	S233	L293	S113		
L176	S234	Y294	Q54		
R177	S235	A295	I55		
L178	L236	N296	L56		
S239	E237	N297	V57		
	K238	V298	A118		
		M299	S119		

• Molecule 2: Cofilin-2

Chain K:

100%

ACE0	M1	T60	S120
A2	G61	G61	K121
S3	D62	D62	A122
G4	T63	T63	A123
V5	V64	V64	I124
T6	E65	E65	K125
V7	D66	D66	K126
N8	P67	P67	K127
D9	Y68	Y68	F128
E10	T69	T69	T129
V11	S70	S70	G130
I12	F71	F71	I131
K13	V72	V72	K132
L14	K73	K73	H133
F15	L74	L74	E134
N16	P76	P76	W135
D17	F77	F77	Q136
M18	L78	L78	V137
K19	D79	D79	N138
V20	C80	C80	G139
R21	R81	R81	L140
K22	Y82	Y82	D141
S23	A83	A83	D142
S24	K84	K84	I143
T25	L84	L84	K144
Q26	Y85	Y85	D145
E27	D86	D86	R146
E28	A87	A87	S147
I29	T88	T88	L148
K30	Y89	Y89	L149
K31	E90	E90	G150
R32	T91	T91	E151
E33	K92	K92	K152
S34	E93	E93	L153
A35	S94	S94	G154
V36	K95	K95	G155
L37	E97	E97	N156
F38	D98	D98	V157
C39	L99	L99	V158
L40	V100	V100	V159
S41	F101	F101	S160
D42	I102	I102	L161
D43	F103	F103	E162
K44	W104	W104	G163
R45	A105	A105	K164
Q46	P106	P106	P165
I47	E107	E107	L166
I48	S108	S108	NH2167
V49	A109	A109	
E50	F110	F110	
E51	L111	L111	
A52	K112	K112	
K53	S113	S113	
Q54	K114	K114	
I55	M115	M115	
L56	T116	T116	
V57	Y117	Y117	
G58	A118	A118	
D59	S119	S119	

• Molecule 2: Cofilin-2

Chain L:

100%

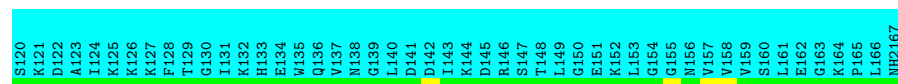
ACE0	M1	T60	S120
A2	G61	G61	K121
S3	D62	D62	A122
G4	T63	T63	A123
V5	V64	V64	I124
T6	E65	E65	K125
V7	D66	D66	K126
N8	P67	P67	K127
D9	Y68	Y68	F128
E10	T69	T69	T129
V11	S70	S70	G130
I12	F71	F71	I131
K13	V72	V72	K132
L14	K73	K73	H133
F15	L74	L74	E134
N16	P76	P76	W135
D17	F77	F77	Q136
M18	L78	L78	V137
K19	D79	D79	N138
V20	C80	C80	G139
R21	R81	R81	L140
K22	Y82	Y82	D141
S23	A83	A83	D142
S24	K84	K84	I143
T25	L84	L84	K144
Q26	Y85	Y85	D145
E27	D86	D86	R146
E28	A87	A87	S147
I29	T88	T88	L148
K30	Y89	Y89	L149
K31	E90	E90	G150
R32	T91	T91	E151
E33	K92	K92	K152
S34	E93	E93	L153
A35	S94	S94	G154
V36	K95	K95	G155
L37	E97	E97	N156
F38	D98	D98	V157
C39	L99	L99	V158
L40	V100	V100	V159
S41	F101	F101	S160
D42	I102	I102	L161
D43	F103	F103	E162
K44	W104	W104	G163
R45	A105	A105	K164
Q46	P106	P106	P165
I47	E107	E107	L166
I48	S108	S108	NH2167
V49	A109	A109	
E50	F110	F110	
E51	L111	L111	
A52	K112	K112	
K53	S113	S113	
Q54	K114	K114	
I55	M115	M115	
L56	T116	T116	
V57	Y117	Y117	
G58	A118	A118	
D59	S119	S119	

• Molecule 2: Cofilin-2

Chain M:

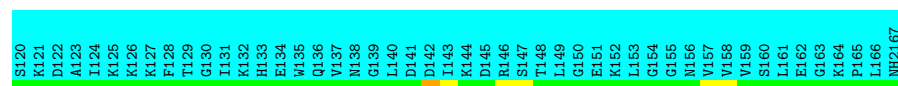
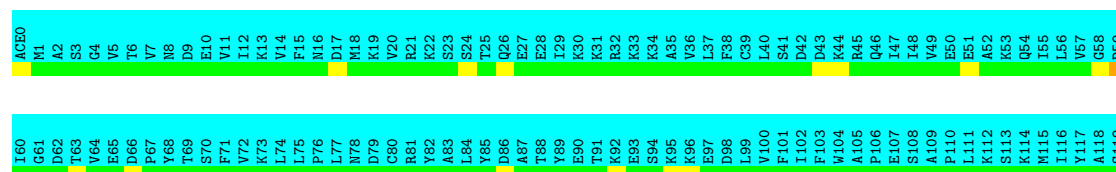
100%

ACE0	M1	I60	S120
A2	G61	G61	K121
S3	D62	D62	A122
G4	T63	T63	A123
V5	V64	V64	I124
T6	E65	E65	K125
V7	D66	D66	K126
N8	P67	P67	K127
D9	Y68	Y68	F128
E10	T69	T69	T129
V11	S70	S70	G130
I12	F71	F71	I131
K13	V72	V72	K132
L14	K73	K73	H133
F15	L74	L74	E134
N16	P76	P76	W135
D17	F77	F77	Q136
M18	L78	L78	V137
K19	D79	D79	N138
V20	C80	C80	G139
R21	R81	R81	L140
K22	Y82	Y82	D141
S23	A83	A83	D142
S24	K84	K84	I143
T25	L84	L84	K144
Q26	Y85	Y85	D145
E27	D86	D86	R146
E28	A87	A87	S147
I29	T88	T88	L148
K30	Y89	Y89	L149
K31	E90	E90	G150
R32	T91	T91	E151
E33	K92	K92	K152
S34	E93	E93	L153
A35	S94	S94	G154
V36	K95	K95	G155
L37	E97	E97	N156
F38	D98	D98	V157
C39	L99	L99	V158
L40	V100	V100	V159
S41	F101	F101	S160
D42	I102	I102	L161
D43	F103	F103	E162
K44	W104	W104	G163
R45	A105	A105	K164
Q46	P106	P106	P165
I47	E107	E107	L166
I48	S108	S108	NH2167
V49	A109	A109	
E50	F110	F110	
E51	L111	L111	
A52	K112	K112	
K53	S113	S113	
Q54	K114	K114	
I55	M115	M115	
L56	T116	T116	
V57	Y117	Y117	
G58	A118	A118	
D59	S119	S119	



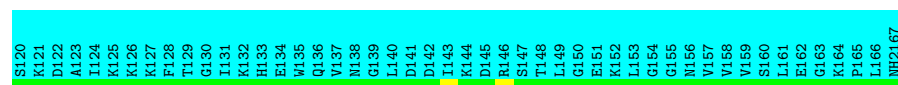
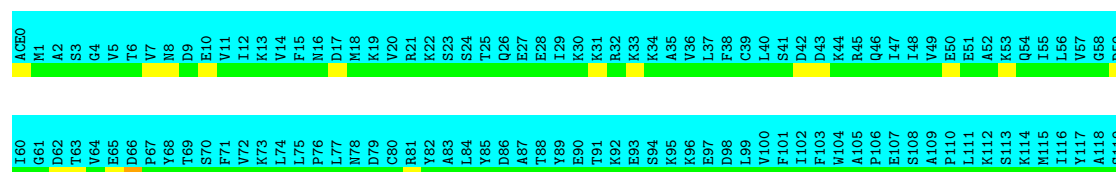
• Molecule 2: Cofilin-2

Chain N: 100%



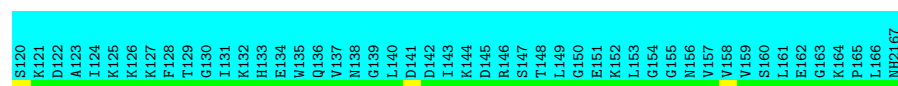
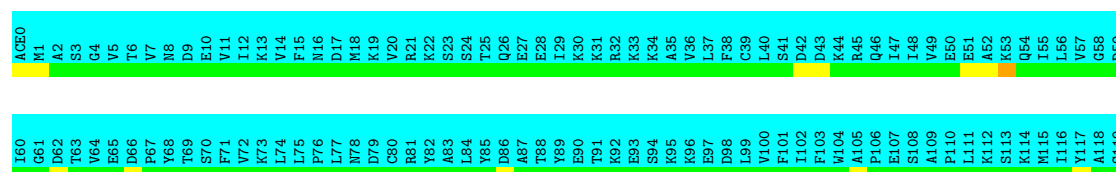
• Molecule 2: Cofilin-2

Chain O: 100%



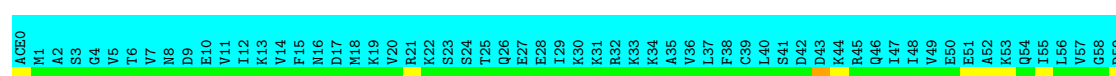
• Molecule 2: Cofilin-2

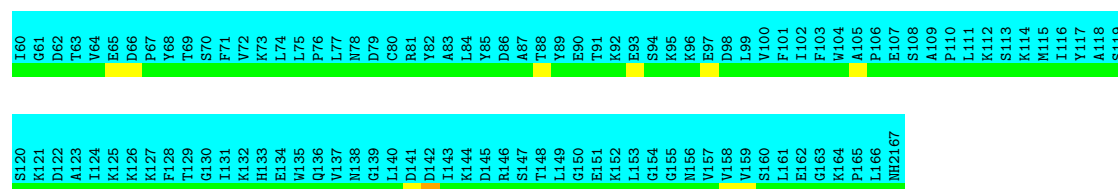
Chain P: 100%



• Molecule 2: Cofilin-2

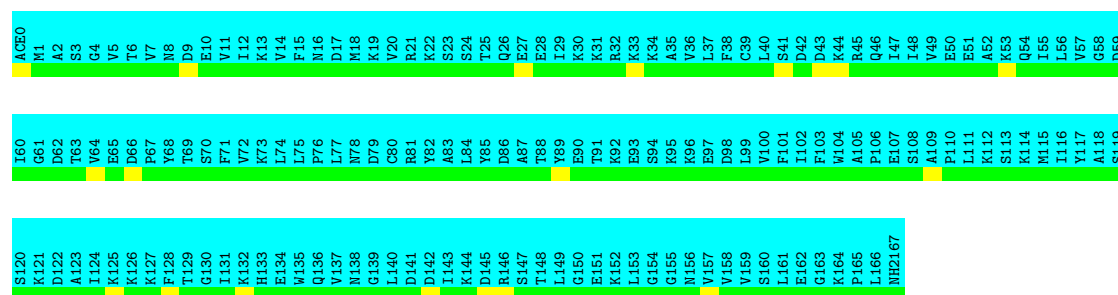
Chain Q: 100%





• Molecule 2: Cofilin-2

Chain R:  100%

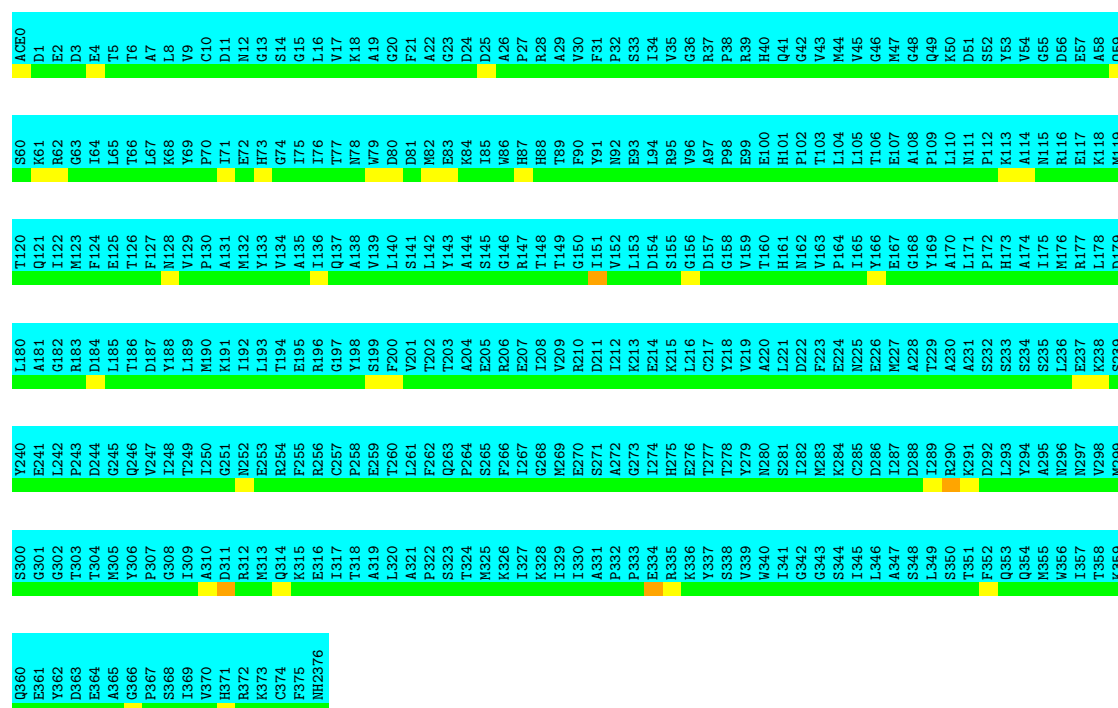


4.2 Residue scores for the representative (author defined) model from the NMR ensemble

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

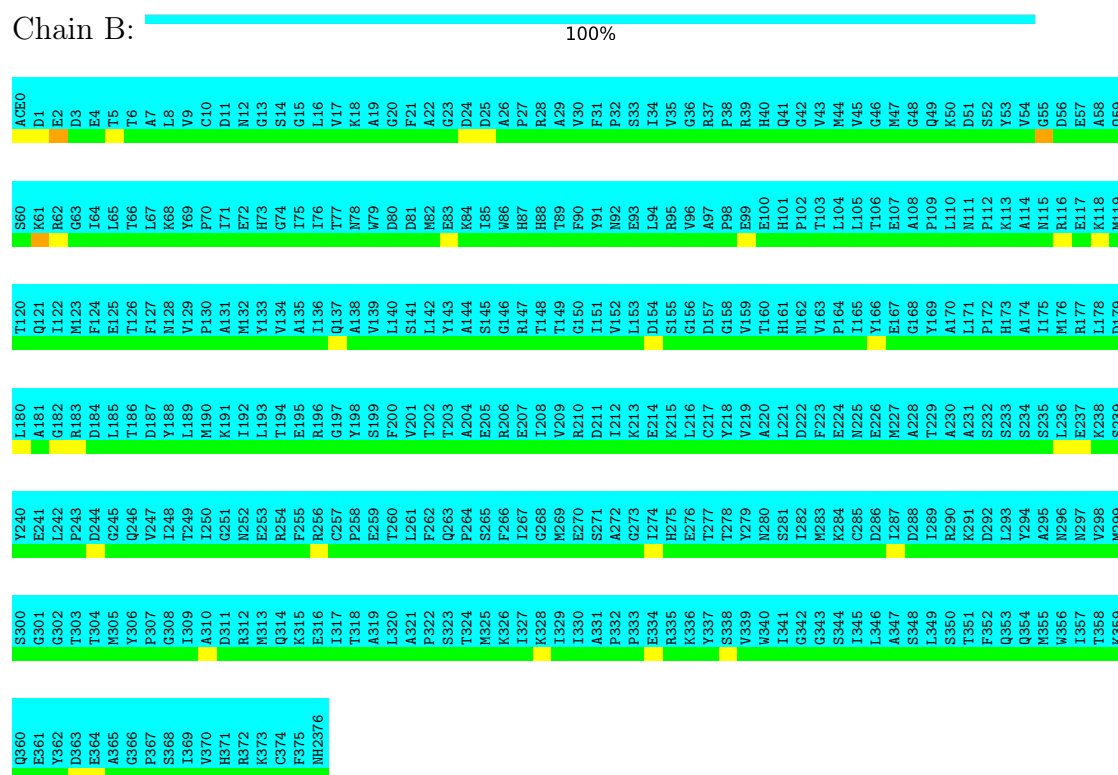
• Molecule 1: Actin, alpha skeletal muscle

Chain A:  100%



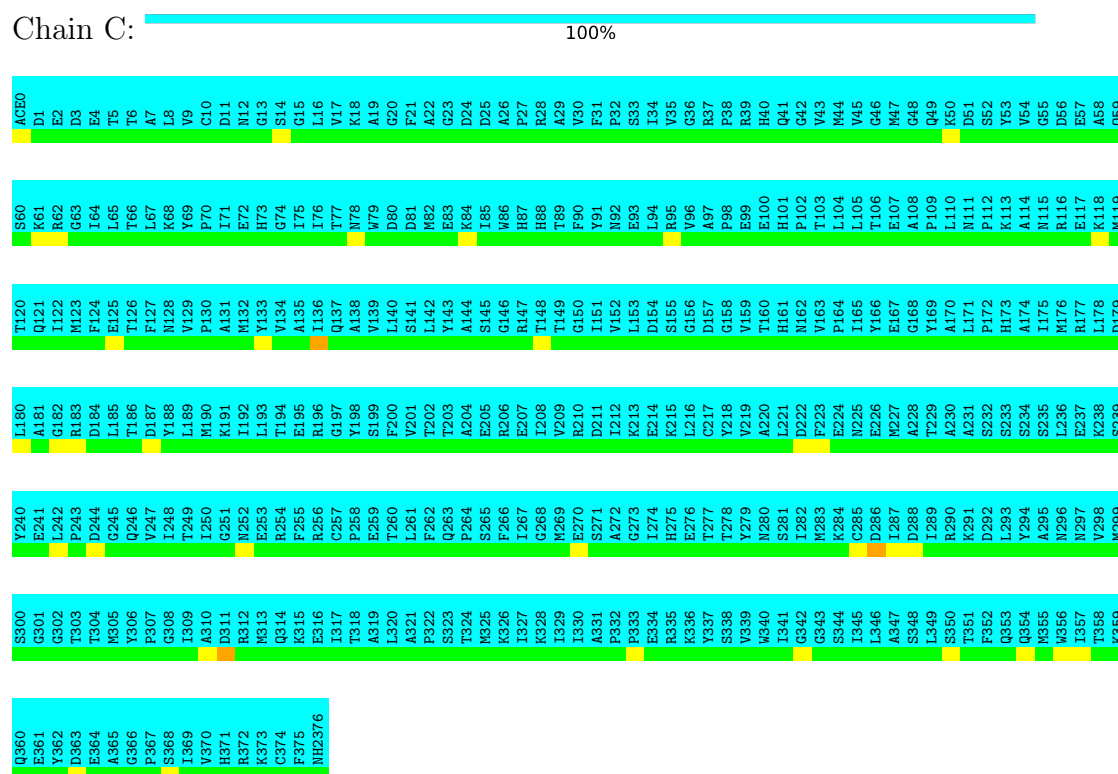
- Molecule 1: Actin, alpha skeletal muscle

Chain B:



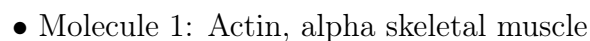
- Molecule 1: Actin, alpha skeletal muscle

Chain C:

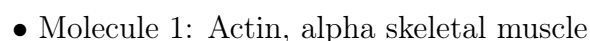


- Molecule 1: Actin, alpha skeletal muscle

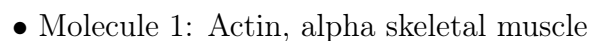
100%



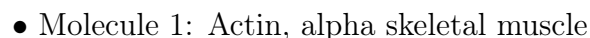
100%



100%

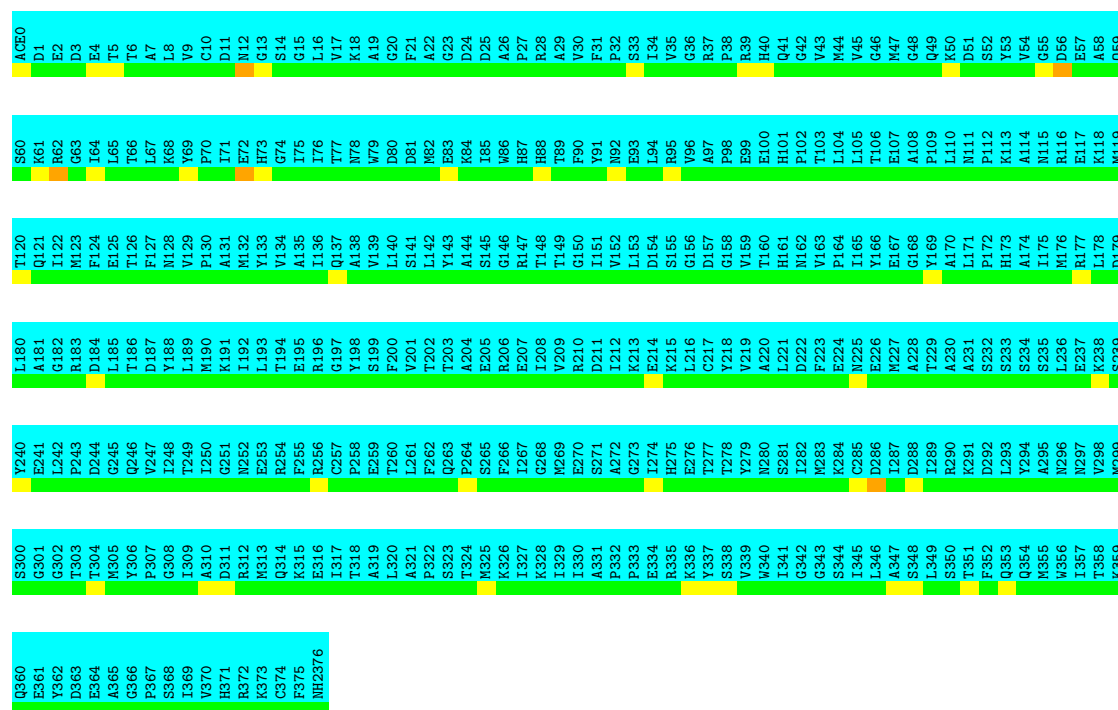


100%



Chain H:

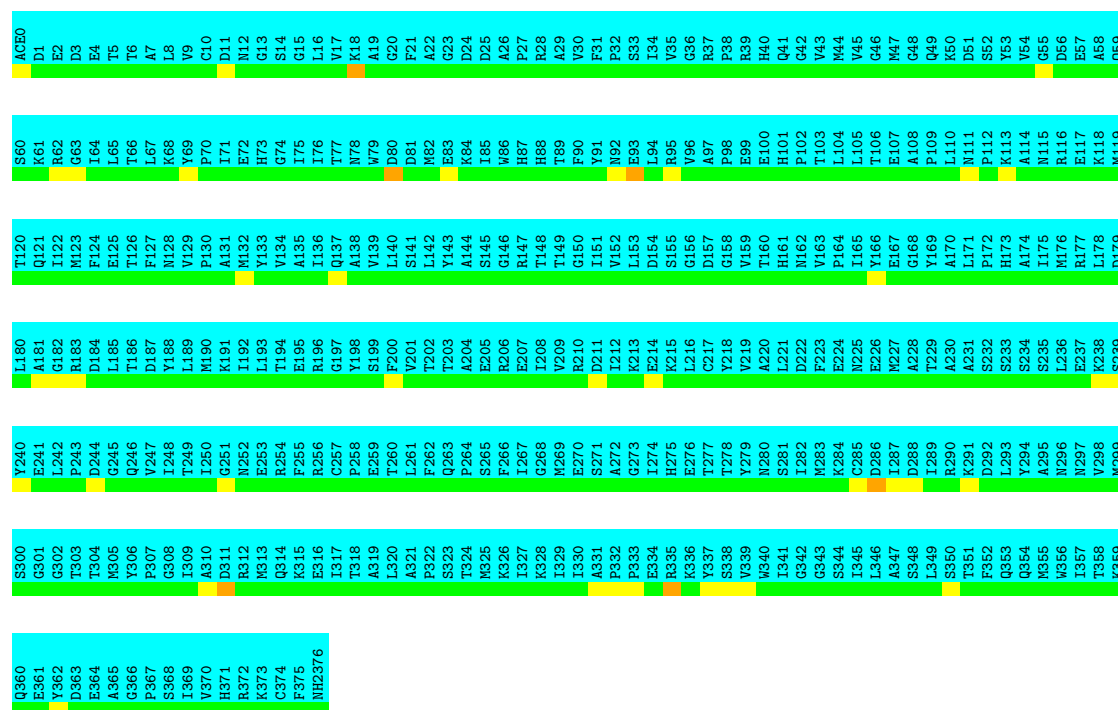
100%



- Molecule 1: Actin, alpha skeletal muscle

Chain I:

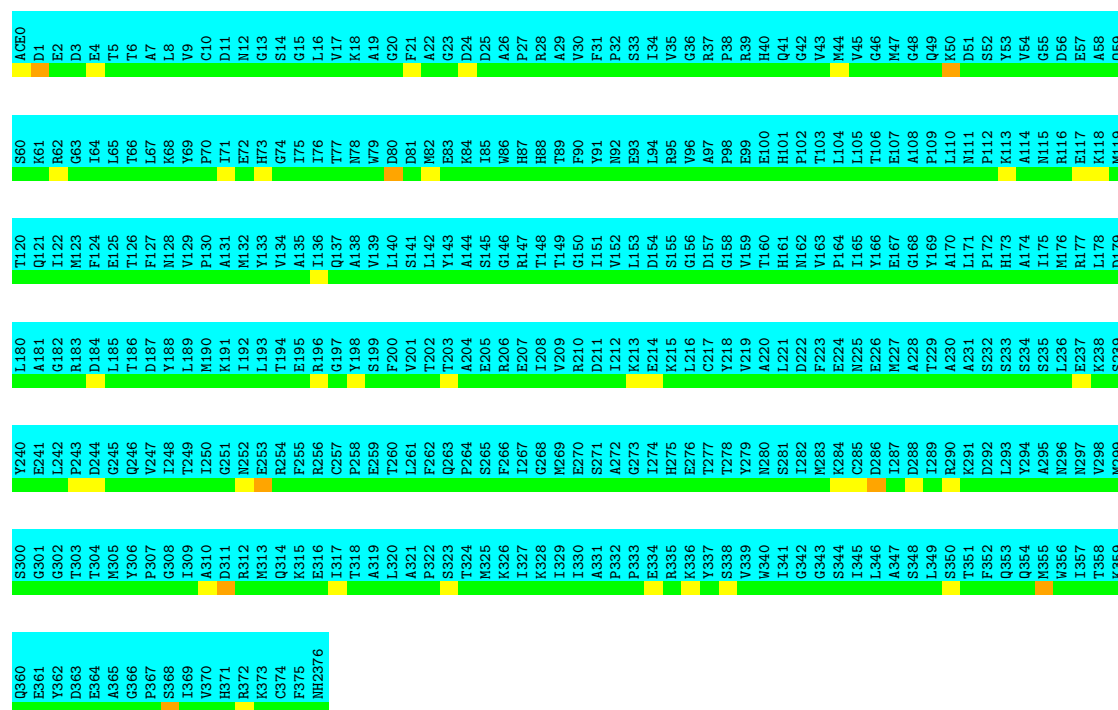
100%



- Molecule 1: Actin, alpha skeletal muscle

Chain J:

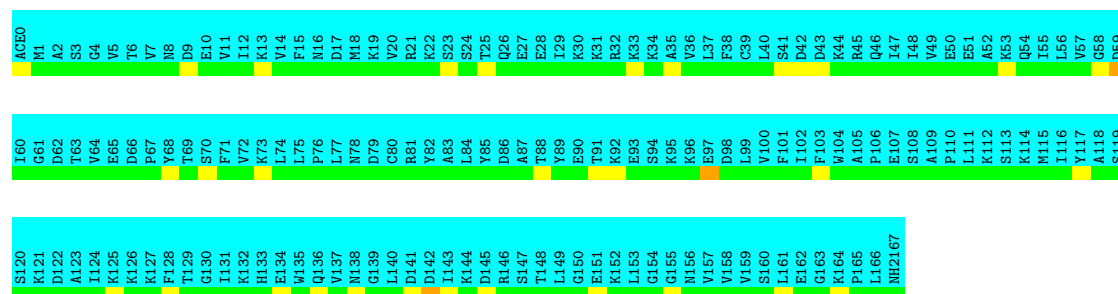
100%



• Molecule 2: Cofilin-2

Chain K:

100%



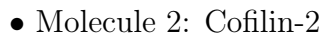
100%



100%



100%



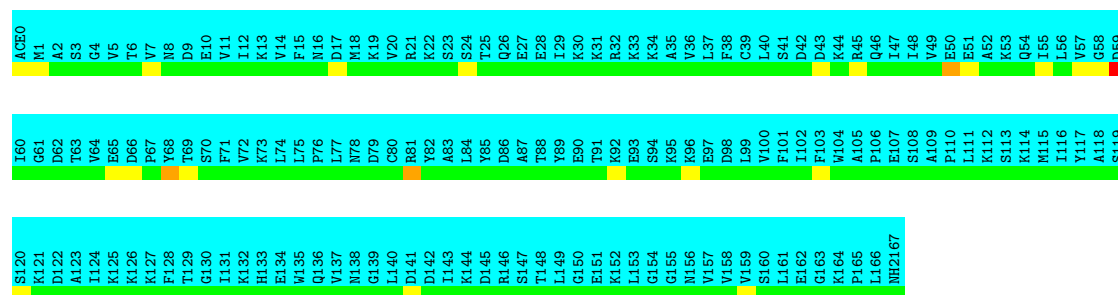
100%



● Molecule 2: Cofilin-2

Chain Q:

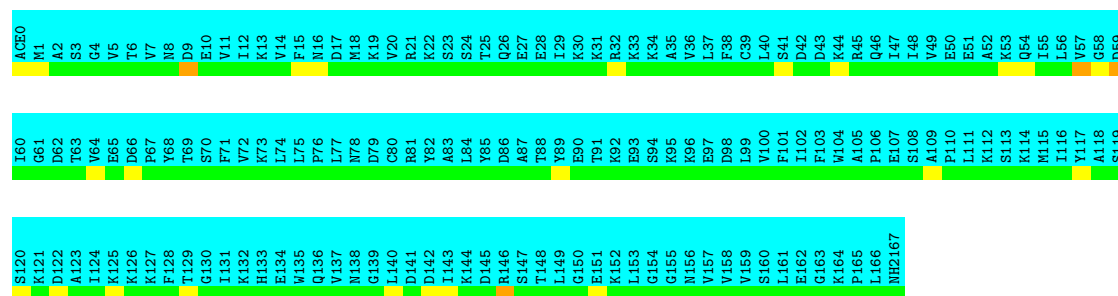
100%



● 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 [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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	E	0	0	0	0±0
1	F	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	B	0	0	0	0±0
1	D	0	0	0	0±0
1	A	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 oligosaccharides 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.