



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 10, 2018 – 11:36 PM EST

PDB ID : 6F1T  
EMDB ID: : EMD-4168  
Title : Cryo-EM structure of two dynein tail domains bound to dynactin and BICDR1  
Authors : Urnavicius, L.; Lau, C.K.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.;  
Yildiz, A.; Carter, A.P.  
Deposited on : 2017-11-23  
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

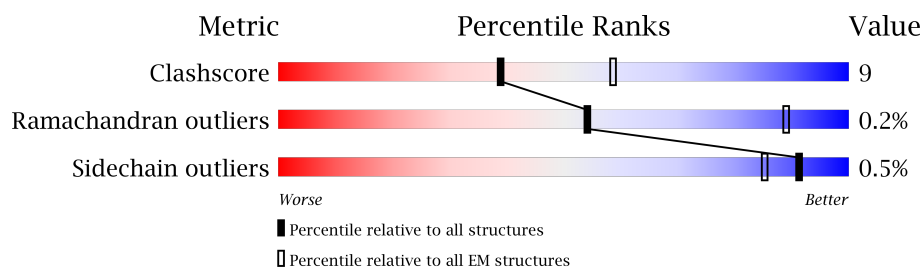
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















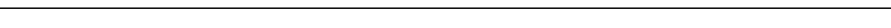











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	
1	C	376	
1	D	376	
1	E	376	
1	F	376	
1	G	376	
1	I	376	
2	H	375	

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Mol	Chain	Length	Quality of chain
3	J	390	
4	K	286	
5	L	272	
6	M	589	
7	N	618	
8	O	65	
8	P	65	
9	Q	87	
9	R	87	
10	U	190	
11	V	182	
12	X	389	
13	Y	263	
14	Z	52	
15	a	66	
16	b	89	
17	c	50	
18	d	26	
19	e	1053	
19	f	1053	
19	m	1053	
19	n	1053	
20	g	612	
20	h	612	
20	o	612	

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Mol	Chain	Length	Quality of chain
20	p	612	 65% 34%
21	i	492	 54% 46%
21	j	492	 55% 41% .
21	q	492	 54% 46%
21	r	492	 54% 46%
22	k	96	 97% .
22	l	96	 96% . .
22	s	96	 95% . .
22	t	96	 96% . .
23	x	392	 73% 27% .
24	z	53	 100%

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 92795 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	B	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	C	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	D	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	E	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	F	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	G	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	I	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		

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

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

- Molecule 3 is a protein called Actin related protein 10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	369	Total	C	N	O	S	0	0
			2883	1859	486	522	16		

- Molecule 4 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	278	Total	C	N	O	S	0	0
			2264	1428	396	434	6		

- Molecule 5 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	269	Total	C	N	O	S	0	0
			2122	1323	370	418	11		

- Molecule 6 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	587	Total	C	N	O		0	0
			2935	1761	587	587			

- Molecule 7 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	616	Total	C	N	O		0	0
			3080	1848	616	616			

- Molecule 8 is a protein called Dynactin Subunit 3.

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

- Molecule 9 is a protein called Dynactin Subunit 2.

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

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	172	Total	C	N	O		0	1
			843	500	171	172			

- Molecule 11 is a protein called Dynactin subunit 5.

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

- Molecule 12 is a protein called BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICDR-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	285	Total	C	N	O	S	0	0
			1715	1028	340	346	1		

- Molecule 13 is a protein called Dynactin Subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Y	263	Total	C	N	O	0	0
			1315	789	263	263		

- Molecule 14 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Z	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 15 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	a	52	Total	C	N	O	0	0
			405	255	64	86		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	37	LEU	GLN	conflict	UNP F1SKF9

- Molecule 16 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	b	75	Total	C	N	O	0	0
			585	365	99	121		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	37	LEU	GLN	conflict	UNP F1SKF9

- Molecule 17 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	c	37	Total	C	N	O	S	0	0
			256	159	42	54	1		

- Molecule 18 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	d	24	Total	C	N	O	0	0
			188	118	29	41		

- Molecule 19 is a protein called Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	926	Total	C	N	O	S	0	0
			5034	3049	982	1000	3		
19	f	929	Total	C	N	O	S	0	0
			6939	4365	1267	1288	19		
19	m	926	Total	C	N	O	S	0	0
			6260	3888	1182	1176	14		
19	n	928	Total	C	N	O	S	0	0
			5730	3518	1099	1104	9		

- Molecule 20 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace	
20	g	397	Total 1961	C 1167	N 397	O 397	0	0	
20	h	400	Total 3010	C 1892	N 532	O 571	S 15	0	0
20	o	397	Total 3126	C 1969	N 546	O 596	S 15	0	0
20	p	401	Total 2116	C 1273	N 416	O 427		0	0

There are 8 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
g	484	SER	THR	conflict	UNP Q13409
g	499	GLY	ASP	conflict	UNP Q13409
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409
o	484	SER	THR	conflict	UNP Q13409
o	499	GLY	ASP	conflict	UNP Q13409
p	484	SER	THR	conflict	UNP Q13409
p	499	GLY	ASP	conflict	UNP Q13409

- Molecule 21 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	268	Total	C	N	O		0	0
			1327	791	268	268			
21	j	288	Total	C	N	O	S	0	0
			2284	1463	379	431	11		
21	q	268	Total	C	N	O		0	0
			1327	791	268	268			
21	r	268	Total	C	N	O		0	0
			1327	791	268	268			

- Molecule 22 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	93	Total	C	N	O		0	0
			462	276	93	93			
22	l	93	Total	C	N	O		0	0
			462	276	93	93			
22	s	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
22	t	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

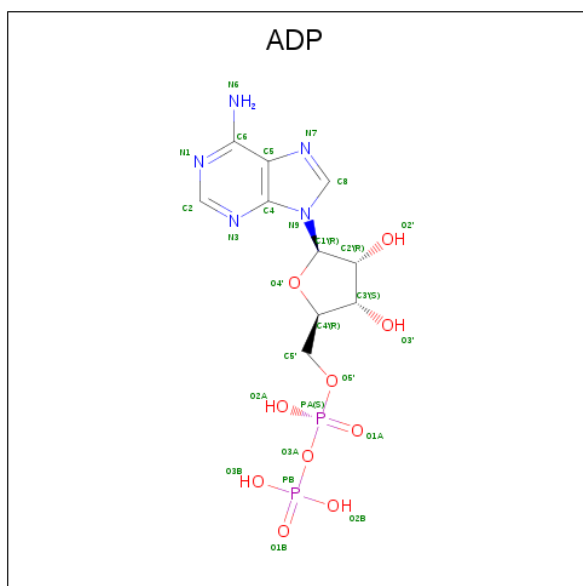
- Molecule 23 is a protein called BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1.

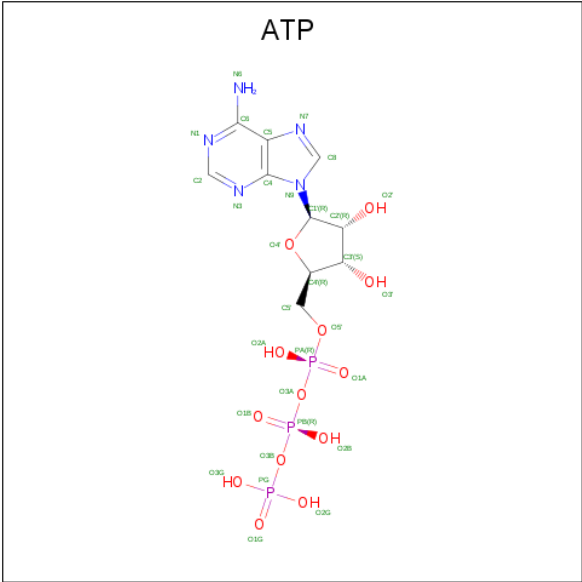
Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	288	Total	C	N	O	S	0	0
			1695	1018	336	340	1		

- Molecule 24 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 25 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



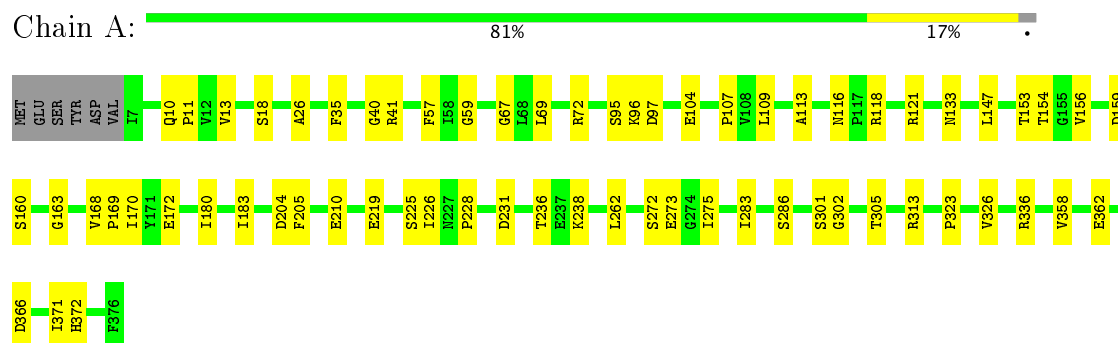


Mol	Chain	Residues	Atoms					AltConf
26	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

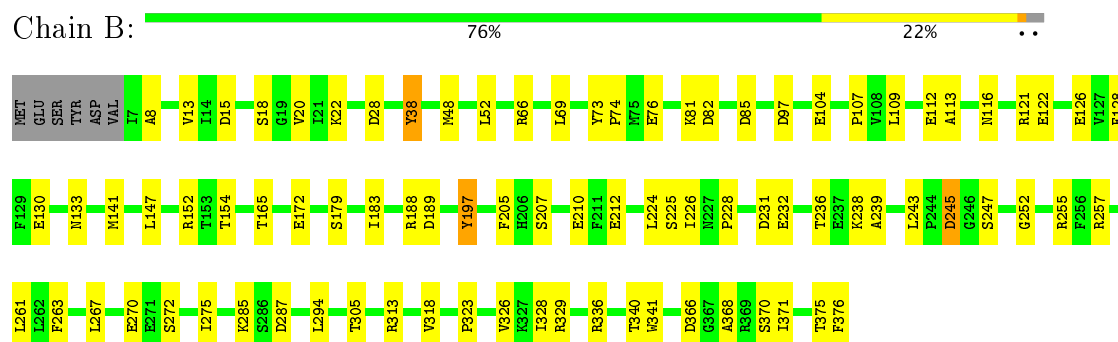
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

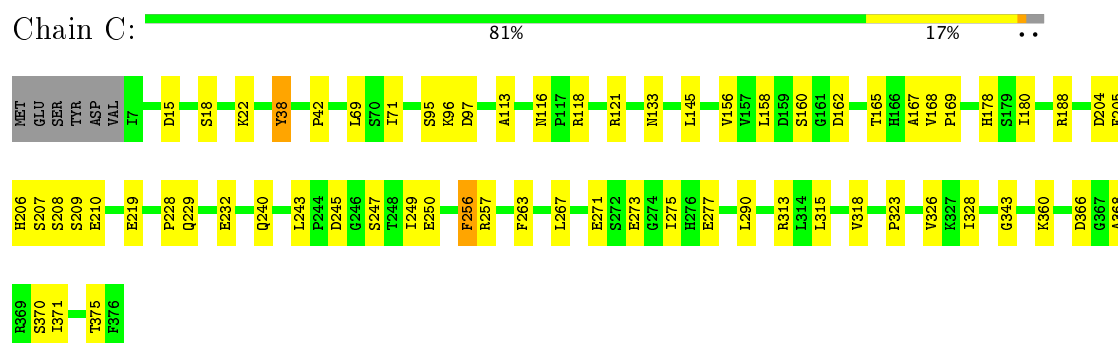
- Molecule 1: ARP1 actin related protein 1 homolog A



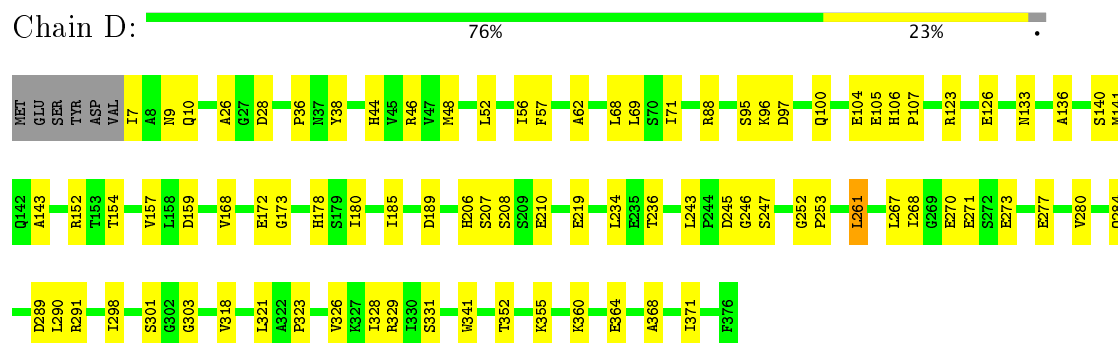
- Molecule 1: ARP1 actin related protein 1 homolog A



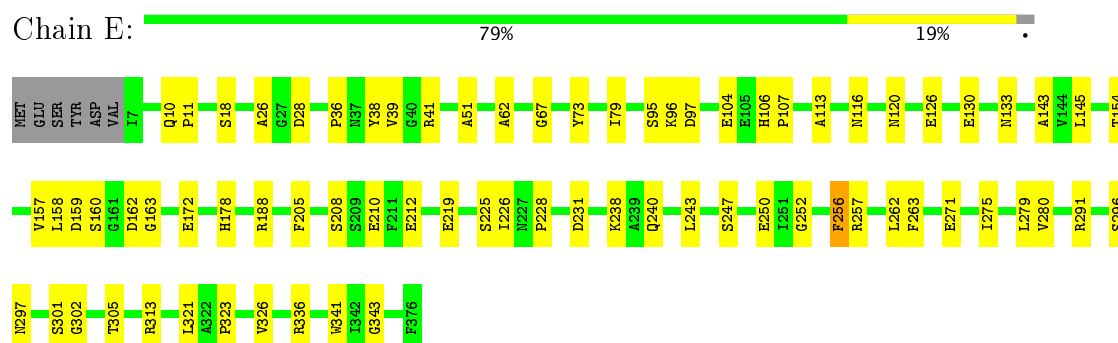
- Molecule 1: ARP1 actin related protein 1 homolog A



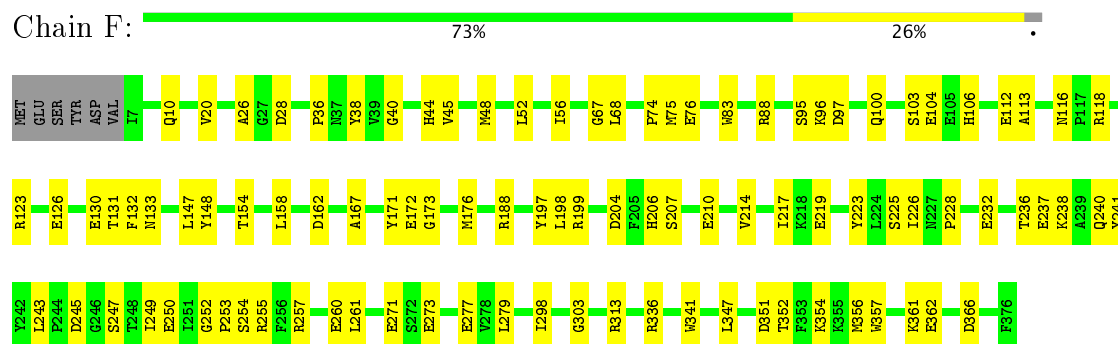
- Molecule 1: ARP1 actin related protein 1 homolog A



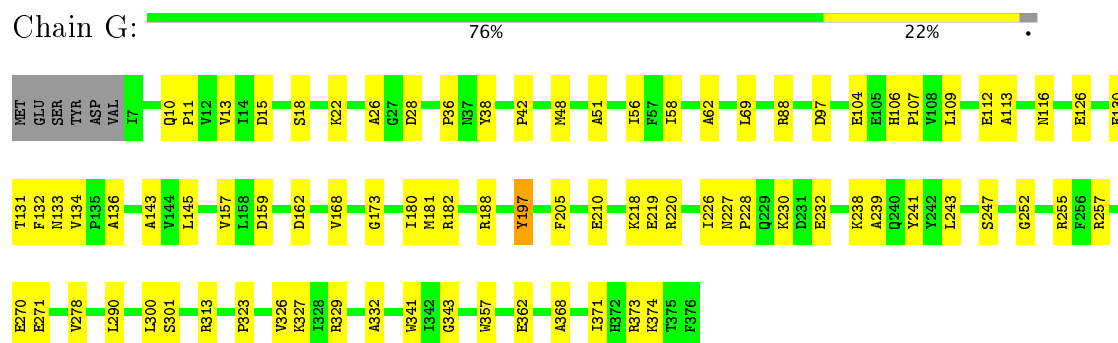
- Molecule 1: ARP1 actin related protein 1 homolog A



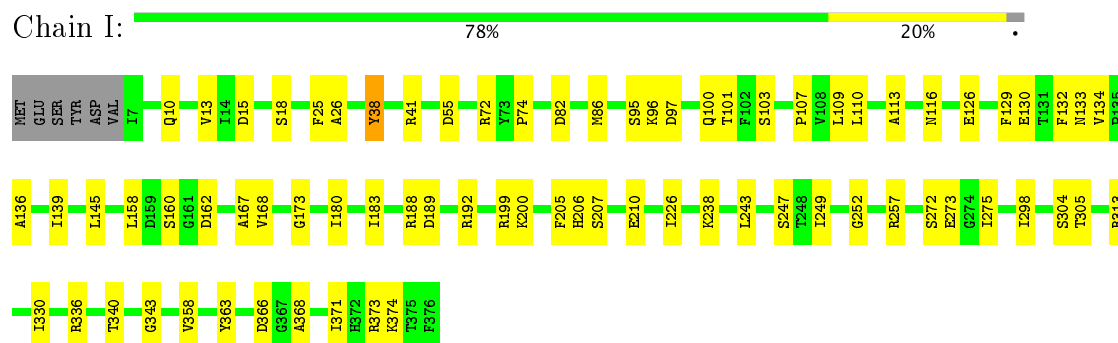
- Molecule 1: ARP1 actin related protein 1 homolog A



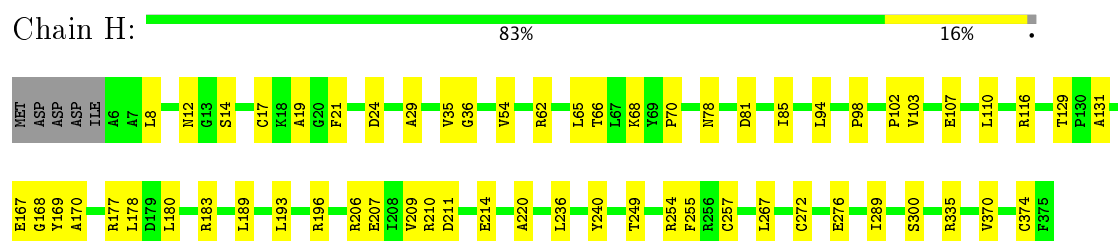
- Molecule 1: ARP1 actin related protein 1 homolog A



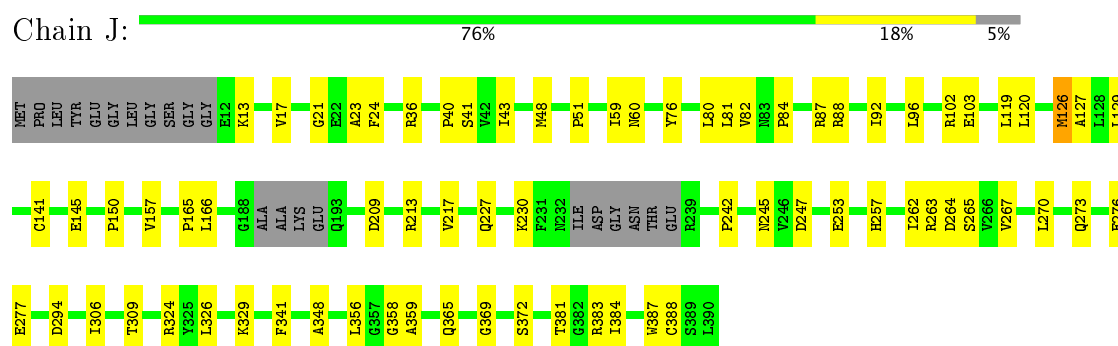
- Molecule 1: ARP1 actin related protein 1 homolog A



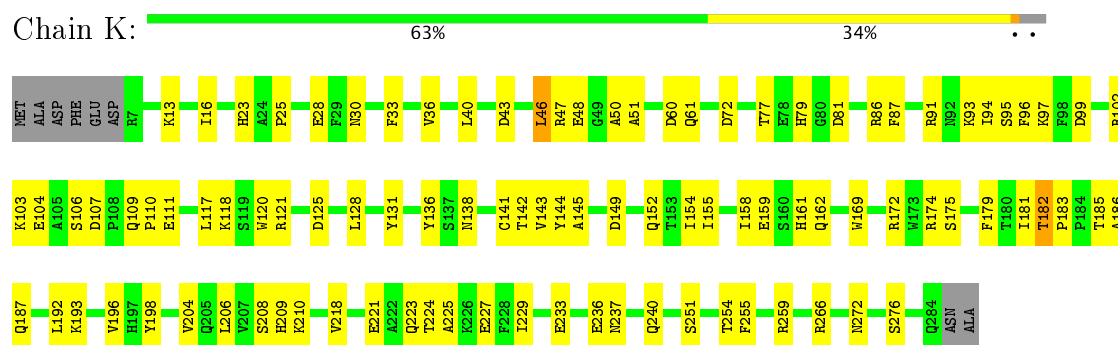
- Molecule 2: Actin, cytoplasmic 1



- Molecule 3: Actin related protein 10 homolog

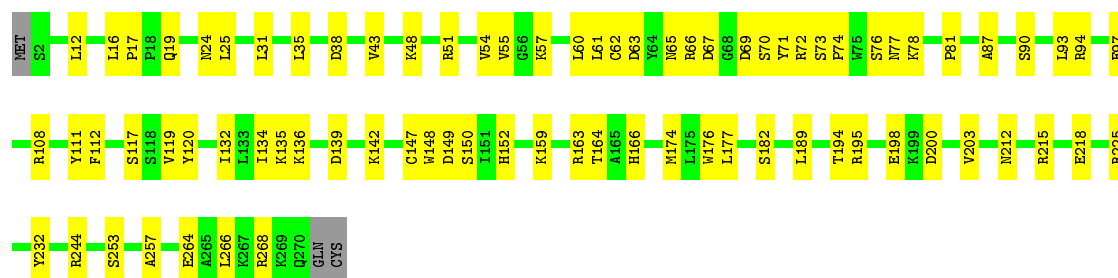


- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1



- Molecule 5: F-actin capping protein beta subunit





• Molecule 6: Dynactin Subunit 2

Chain M: 97%



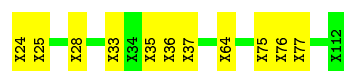
• Molecule 7: Dynactin Subunit 2

Chain N: 97%



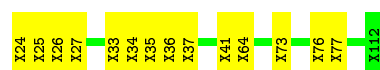
• Molecule 8: Dynactin Subunit 3

Chain O: 83% 17%



• Molecule 8: Dynactin Subunit 3

Chain P: 78% 22%



• Molecule 9: Dynactin Subunit 2

Chain Q: 75% 25%




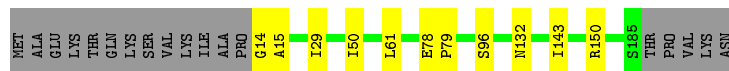
• Molecule 9: Dynactin Subunit 2

Chain R: 97%



- Molecule 10: Dynactin 6

Chain U:  85% 6% 9%



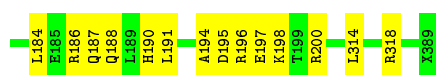
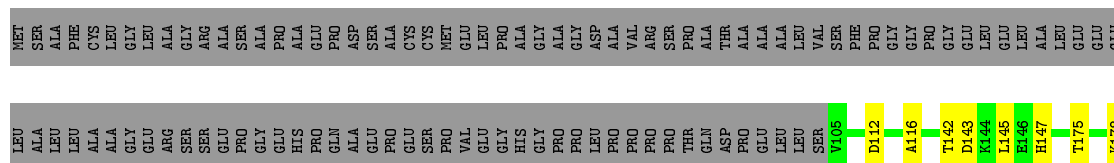
- Molecule 11: Dynactin subunit 5

Chain V:  86% 9%



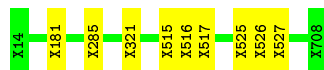
- Molecule 12: BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICDR-1

Chain X:  68% 6% 27%



- Molecule 13: Dynactin Subunit 4

Chain Y:  97%



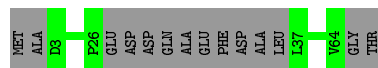
- Molecule 14: Dynactin Subunit 1

Chain Z:  71% 29%




- Molecule 15: Dynactin subunit 2

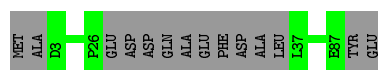
Chain a:  79% 21%



- Molecule 16: Dynactin subunit 2

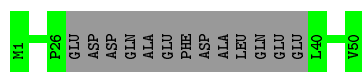


Chain b:  84% 16%

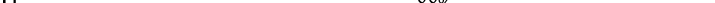


- Molecule 17: Dynactin subunit 2

Chain c:  74% 26%



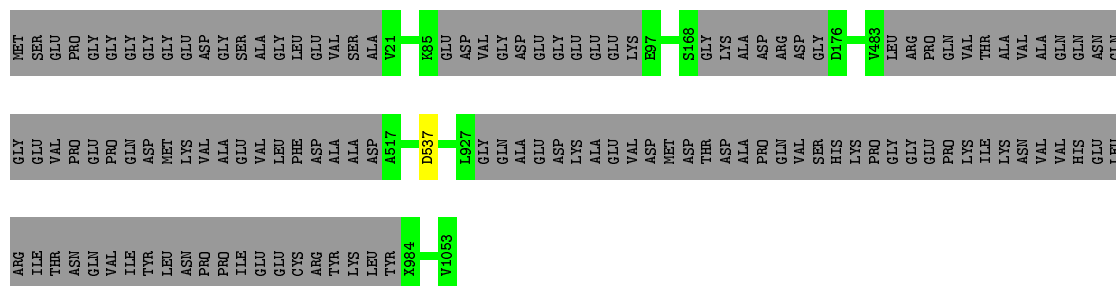
- Molecule 18: Dynactin subunit 2

Chain d:  88% • 8%

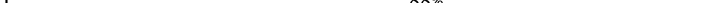


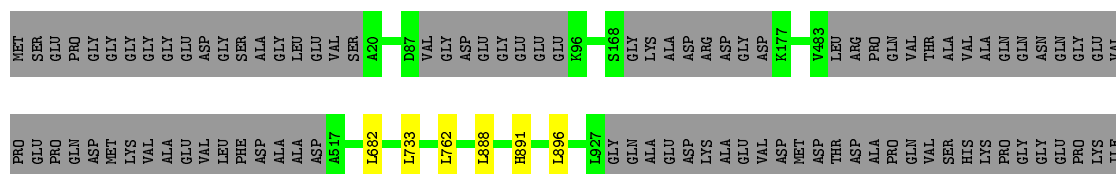
- Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1

Chain e:  88% 12%



- Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1

Chain f:  88% • 12%

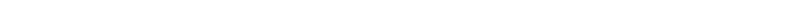


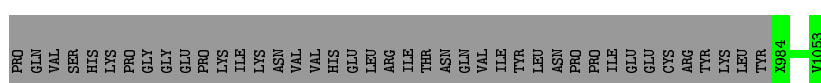
- Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1

Chain m:  86% • 12%



- Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1

Chain n: 



- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

Chain g:  65% 35%

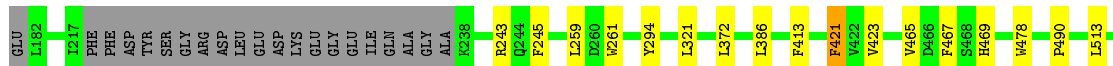




- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

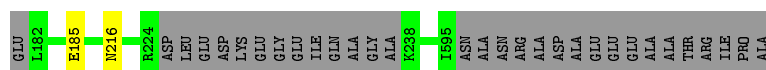


- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2



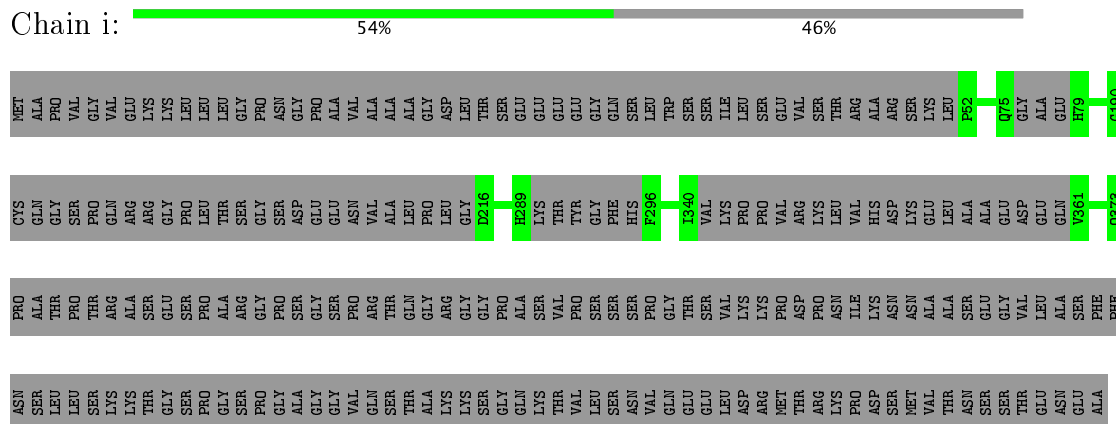
- Molecule 20: Cytoplasmic dynein 1 intermediate chain 2





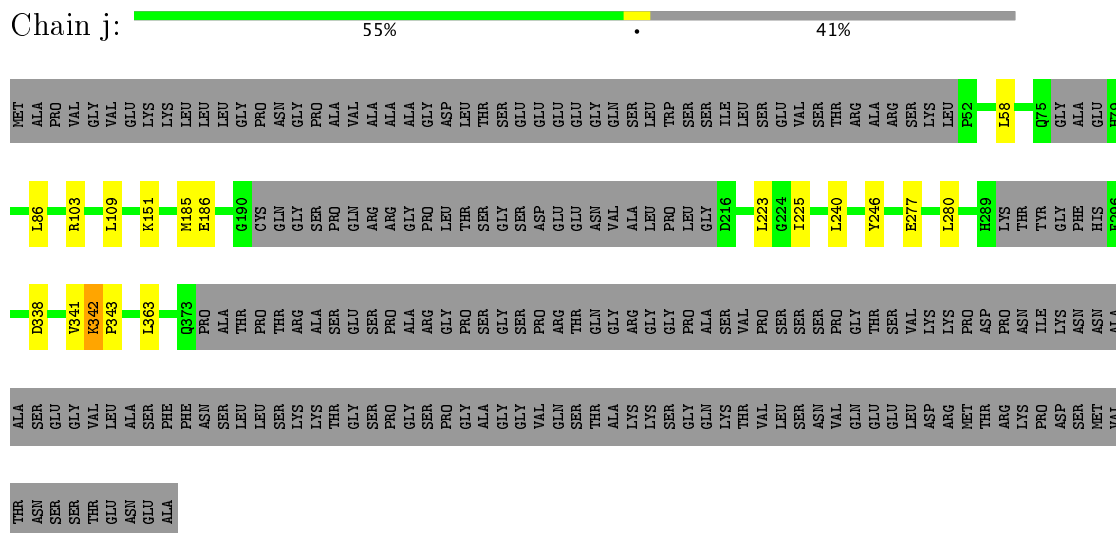
- Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

Chain i:



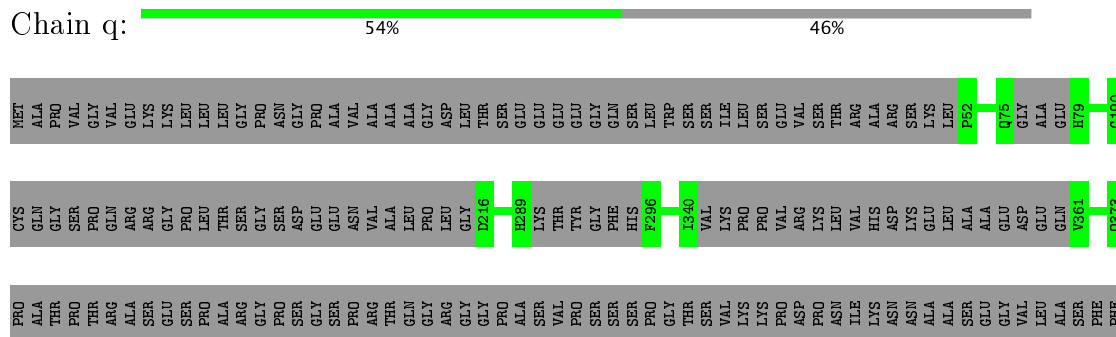
- Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

Chain j:



- Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

Chain q:



ASN	SER	LEU	LEU	SER	LYS	LYS	THR	GLY	SER	PRO	GLY	ALA	GLY	GLY	VAL	GLN	SER	THR	ALA	LYS	LYS	SER	GLY	GLN	LYS	THR	VAL	VAL	SER	ASN	VAL	GLN	GLU	GLU	LEU	ASP	ARG	MET	THR	ARG	LYS	PRO	ASP	SER	MET	VAL	THR	ASN	SER	THR	GLU	ASN	GLU	ALA
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- Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

Chain r:  54% 46%

Met	Ala	Pro	Val	Gly	Val	Glu	Lys	Lys	Leu	Leu	Leu	Gly	Pro	Asn	Gly	Pro	Ala	Ala	Ala	Gly	Asp	Leu	Ser	Ser	Glu	Glu	Glu	Gly	Gln	Ser	Ser	Thr	Trp	Ser	Ser	Ser	Leu	Ser	Glu	Val	Gly	Val	Ala	Ala	Arg	Ser	Lys	Glu	Gly	Pro	Met
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CYS	GLY	GLN	SER	PRO	GLN	ARG	ARG	GLY	PRO	LEU	THR	SER	GLY	SER	ASP	GLU	GLU	GLY	D216	H289	R289	THR	TYR	GLY	PHE	HIS	F296	I340	VAL	LNS	PRO	PRO	VAL	ARG	LNS	LEU	VAL	HIS	ASP	LNS	GLU	ALA	ALA	GLU	ASP	GLU	GLU	V361	G372
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PRO	ALA	THR	PRO	THR	THR	ARG	ALA	SER	GLU	SER	PRO	ALA	ARG	GLY	PRO	GLY	SER	GLY	SER	PRO	ARG	ARG	THR	GLN	GLY	ARG	GLY	GLY	ALA	ALA	SER	SER	SER	PRO	PRO	VAL	VAL	SER	SER	SER	SER	PRO	GLY	GLY	THR	GLY	ASN	LYS	LYS	LYS	PRO	ASP	PRO	PRO	ASN	ILE	LYS	LYS	ASN	ASN	ALA	ALA	SER	SER	GLU	GLY	VAL	LEU	ALA	ALA	SER	SER	PHE	THR	PRO
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ASN	SER	LEU	LEU	SER	LYS	LYS	THR	GLY	SER	PRO	GLY	GLY	ALA	GLY	GLY	VAL	GLN	SER	THR	ALA	LYS	LYS	GLY	GLN	LYS	THR	VAL	VAL	LEU	SER	ASN	VAL	GLN	GLN	THR	THR	ARG	ASP	LEU	ASP	LYS	PRO	ASP	SER	SER	THR	GLU	ASN	GLU	ALA
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- Molecule 22: Dynein light chain roadblock-type 1

Chain k:  97%

MET  
ALA  
E3  
T95  
GLU

- Molecule 22: Dynein light chain roadblock-type 1

Chain 1:  96% ..

MET  
ALA  
E3  
P82  
T95  
GLU

- Molecule 22: Dynein light chain roadblock-type 1

Chain s:  95% • •

**MET**  
**ALA**  
**E3** — **N36** — **R70** — **T95**  
**GLU**

- Molecule 22: Dynein light chain roadblock-type 1

Chain t:  96% ..

MET  
ALA  
E3  
N36  
T95  
GLU

- Molecule 23: BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1

Chain x:  73% . 27%



● Molecule 24: Dynactin Subunit 1

Chain z: 

100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	205611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.57	0/3025	0.67	1/4085 (0.0%)
1	B	0.82	0/3025	0.80	5/4085 (0.1%)
1	C	0.70	0/3025	0.77	6/4085 (0.1%)
1	D	0.83	0/3025	0.79	2/4085 (0.0%)
1	E	0.69	0/3025	0.73	3/4085 (0.1%)
1	F	0.89	1/3025 (0.0%)	0.84	3/4085 (0.1%)
1	G	0.61	0/3025	0.69	1/4085 (0.0%)
1	I	0.34	0/3025	0.66	4/4085 (0.1%)
10	U	0.38	0/841	0.65	0/1168
11	V	0.31	0/811	0.61	0/1126
12	X	0.39	0/1402	0.56	0/1914
15	a	0.39	0/413	0.65	0/563
16	b	0.43	0/595	0.69	0/803
17	c	0.57	0/260	0.78	0/356
18	d	0.79	1/193 (0.5%)	0.74	0/265
19	e	0.32	0/4807	0.62	0/6656
19	f	0.54	0/6791	0.82	7/9196 (0.1%)
19	m	0.61	5/6087 (0.1%)	0.84	14/8287 (0.2%)
19	n	0.42	1/5527 (0.0%)	0.74	8/7571 (0.1%)
2	H	0.49	0/2948	0.64	0/3991
20	g	0.37	0/1959	0.76	0/2725
20	h	0.68	2/3087 (0.1%)	0.88	2/4213 (0.0%)
20	o	0.78	5/3209 (0.2%)	1.03	14/4369 (0.3%)
20	p	0.32	0/2121	0.74	0/2933
21	i	0.26	0/1322	0.61	0/1835
21	j	0.61	1/2333 (0.0%)	1.07	13/3157 (0.4%)
21	q	0.29	0/1322	0.68	0/1835
21	r	0.28	0/1322	0.69	0/1835
22	k	0.33	0/461	0.81	0/642
22	l	0.31	0/461	0.69	0/642
22	s	0.28	0/752	0.57	0/1017
22	t	0.26	0/752	0.53	0/1017



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
23	x	0.37	0/1367	0.57	1/1870 (0.1%)
3	J	0.35	0/2943	0.65	2/3992 (0.1%)
4	K	0.64	0/2316	0.78	3/3135 (0.1%)
5	L	0.63	0/2156	0.77	0/2906
All	All	0.57	16/82758 (0.0%)	0.76	89/112699 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
14	Z	0	1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	n	553	TYR	CD1-CE1	-7.94	1.27	1.39
20	o	552	TRP	CB-CG	-7.30	1.37	1.50
19	m	702	TRP	CB-CG	-6.92	1.37	1.50
19	m	546	TRP	CB-CG	-6.77	1.38	1.50
19	m	749	GLU	CG-CD	-6.26	1.42	1.51

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	38	TYR	CB-CG-CD2	-10.52	114.69	121.00
20	o	513	LEU	CA-CB-CG	10.41	139.24	115.30
1	E	256	PHE	CB-CG-CD2	-10.13	113.71	120.80
1	C	38	TYR	CB-CG-CD2	-10.10	114.94	121.00
1	C	256	PHE	CB-CG-CD2	-9.94	113.84	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	Z	1038	UNK	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2956	0	2947	38	0
1	B	2956	0	2950	54	0
1	C	2956	0	2950	42	0
1	D	2956	0	2950	52	0
1	E	2956	0	2950	45	0
1	F	2956	0	2948	62	0
1	G	2956	0	2947	56	0
1	I	2956	0	2950	46	0
2	H	2885	0	2856	36	0
3	J	2883	0	2972	45	0
4	K	2264	0	2186	77	0
5	L	2122	0	2113	56	0
6	M	2935	0	599	7	0
7	N	3080	0	633	11	0
8	O	323	0	73	7	0
8	P	323	0	74	8	0
9	Q	435	0	93	11	0
9	R	435	0	93	2	0
10	U	843	0	376	5	0
11	V	812	0	344	4	0
12	X	1715	0	1026	15	0
13	Y	1315	0	344	5	0
14	Z	260	0	55	7	0
15	a	405	0	378	0	0
16	b	585	0	565	0	0
17	c	256	0	210	0	0
18	d	188	0	171	0	0
19	e	5034	0	2812	0	0
19	f	6939	0	6419	0	0
19	m	6260	0	5109	0	0
19	n	5730	0	4114	0	0
20	g	1961	0	883	0	0
20	h	3010	0	2751	0	0
20	o	3126	0	2973	0	0
20	p	2116	0	1120	0	0
21	i	1327	0	574	0	0
21	j	2284	0	2207	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	q	1327	0	574	0	0
21	r	1327	0	574	0	0
22	k	462	0	192	0	0
22	l	462	0	192	0	0
22	s	742	0	768	0	0
22	t	742	0	768	0	0
23	x	1695	0	968	0	0
24	z	265	0	56	0	0
25	A	27	0	11	2	0
25	B	27	0	12	0	0
25	C	27	0	12	2	0
25	D	27	0	12	2	0
25	E	27	0	12	2	0
25	F	27	0	11	3	0
25	G	27	0	12	3	0
25	I	27	0	12	0	0
25	J	27	0	11	1	0
26	H	31	0	12	1	0
All	All	92795	0	71924	640	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 9.

The worst 5 of 640 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:46:LEU:O	4:K:50:ALA:HB3	1.69	0.92
8:O:64:UNK:HA	8:O:76:UNK:O	1.71	0.89
1:G:36:PRO:HB2	1:G:38:TYR:CE1	2.07	0.89
4:K:43:ASP:O	4:K:47:ARG:HB2	1.73	0.88
1:D:206:HIS:N	1:D:210:GLU:OE2	2.08	0.86

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	334 (91%)	34 (9%)	0	100	100
1	B	368/376 (98%)	338 (92%)	30 (8%)	0	100	100
1	C	368/376 (98%)	341 (93%)	27 (7%)	0	100	100
1	D	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	E	368/376 (98%)	335 (91%)	33 (9%)	0	100	100
1	F	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	G	368/376 (98%)	342 (93%)	26 (7%)	0	100	100
1	I	368/376 (98%)	342 (93%)	26 (7%)	0	100	100
2	H	368/375 (98%)	345 (94%)	23 (6%)	0	100	100
3	J	363/390 (93%)	336 (93%)	27 (7%)	0	100	100
4	K	276/286 (96%)	244 (88%)	32 (12%)	0	100	100
5	L	267/272 (98%)	233 (87%)	34 (13%)	0	100	100
10	U	169/190 (89%)	126 (75%)	41 (24%)	2 (1%)	15	57
11	V	163/182 (90%)	125 (77%)	36 (22%)	2 (1%)	15	57
12	X	220/389 (57%)	216 (98%)	4 (2%)	0	100	100
15	a	48/66 (73%)	43 (90%)	5 (10%)	0	100	100
16	b	71/89 (80%)	58 (82%)	13 (18%)	0	100	100
17	c	33/50 (66%)	26 (79%)	7 (21%)	0	100	100
18	d	22/26 (85%)	16 (73%)	6 (27%)	0	100	100
19	e	868/1053 (82%)	807 (93%)	60 (7%)	1 (0%)	55	88
19	f	871/1053 (83%)	796 (91%)	75 (9%)	0	100	100
19	m	868/1053 (82%)	797 (92%)	70 (8%)	1 (0%)	55	88
19	n	870/1053 (83%)	797 (92%)	73 (8%)	0	100	100
20	g	393/612 (64%)	314 (80%)	77 (20%)	2 (0%)	32	73
20	h	394/612 (64%)	332 (84%)	59 (15%)	3 (1%)	22	65
20	o	393/612 (64%)	321 (82%)	70 (18%)	2 (0%)	32	73
20	p	397/612 (65%)	329 (83%)	68 (17%)	0	100	100
21	i	258/492 (52%)	226 (88%)	32 (12%)	0	100	100
21	j	280/492 (57%)	216 (77%)	60 (21%)	4 (1%)	13	53
21	q	258/492 (52%)	215 (83%)	43 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	r	258/492 (52%)	217 (84%)	41 (16%)	0	100	100
22	k	91/96 (95%)	72 (79%)	19 (21%)	0	100	100
22	l	91/96 (95%)	76 (84%)	14 (15%)	1 (1%)	17	59
22	s	91/96 (95%)	82 (90%)	9 (10%)	0	100	100
22	t	91/96 (95%)	83 (91%)	8 (9%)	0	100	100
23	x	220/392 (56%)	218 (99%)	2 (1%)	0	100	100
All	All	11636/14727 (79%)	10362 (89%)	1256 (11%)	18 (0%)	54	85

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	U	79	PRO
20	o	467	PHE
20	h	491	LEU
21	j	246	TYR
20	o	469	HIS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/324 (98%)	318 (100%)	0	100	100
1	B	318/324 (98%)	315 (99%)	3 (1%)	82	93
1	C	318/324 (98%)	316 (99%)	2 (1%)	89	96
1	D	318/324 (98%)	318 (100%)	0	100	100
1	E	318/324 (98%)	317 (100%)	1 (0%)	94	98
1	F	318/324 (98%)	317 (100%)	1 (0%)	94	98
1	G	318/324 (98%)	316 (99%)	2 (1%)	89	96
1	I	318/324 (98%)	317 (100%)	1 (0%)	94	98
2	H	313/318 (98%)	313 (100%)	0	100	100
3	J	323/338 (96%)	323 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	K	247/254 (97%)	247 (100%)	0	100	100
5	L	238/241 (99%)	238 (100%)	0	100	100
12	X	74/282 (26%)	74 (100%)	0	100	100
15	a	45/57 (79%)	45 (100%)	0	100	100
16	b	64/76 (84%)	64 (100%)	0	100	100
17	c	22/44 (50%)	22 (100%)	0	100	100
18	d	21/22 (96%)	21 (100%)	0	100	100
19	e	125/891 (14%)	125 (100%)	0	100	100
19	f	643/891 (72%)	643 (100%)	0	100	100
19	m	453/891 (51%)	450 (99%)	3 (1%)	87	95
19	n	307/891 (34%)	302 (98%)	5 (2%)	68	87
20	h	307/531 (58%)	305 (99%)	2 (1%)	87	95
20	o	344/531 (65%)	341 (99%)	3 (1%)	82	93
20	p	37/531 (7%)	35 (95%)	2 (5%)	26	63
21	j	244/422 (58%)	242 (99%)	2 (1%)	85	94
22	s	87/89 (98%)	85 (98%)	2 (2%)	56	82
22	t	87/89 (98%)	86 (99%)	1 (1%)	78	91
23	x	64/282 (23%)	63 (98%)	1 (2%)	68	87
All	All	6589/10263 (64%)	6558 (100%)	31 (0%)	91	96

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	m	264	ARG
19	n	264	ARG
22	s	70	ARG
19	m	658	LEU
19	n	292	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
19	f	311	HIS
19	f	891	HIS
22	s	36	ASN

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Mol	Chain	Res	Type
19	f	421	GLN
19	f	731	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
25	ADP	A	800	-	25,29,29	0.99	2 (8%)	24,45,45	1.98	4 (16%)
25	ADP	B	800	-	25,29,29	1.15	1 (4%)	24,45,45	1.83	5 (20%)
25	ADP	C	800	-	25,29,29	1.05	1 (4%)	24,45,45	1.84	3 (12%)
25	ADP	D	800	-	25,29,29	1.25	4 (16%)	24,45,45	1.47	4 (16%)
25	ADP	E	800	-	25,29,29	1.05	0	24,45,45	1.55	3 (12%)
25	ADP	F	800	-	25,29,29	1.16	1 (4%)	24,45,45	1.74	3 (12%)
25	ADP	G	800	-	25,29,29	1.06	2 (8%)	24,45,45	1.44	2 (8%)
26	ATP	H	401	-	27,33,33	0.92	1 (3%)	25,52,52	1.68	2 (8%)
25	ADP	I	800	-	25,29,29	0.97	1 (4%)	24,45,45	1.56	3 (12%)
25	ADP	J	800	-	25,29,29	0.96	1 (4%)	24,45,45	1.70	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	ADP	A	800	-	-	0/12/32/32	0/3/3/3
25	ADP	B	800	-	-	0/12/32/32	0/3/3/3
25	ADP	C	800	-	-	0/12/32/32	0/3/3/3
25	ADP	D	800	-	-	0/12/32/32	0/3/3/3
25	ADP	E	800	-	-	0/12/32/32	0/3/3/3
25	ADP	F	800	-	-	0/12/32/32	0/3/3/3
25	ADP	G	800	-	-	0/12/32/32	0/3/3/3
26	ATP	H	401	-	-	0/18/38/38	0/3/3/3
25	ADP	I	800	-	-	0/12/32/32	0/3/3/3
25	ADP	J	800	-	-	0/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	800	ADP	C2'-C1'	-2.90	1.49	1.53
25	F	800	ADP	C2'-C1'	-2.63	1.49	1.53
25	G	800	ADP	C2'-C1'	-2.55	1.49	1.53
25	D	800	ADP	C2'-C1'	-2.54	1.49	1.53
25	A	800	ADP	C2'-C1'	-2.20	1.50	1.53

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	800	ADP	N3-C2-N1	-6.59	123.12	128.86
25	C	800	ADP	N3-C2-N1	-6.17	123.49	128.86
25	J	800	ADP	N3-C2-N1	-5.90	123.72	128.86
25	F	800	ADP	N3-C2-N1	-5.63	123.96	128.86
25	B	800	ADP	N3-C2-N1	-5.54	124.03	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	800	ADP	2	0
25	C	800	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	800	ADP	2	0
25	E	800	ADP	2	0
25	F	800	ADP	3	0
25	G	800	ADP	3	0
26	H	401	ATP	1	0
25	J	800	ADP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	Y	11
7	N	5
6	M	5
8	P	3
8	O	3
9	Q	2
9	R	2

The worst 5 of 31 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	171:UNK	C	201:UNK	N	99.45
1	M	171:UNK	C	201:UNK	N	95.63
1	N	367:UNK	C	401:UNK	N	94.83
1	M	367:UNK	C	401:UNK	N	83.96
1	M	625:UNK	C	701:UNK	N	67.24