wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 11:14 pm GMT

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 EM 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/EMValidationReportHelp
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:

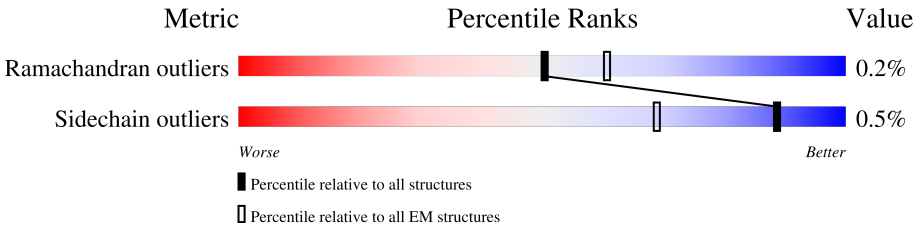
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	98%
1	B	376	97%
1	C	376	98%
1	D	376	98%
1	E	376	98%
1	F	376	97%
1	G	376	98%
1	I	376	98%
2	H	375	99%

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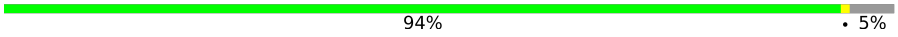
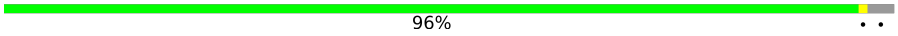
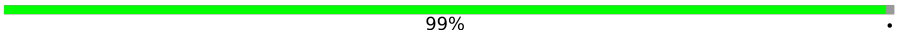
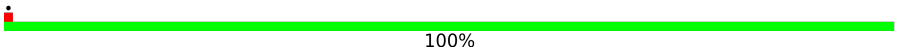
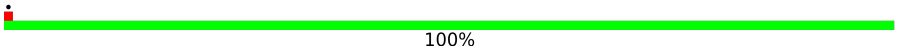
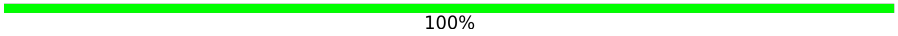
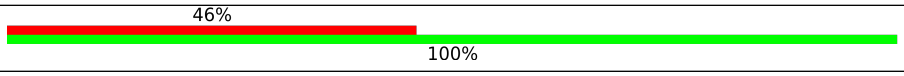
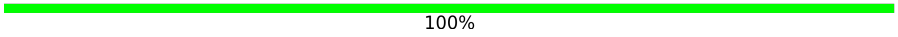
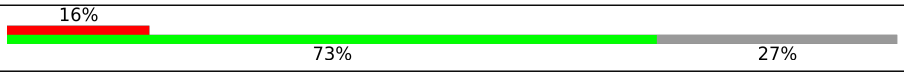
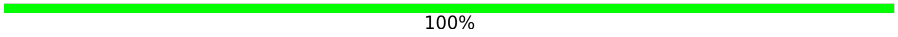
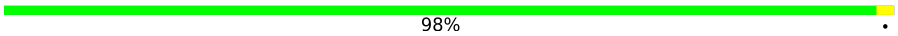
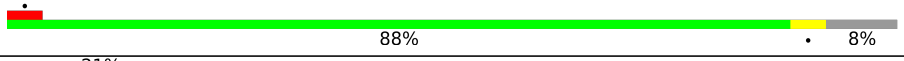
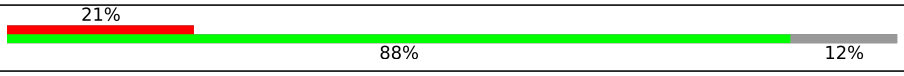
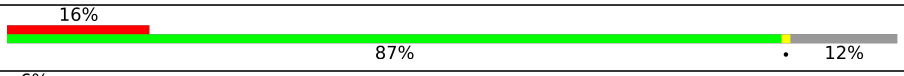
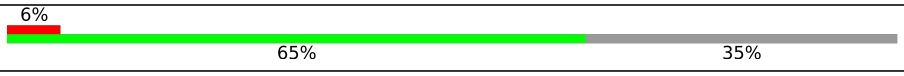
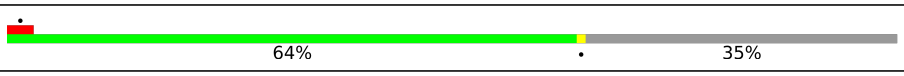
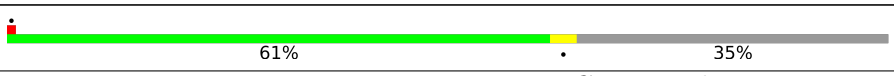
Mol	Chain	Length	Quality of chain
3	J	390	
4	K	286	
5	L	272	
6	M	589	
7	N	618	
8	O	65	
8	P	65	
9	Q	87	
9	R	87	
10	U	190	
11	V	182	
12	X	389	
13	Y	263	
14	Z	52	
15	a	66	
16	b	89	
17	c	50	
18	d	26	
19	e	1053	
19	f	1053	
19	m	1053	
19	n	1053	
20	g	612	
20	h	612	
20	o	612	

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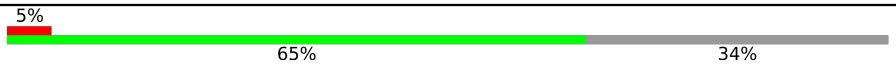
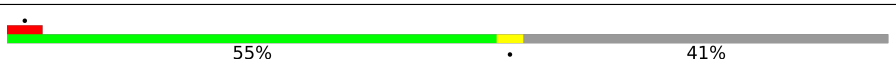
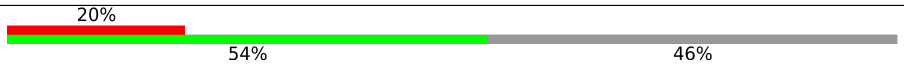
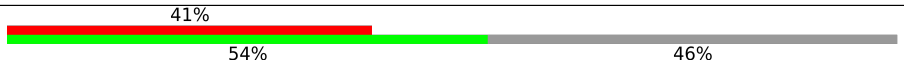
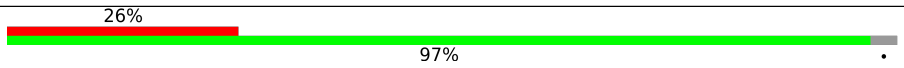
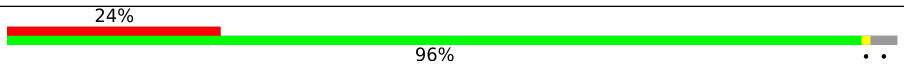
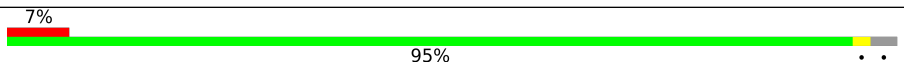
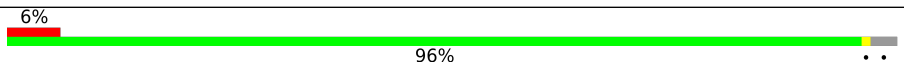
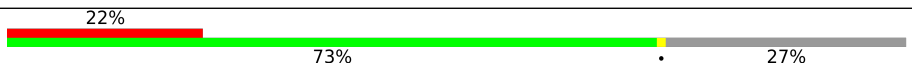
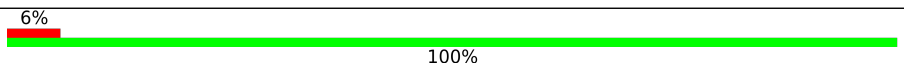
Mol	Chain	Length	Quality of chain
20	p	612	
21	i	492	
21	j	492	
21	q	492	
21	r	492	
22	k	96	
22	l	96	
22	s	96	
22	t	96	
23	x	392	
24	z	53	

2 Entry composition (i)

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

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 1327 791 268 268	0	0
21	j	288	Total C N O S 2284 1463 379 431 11	0	0
21	q	268	Total C N O 1327 791 268 268	0	0
21	r	268	Total C N O 1327 791 268 268	0	0

- 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 462 276 93 93	0	0
22	l	93	Total C N O 462 276 93 93	0	0
22	s	93	Total C N O S 742 468 128 143 3	0	0
22	t	93	Total C N O S 742 468 128 143 3	0	0

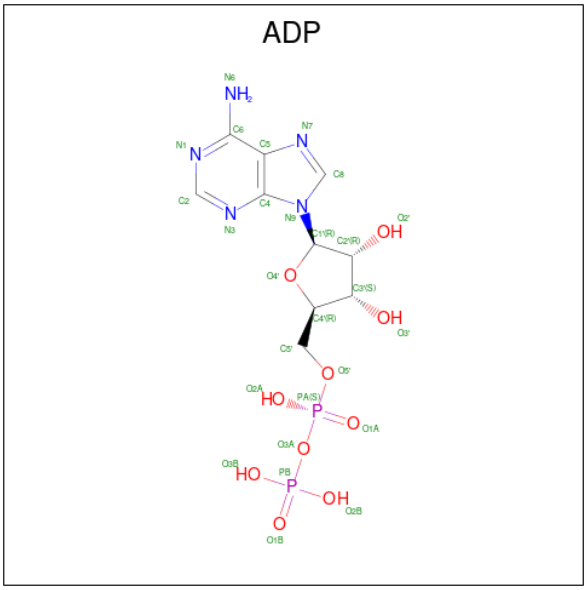
- Molecule 23 is a protein called BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1.

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

- Molecule 24 is a protein called Dynactin Subunit 1.

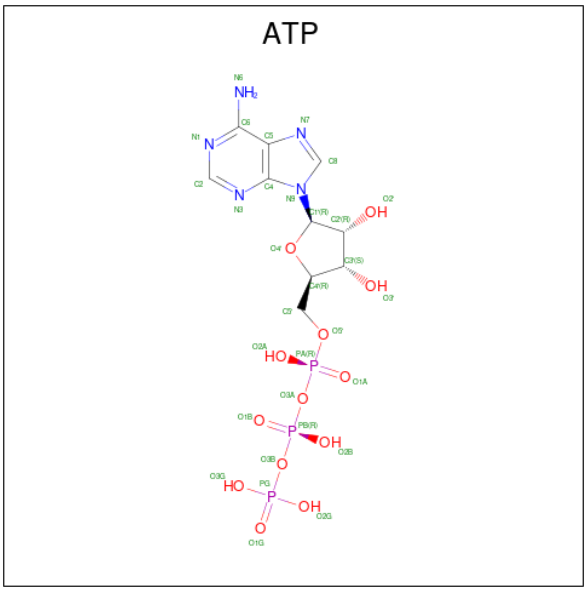
Mol	Chain	Residues	Atoms				AltConf	Trace
24	z	53	Total	C	N	O	0	0
			265	159	53	53		

- 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
25	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
25	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



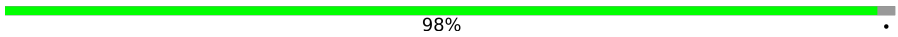
Mol	Chain	Residues	Atoms					AltConf
26	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

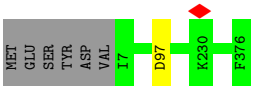
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

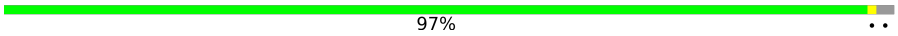
Chain A:

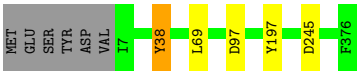




• Molecule 1: ARP1 actin related protein 1 homolog A

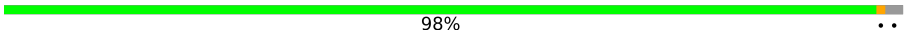
Chain B:

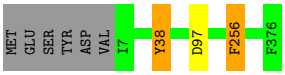




• Molecule 1: ARP1 actin related protein 1 homolog A

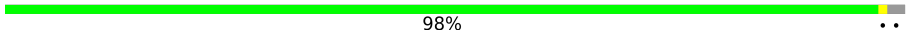
Chain C:

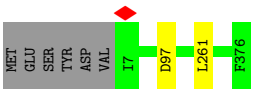




• Molecule 1: ARP1 actin related protein 1 homolog A

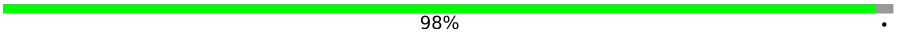
Chain D:

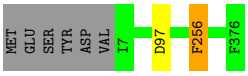




• Molecule 1: ARP1 actin related protein 1 homolog A

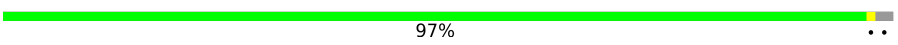
Chain E:

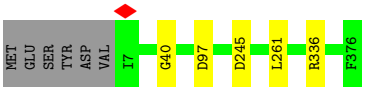




• Molecule 1: ARP1 actin related protein 1 homolog A

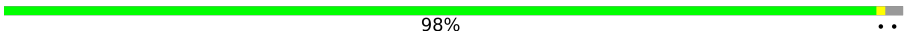
Chain F:

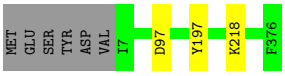




• Molecule 1: ARP1 actin related protein 1 homolog A

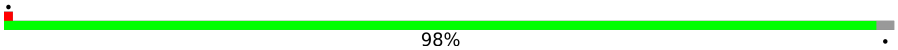
Chain G:

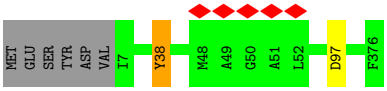




• Molecule 1: ARP1 actin related protein 1 homolog A

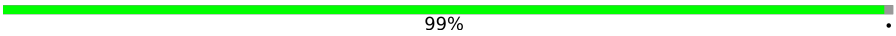
Chain I:

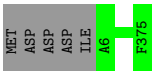




• Molecule 2: Actin, cytoplasmic 1

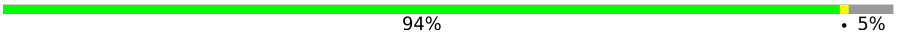
Chain H:

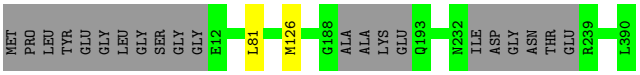




• Molecule 3: Actin related protein 10 homolog

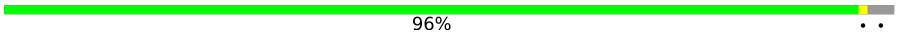
Chain J:





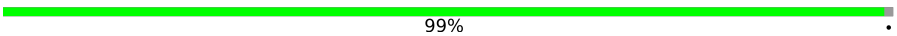
• Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

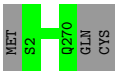
Chain K:



• Molecule 5: F-actin capping protein beta subunit

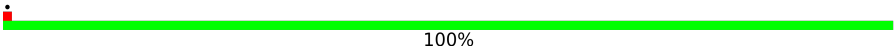
Chain L:

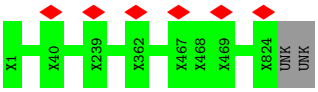




• Molecule 6: Dynactin Subunit 2

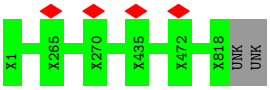
Chain M:





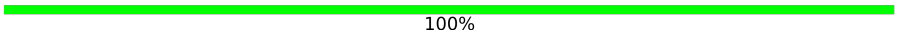
• Molecule 7: Dynactin Subunit 2

Chain N:



• Molecule 8: Dynactin Subunit 3

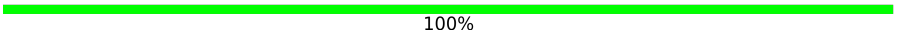
Chain O:



There are no outlier residues recorded for this chain.

• Molecule 8: Dynactin Subunit 3

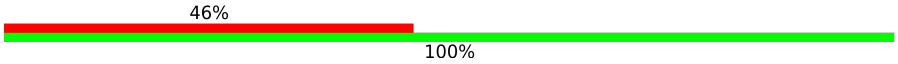
Chain P:

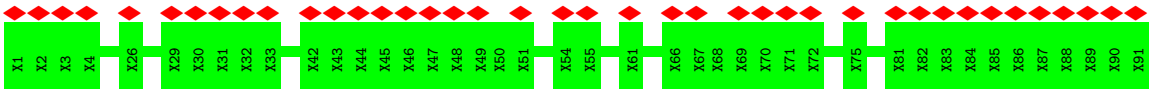


There are no outlier residues recorded for this chain.

• Molecule 9: Dynactin Subunit 2

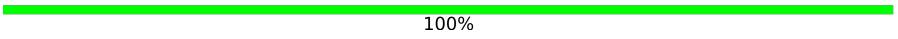
Chain Q:





• Molecule 9: Dynactin Subunit 2

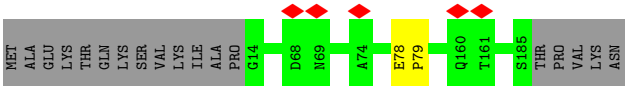
Chain R:



There are no outlier residues recorded for this chain.

• Molecule 10: Dynactin 6

Chain U:

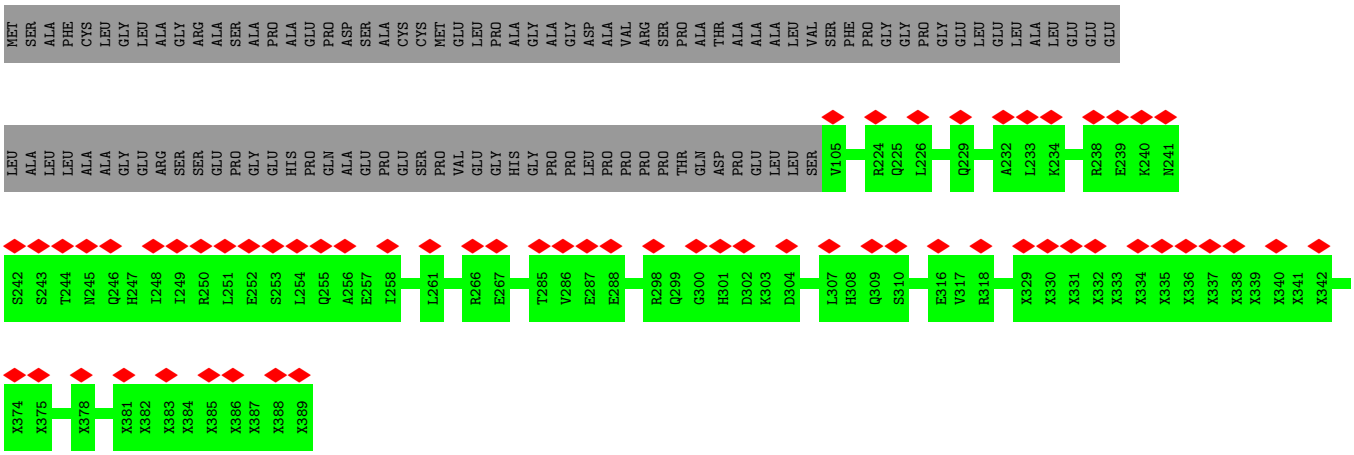


• Molecule 11: Dynactin subunit 5

Chain V:

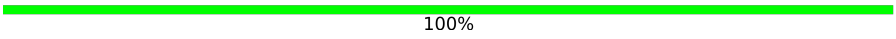
• Molecule 12: BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICDR-1

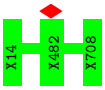
Chain X:



• Molecule 13: Dynactin Subunit 4

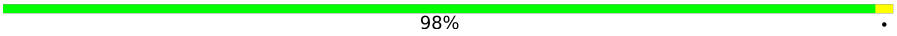
Chain Y:





• Molecule 14: Dynactin Subunit 1

Chain Z:



• Molecule 15: Dynactin subunit 2

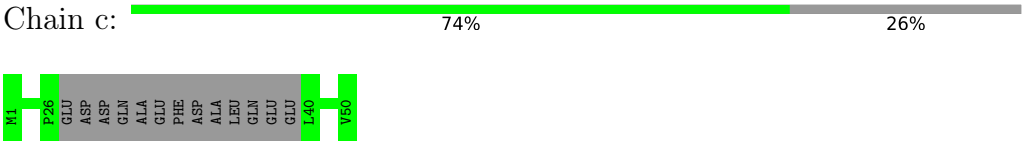
Chain a:

• Molecule 16: Dynactin subunit 2

Chain b:

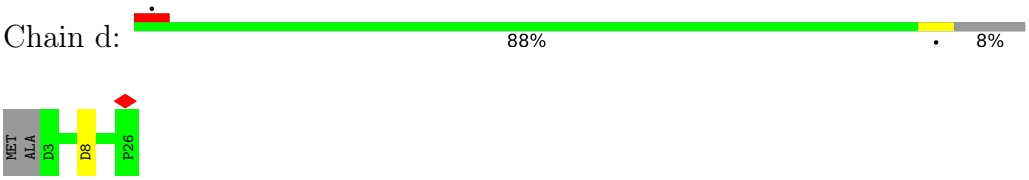
• Molecule 17: Dynactin subunit 2

Chain c:



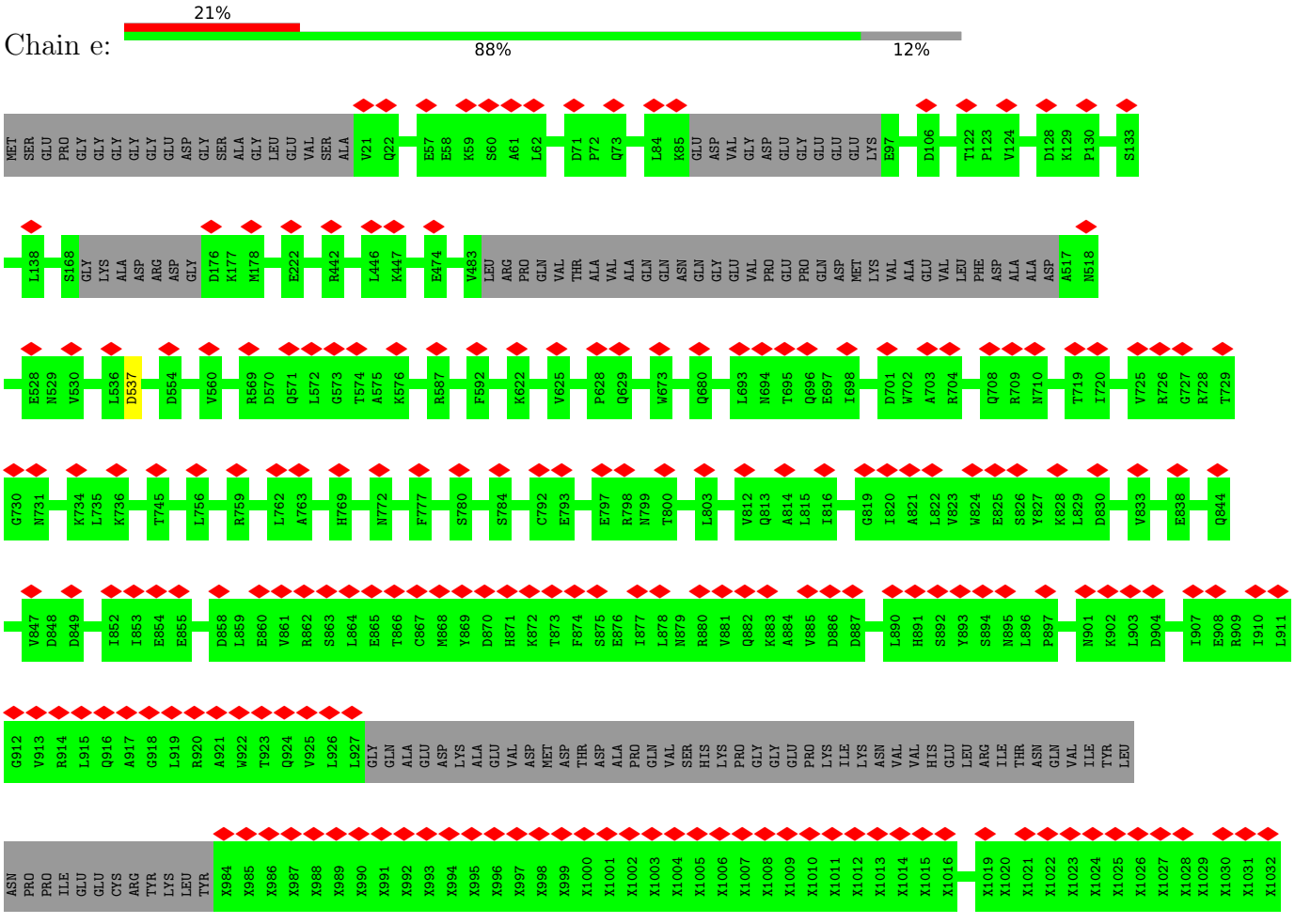
• Molecule 18: Dynactin subunit 2

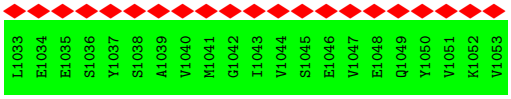
Chain d:



• 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

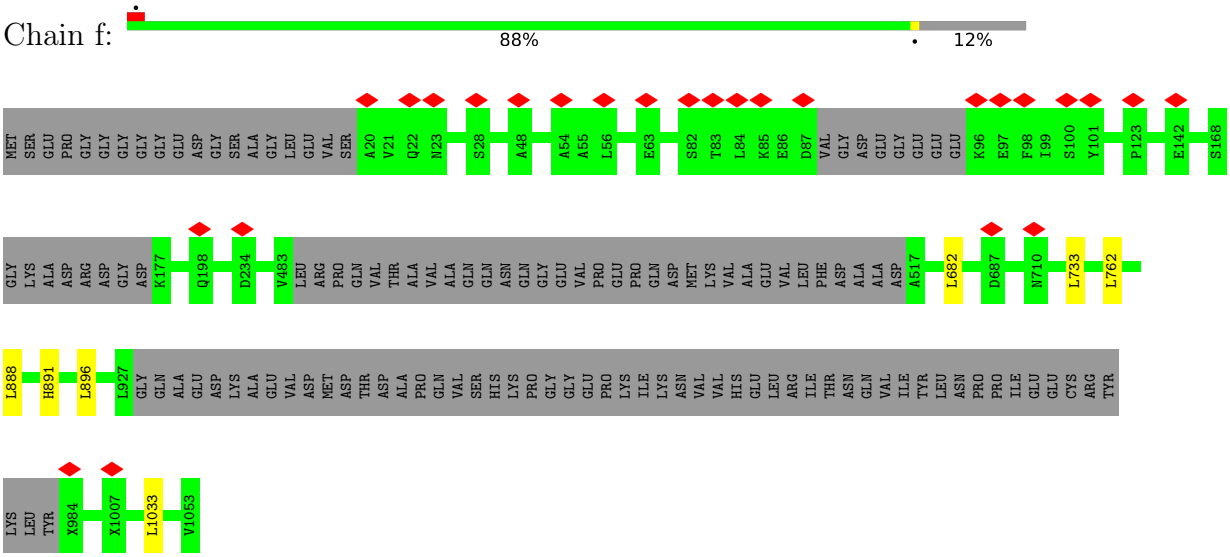
Chain e:





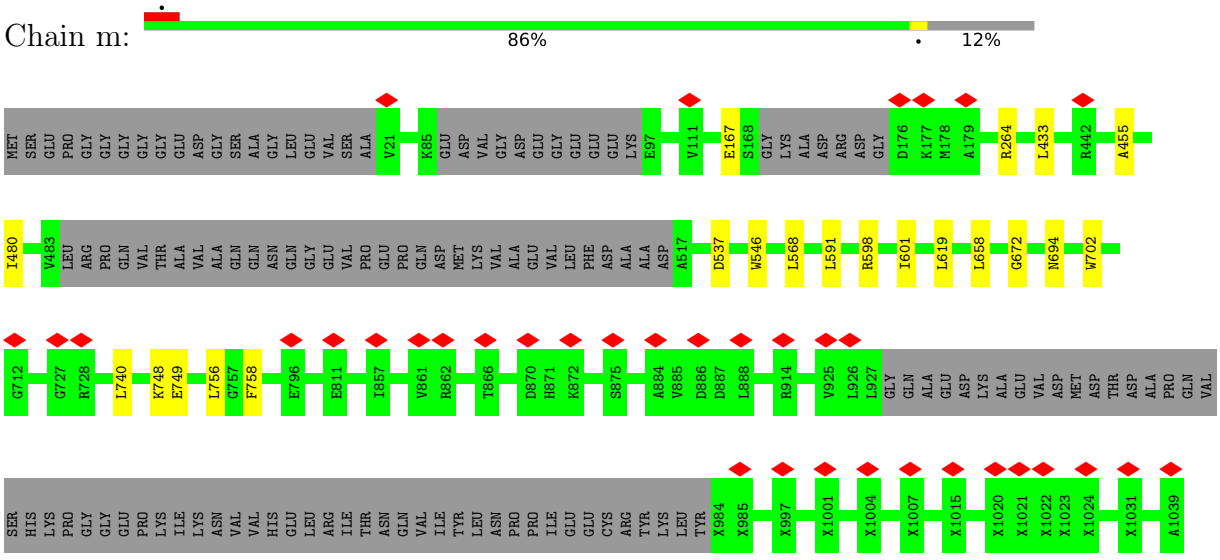
• Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic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

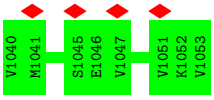
Chain f:



• 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

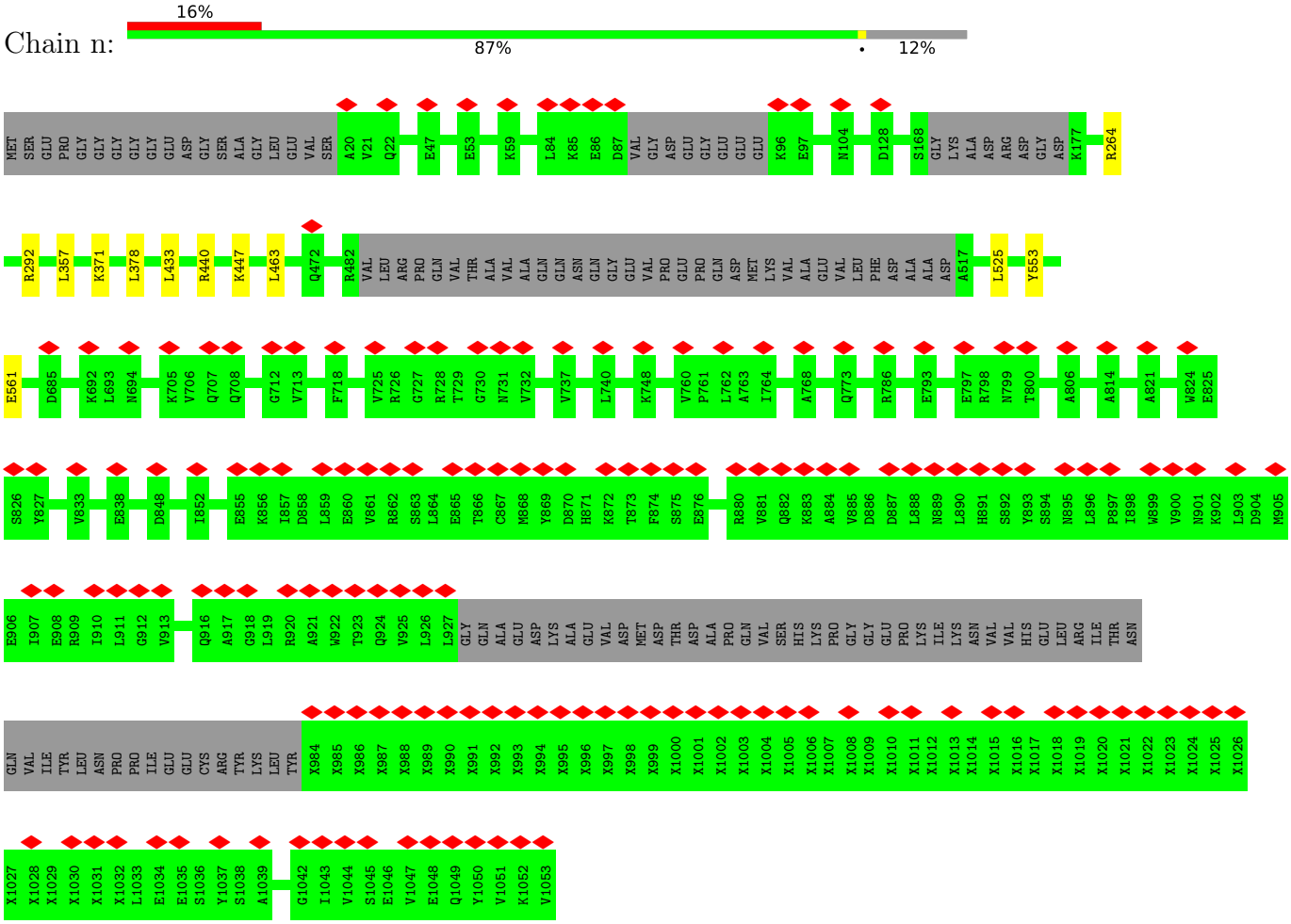
Chain m:





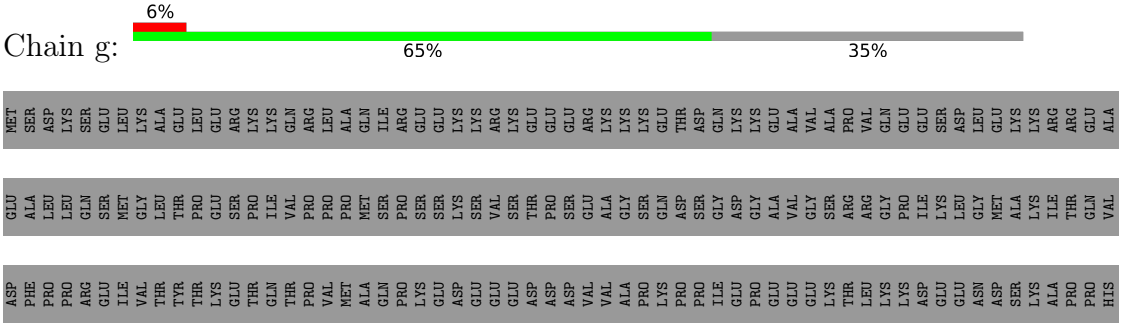
• Molecule 19: Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Cytoplasmic dynein 1 heavy chain 1,Dynein Heavy Chain,Cytoplasmic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

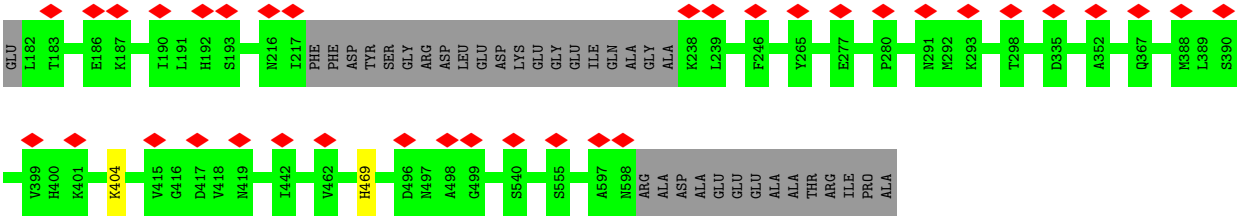
Chain n:



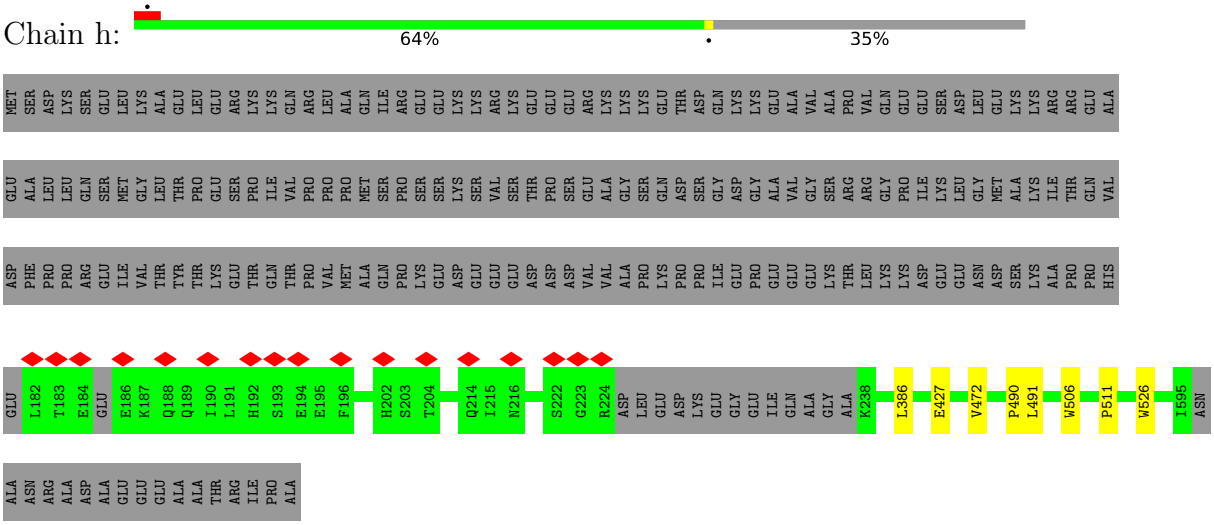
• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

Chain g:

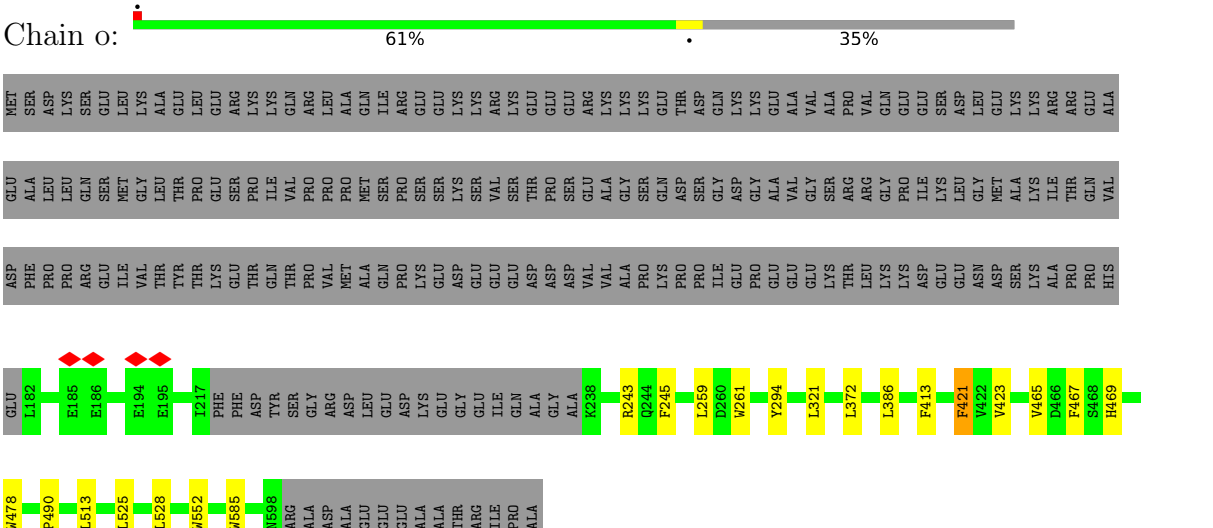




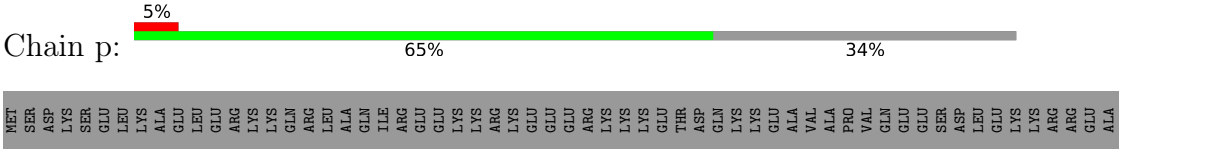
• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2

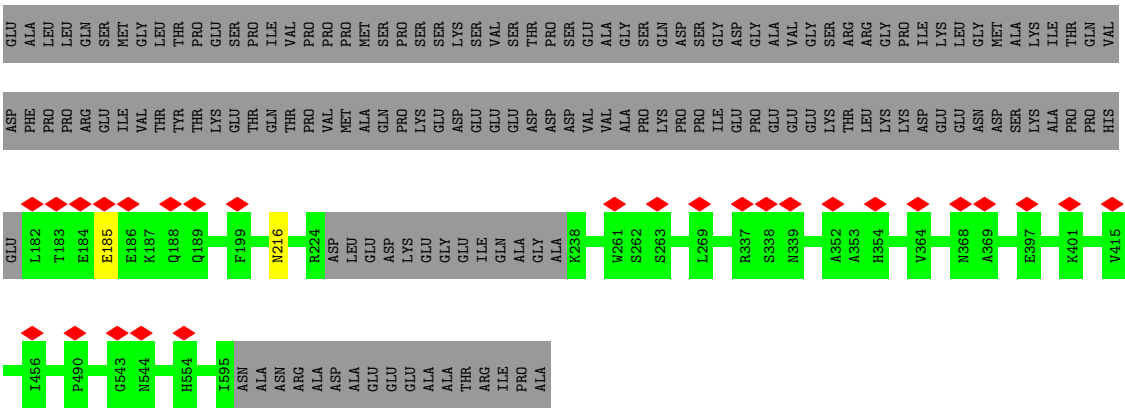


• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2



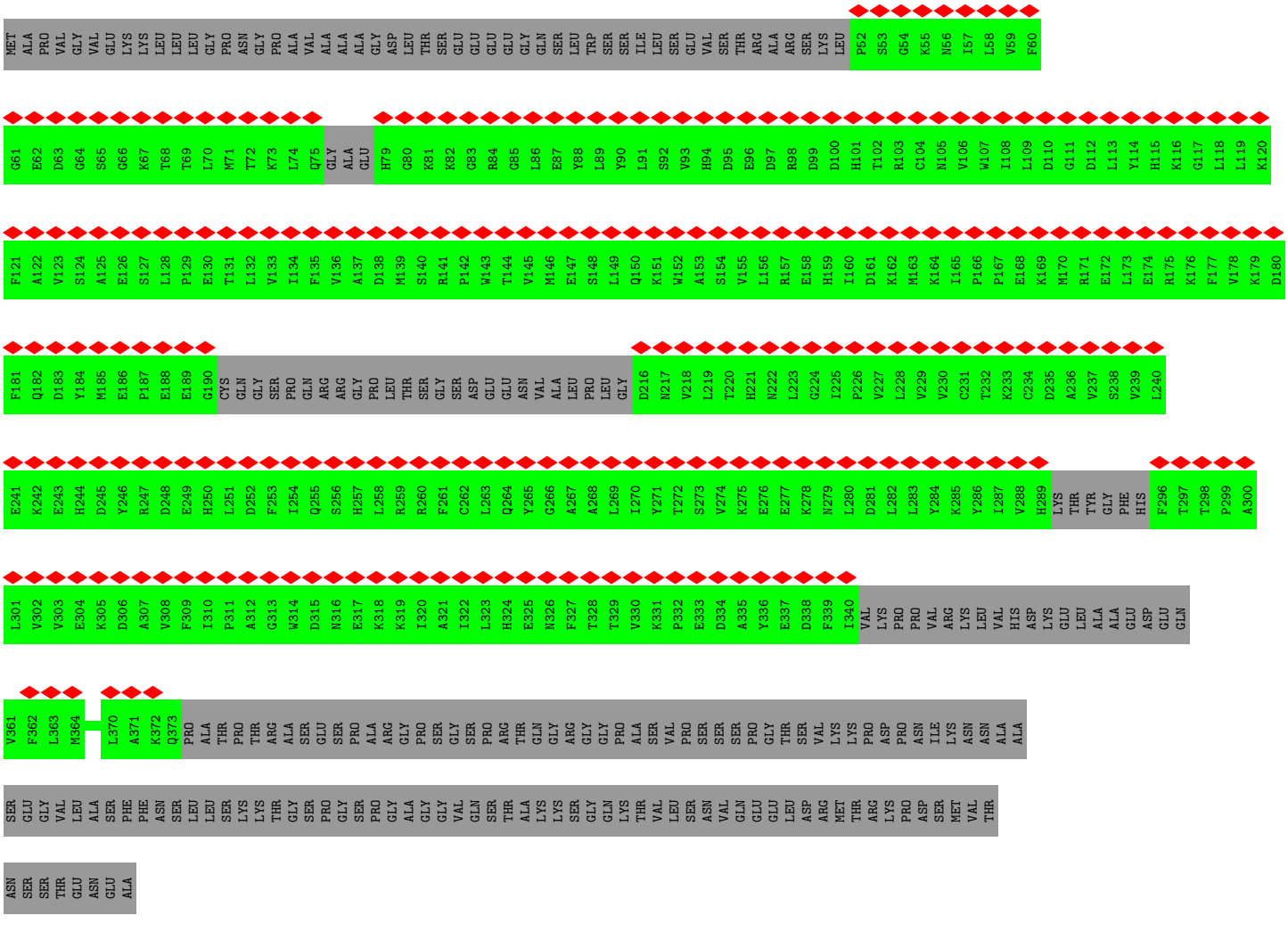
• Molecule 20: Cytoplasmic dynein 1 intermediate chain 2





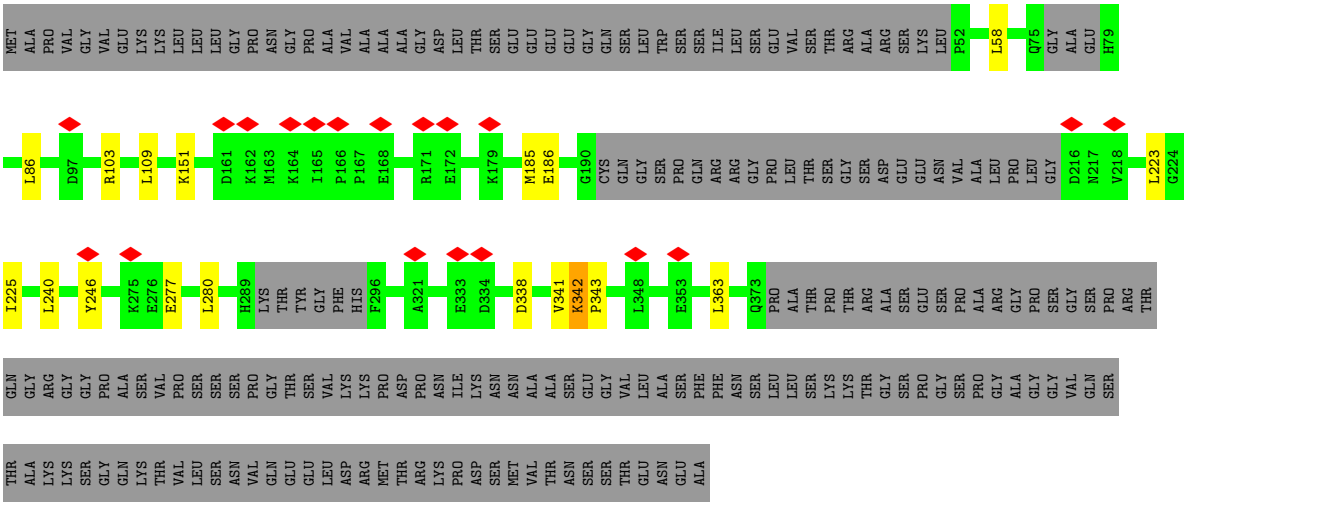
• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

Chain i:



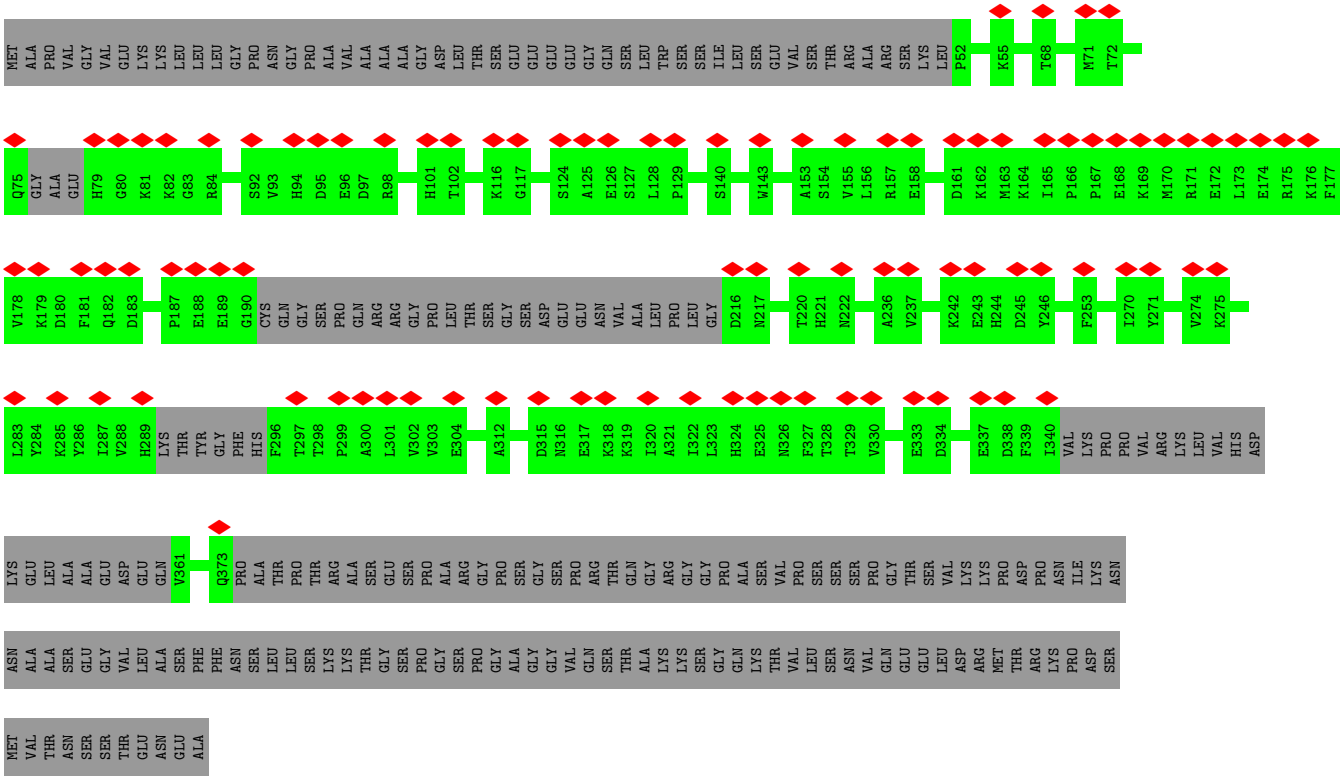
• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

Chain j:



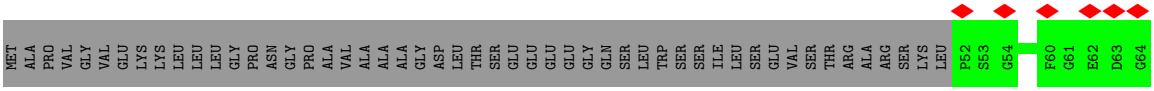
• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

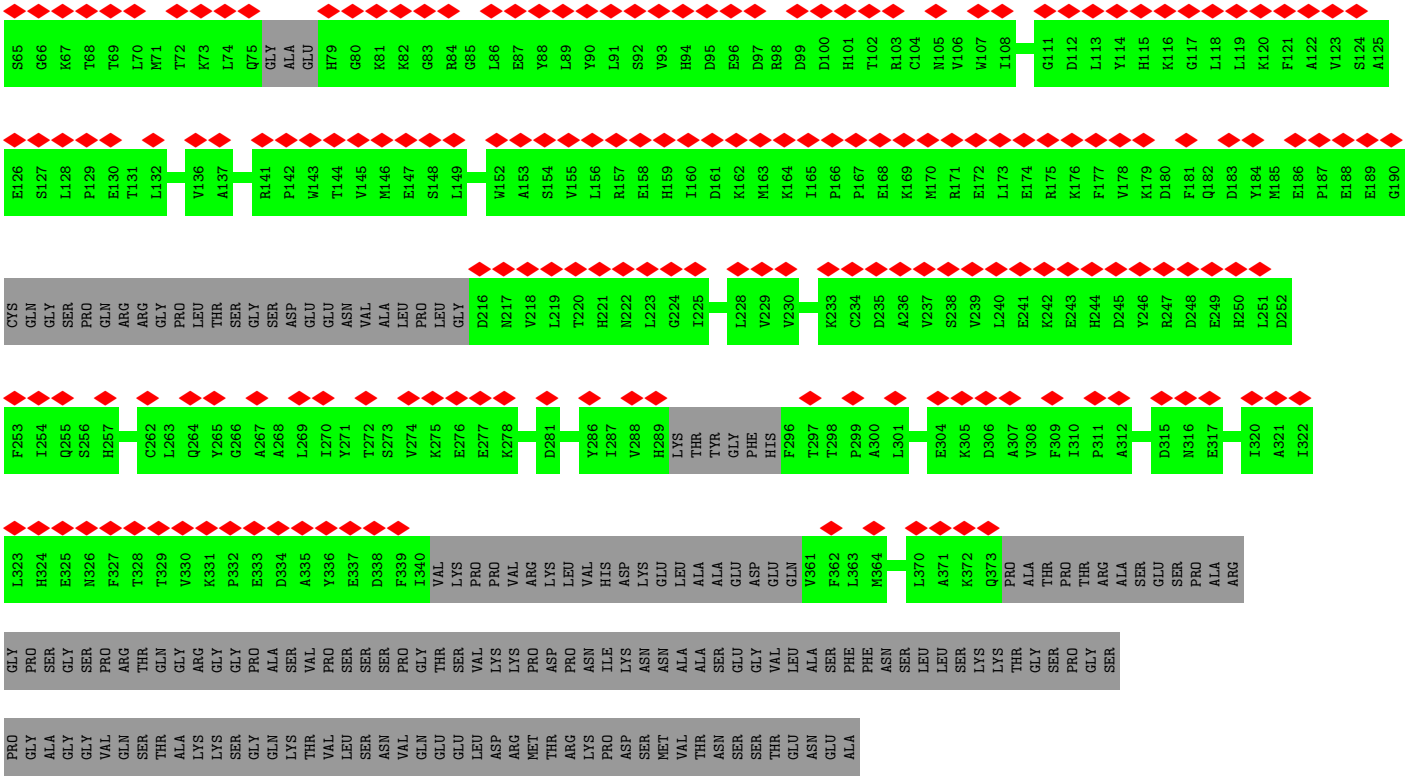
Chain q:



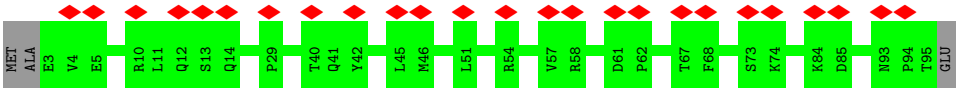
• Molecule 21: Cytoplasmic dynein 1 light intermediate chain 2

Chain r:

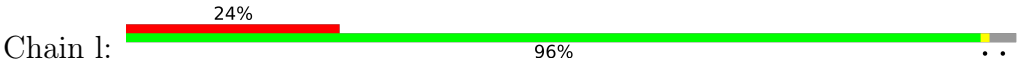


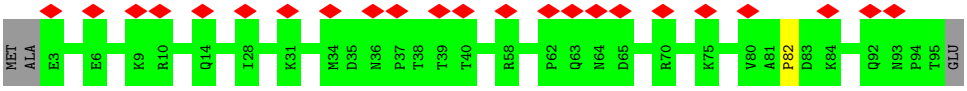


• Molecule 22: Dynein light chain roadblock-type 1

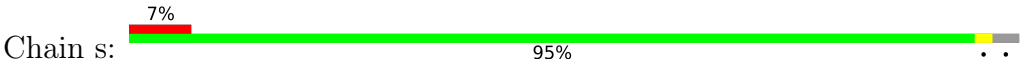


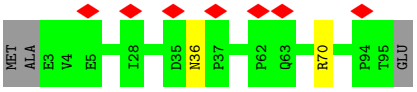
• Molecule 22: Dynein light chain roadblock-type 1



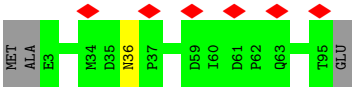


• Molecule 22: Dynein light chain roadblock-type 1



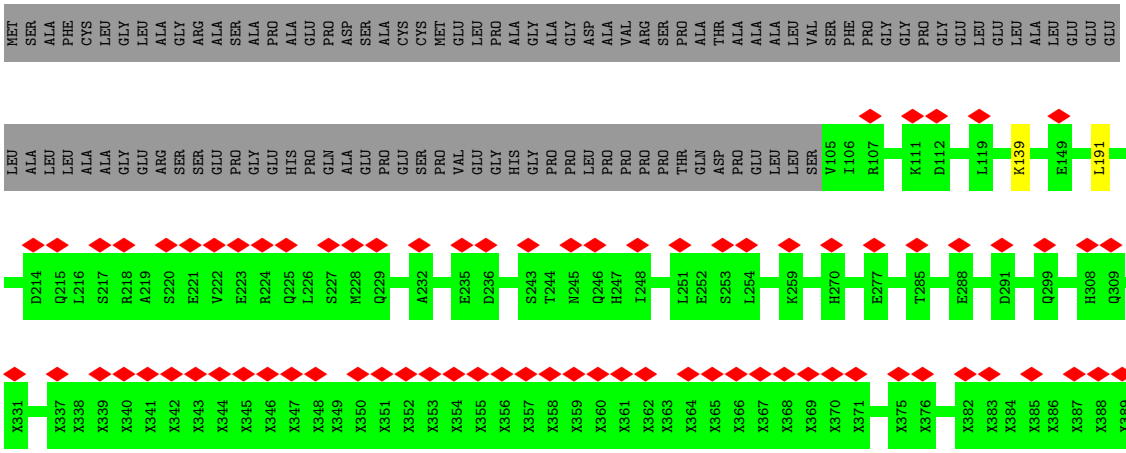


• Molecule 22: Dynein light chain roadblock-type 1



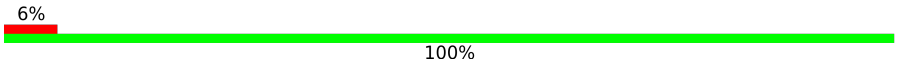
• Molecule 23: BICD family-like cargo adapter 1,BICD family-like cargo adapter 1,BICD family-like cargo adapter 1

Chain x:



• Molecule 24: Dynactin Subunit 1

Chain z:



4 Experimental information (i)

Property	Value	Source
EM 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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.440	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.046	Depositor
Map size (Å)	804.0, 804.0, 804.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
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%)
2	H	0.49	0/2948	0.64	0/3991
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
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%)
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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
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
23	x	0.37	0/1367	0.57	1/1870 (0.1%)
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(^{o})	Ideal(^{o})
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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	13	50
11	V	163/182 (90%)	125 (77%)	36 (22%)	2 (1%)	13	50
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%)	51	84
19	f	871/1053 (83%)	796 (91%)	75 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	m	868/1053 (82%)	797 (92%)	70 (8%)	1 (0%)	51 84
19	n	870/1053 (83%)	797 (92%)	73 (8%)	0	100 100
20	g	393/612 (64%)	314 (80%)	77 (20%)	2 (0%)	29 68
20	h	394/612 (64%)	332 (84%)	59 (15%)	3 (1%)	19 58
20	o	393/612 (64%)	321 (82%)	70 (18%)	2 (0%)	29 68
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%)	11 46
21	q	258/492 (52%)	215 (83%)	43 (17%)	0	100 100
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%)	14 52
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%)	50 81

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	318/324 (98%)	318 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	318/324 (98%)	315 (99%)	3 (1%)	78 90
1	C	318/324 (98%)	316 (99%)	2 (1%)	86 94
1	D	318/324 (98%)	318 (100%)	0	100 100
1	E	318/324 (98%)	317 (100%)	1 (0%)	92 97
1	F	318/324 (98%)	317 (100%)	1 (0%)	92 97
1	G	318/324 (98%)	316 (99%)	2 (1%)	86 94
1	I	318/324 (98%)	317 (100%)	1 (0%)	92 97
2	H	313/318 (98%)	313 (100%)	0	100 100
3	J	323/338 (96%)	323 (100%)	0	100 100
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%)	84 93
19	n	307/891 (34%)	302 (98%)	5 (2%)	62 83
20	h	307/531 (58%)	305 (99%)	2 (1%)	84 93
20	o	344/531 (65%)	341 (99%)	3 (1%)	78 90
20	p	37/531 (7%)	35 (95%)	2 (5%)	22 55
21	j	244/422 (58%)	242 (99%)	2 (1%)	81 91
22	s	87/89 (98%)	85 (98%)	2 (2%)	50 77
22	t	87/89 (98%)	86 (99%)	1 (1%)	73 88
23	x	64/282 (23%)	63 (98%)	1 (2%)	62 83
All	All	6589/10263 (64%)	6558 (100%)	31 (0%)	89 94

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

Mol	Chain	Res	Type
19	m	264	ARG

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Mol	Chain	Res	Type
22	s	36	ASN
19	n	264	ARG
22	t	36	ASN
20	o	465	VAL

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

Mol	Chain	Res	Type
20	p	189	GLN
22	s	24	ASN
3	J	273	GLN
3	J	58	ASN
22	s	36	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	800	-	24,29,29	1.17	2 (8%)	29,45,45	1.87	7 (24%)
25	ADP	I	800	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
25	ADP	A	800	-	24,29,29	1.01	1 (4%)	29,45,45	1.55	4 (13%)
25	ADP	C	800	-	24,29,29	1.07	1 (4%)	29,45,45	1.67	6 (20%)
25	ADP	E	800	-	24,29,29	1.07	1 (4%)	29,45,45	1.54	5 (17%)
25	ADP	F	800	-	24,29,29	1.17	1 (4%)	29,45,45	1.86	5 (17%)
25	ADP	D	800	-	24,29,29	1.24	3 (12%)	29,45,45	1.70	4 (13%)
25	ADP	J	800	-	24,29,29	0.93	1 (4%)	29,45,45	1.51	4 (13%)
25	ADP	G	800	-	24,29,29	1.10	1 (4%)	29,45,45	1.52	3 (10%)
26	ATP	H	401	-	26,33,33	0.91	1 (3%)	31,52,52	1.55	6 (19%)

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	B	800	-	-	3/12/32/32	0/3/3/3
25	ADP	I	800	-	-	0/12/32/32	0/3/3/3
25	ADP	A	800	-	-	4/12/32/32	0/3/3/3
25	ADP	C	800	-	-	4/12/32/32	0/3/3/3
25	ADP	E	800	-	-	3/12/32/32	0/3/3/3
25	ADP	F	800	-	-	4/12/32/32	0/3/3/3
25	ADP	D	800	-	-	4/12/32/32	0/3/3/3
25	ADP	J	800	-	-	6/12/32/32	0/3/3/3
25	ADP	G	800	-	-	0/12/32/32	0/3/3/3
26	ATP	H	401	-	-	7/18/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	800	ADP	C2'-C1'	-3.11	1.49	1.53
25	F	800	ADP	C2'-C1'	-2.83	1.49	1.53
25	G	800	ADP	C2'-C1'	-2.75	1.49	1.53
25	D	800	ADP	C2'-C1'	-2.74	1.49	1.53
25	I	800	ADP	C5-C4	2.55	1.47	1.40

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	F	800	ADP	PA-O3A-PB	-6.65	110.00	132.83
25	B	800	ADP	PA-O3A-PB	-5.71	113.24	132.83
25	D	800	ADP	PA-O3A-PB	-5.17	115.09	132.83
25	C	800	ADP	PA-O3A-PB	-4.75	116.53	132.83
25	G	800	ADP	PA-O3A-PB	-4.18	118.49	132.83

There are no chirality outliers.

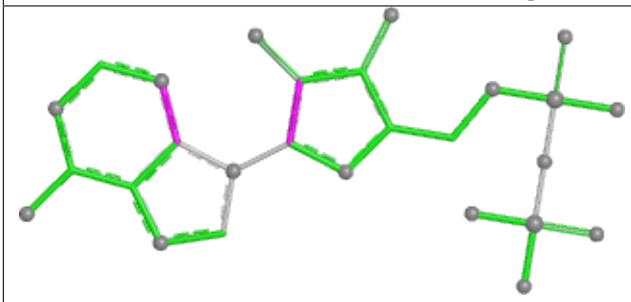
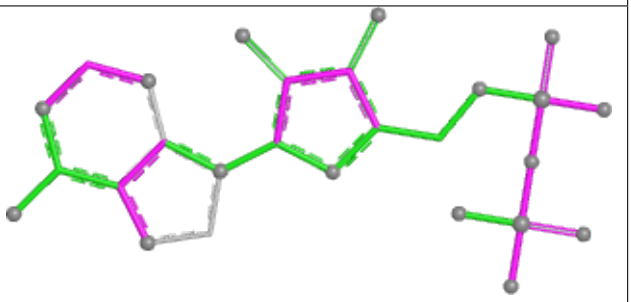
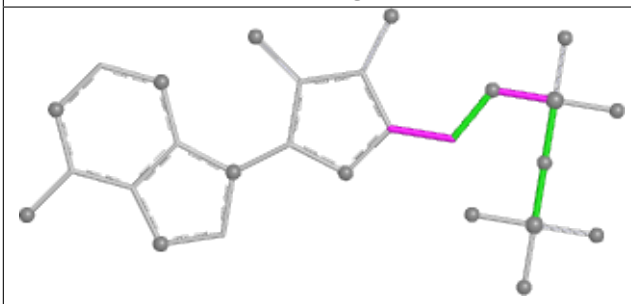
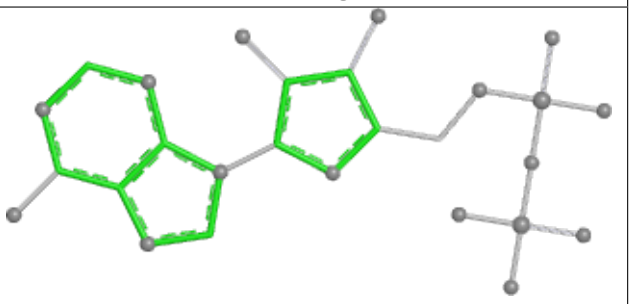
5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	800	ADP	C5'-O5'-PA-O2A
25	A	800	ADP	C5'-O5'-PA-O3A
25	A	800	ADP	O4'-C4'-C5'-O5'
25	A	800	ADP	C3'-C4'-C5'-O5'
25	B	800	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP B 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

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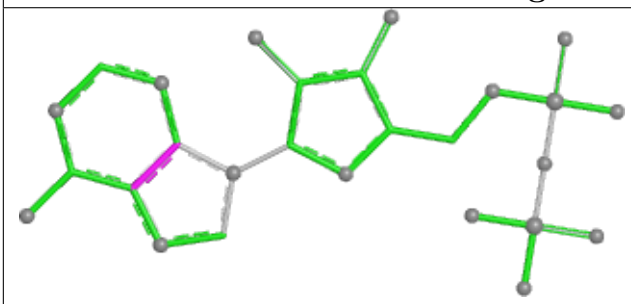
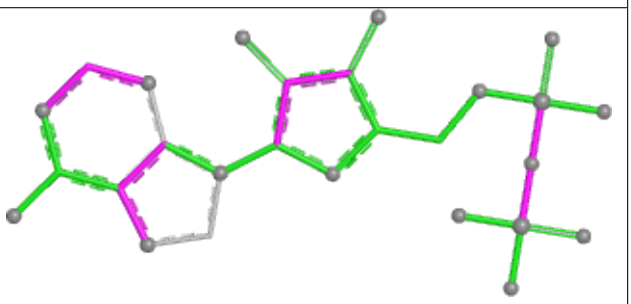
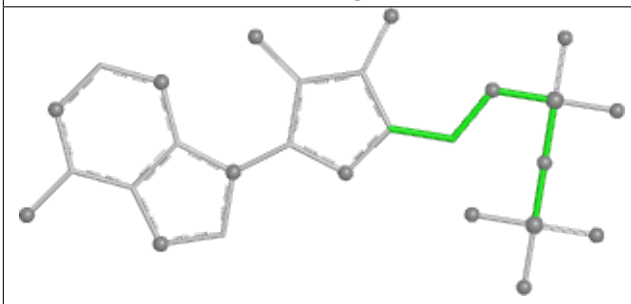
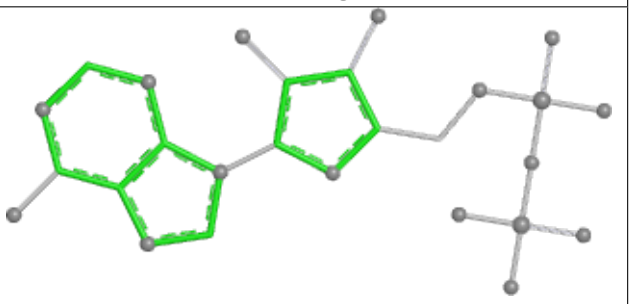
 Bond lengths	 Bond angles
 Torsions	 Rings

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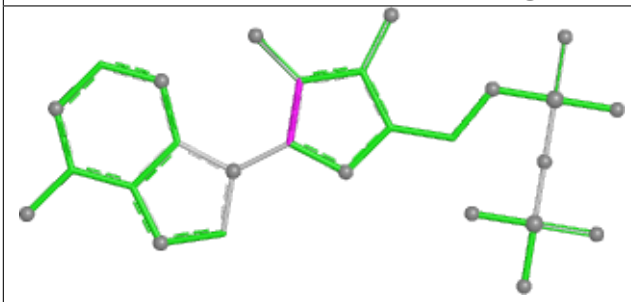
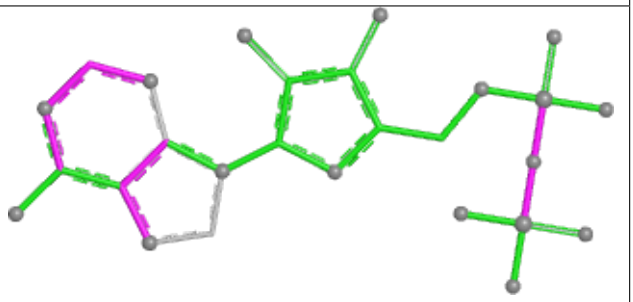
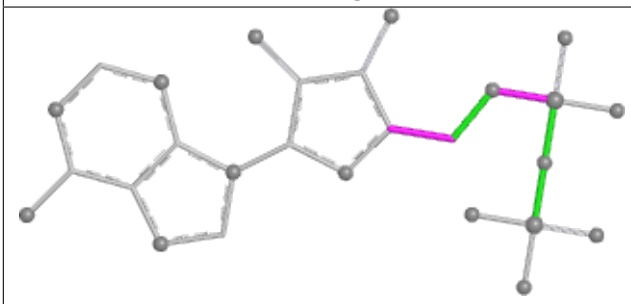


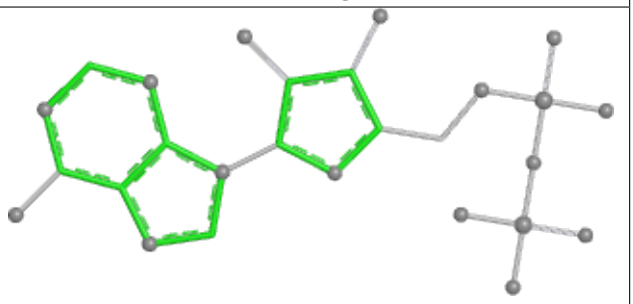
Bond lengths



Bond angles

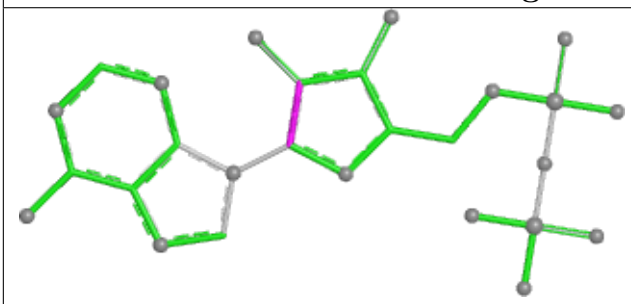


Torsions

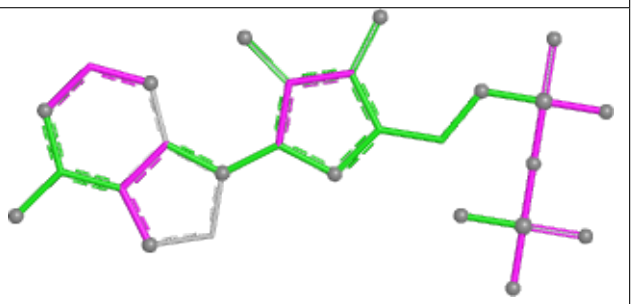


Rings

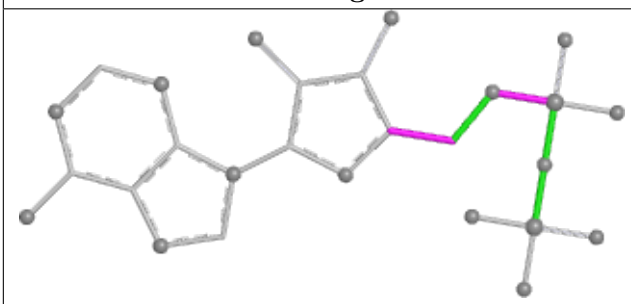
Ligand ADP C 800



Bond lengths



Bond angles



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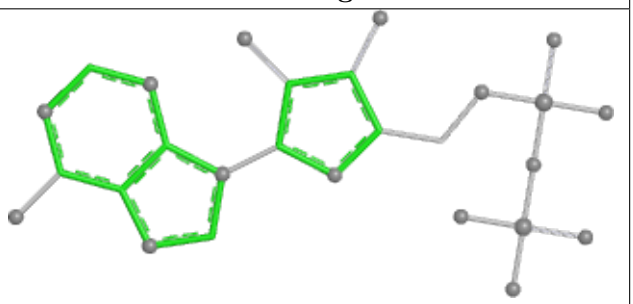

Rings

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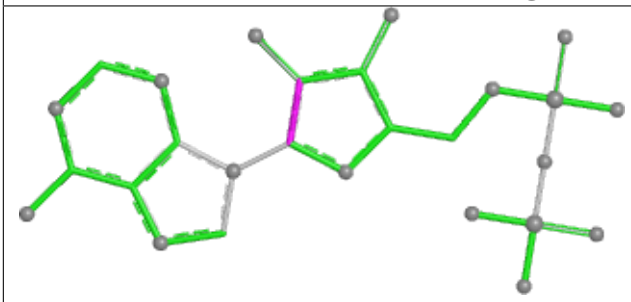
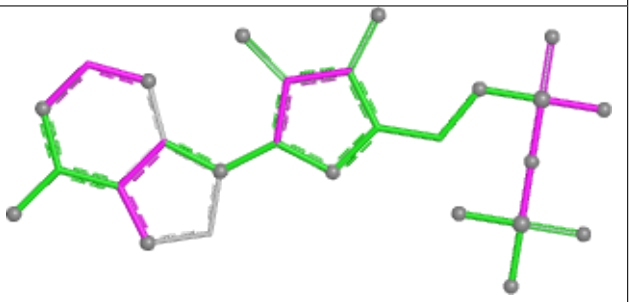
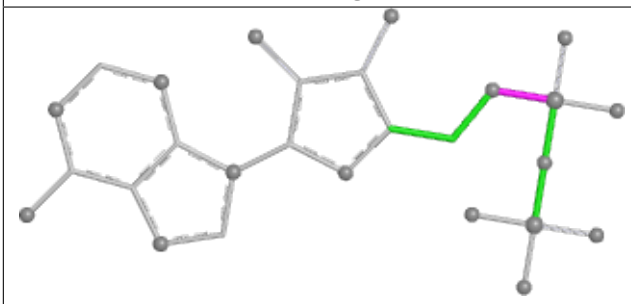
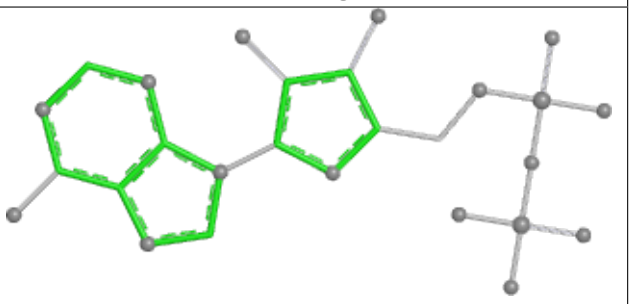
 Bond lengths	 Bond angles
 Torsions	 Rings

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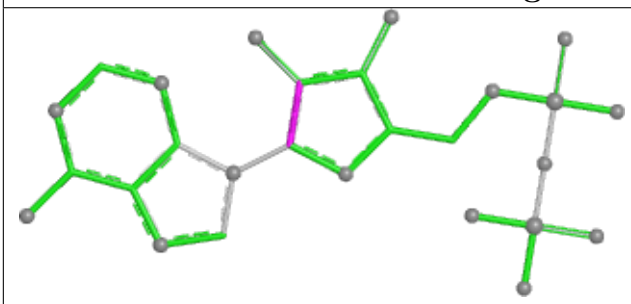
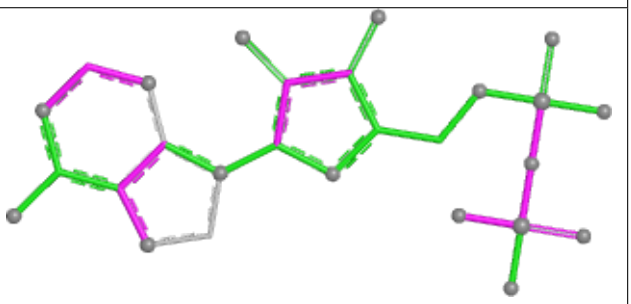
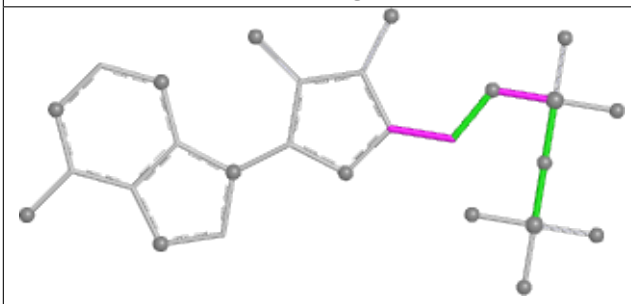
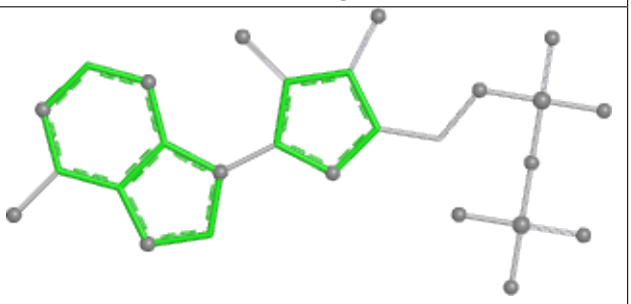
 Bond lengths	 Bond angles
 Torsions	 Rings

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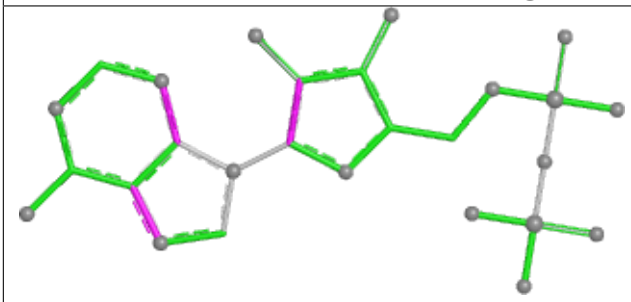
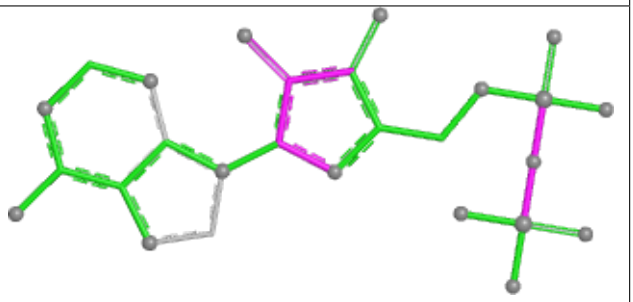
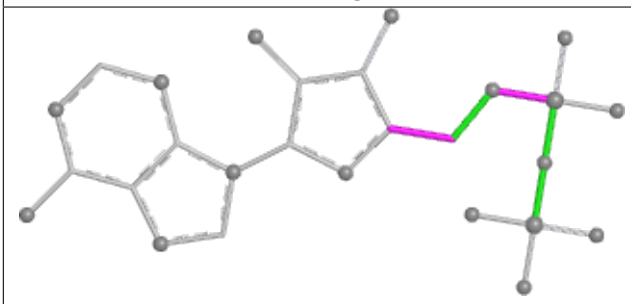


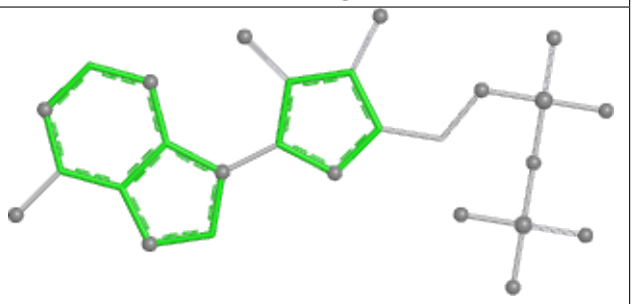
Bond lengths



Bond angles

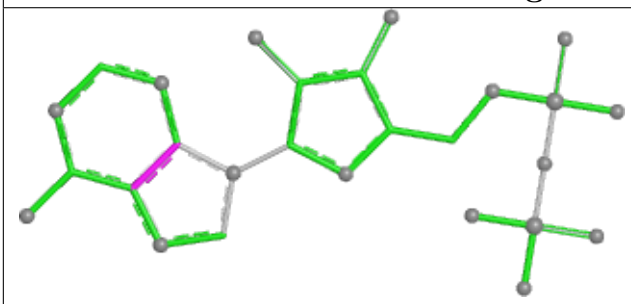


Torsions

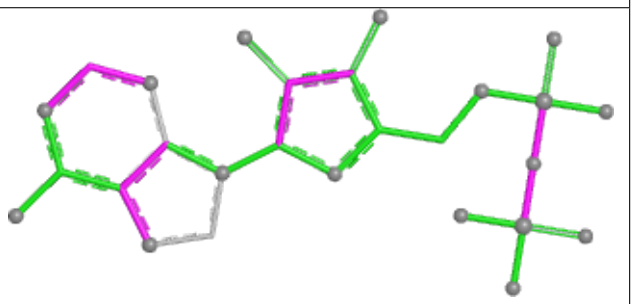


Rings

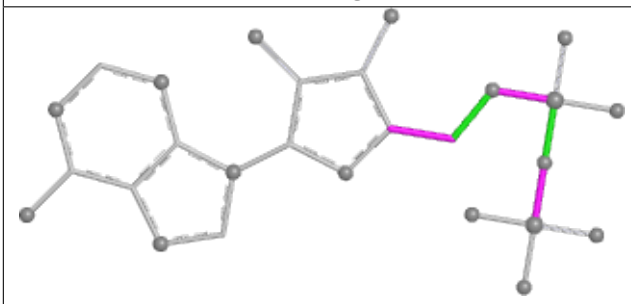
Ligand ADP J 800



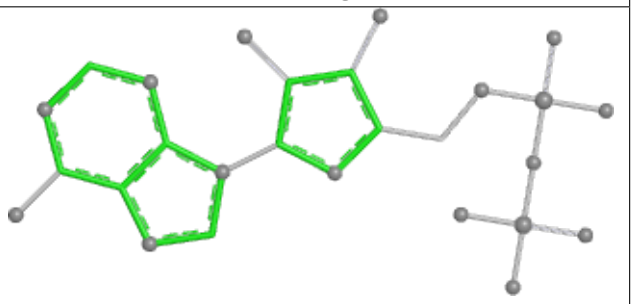
Bond lengths



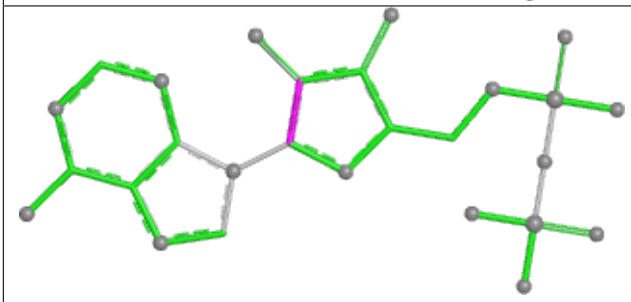
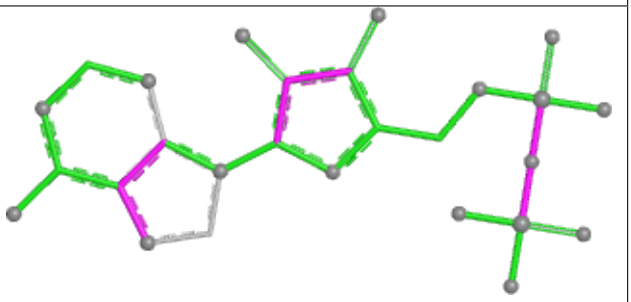
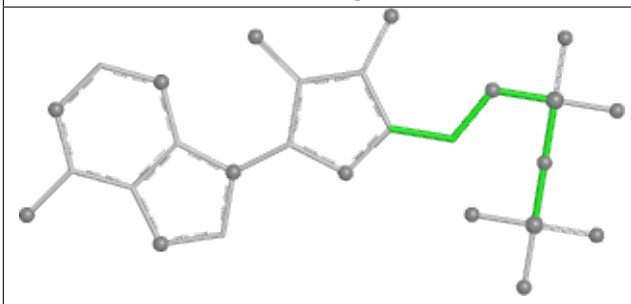
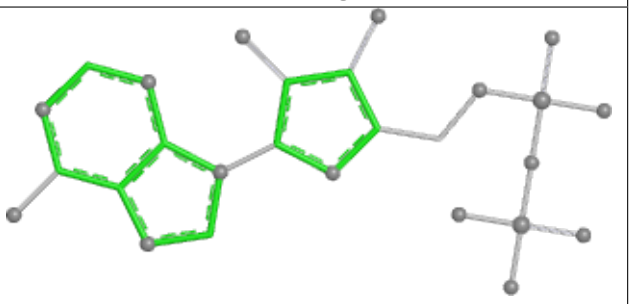
Bond angles

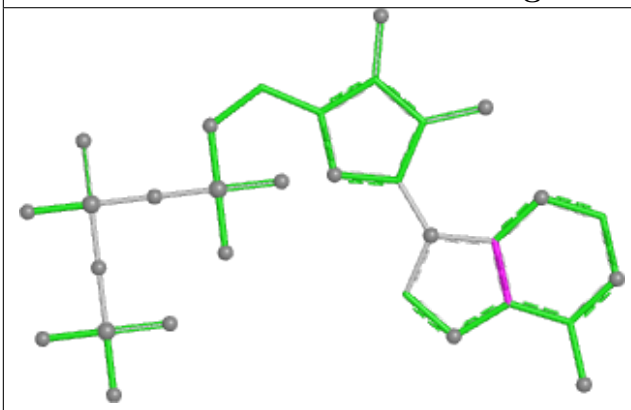
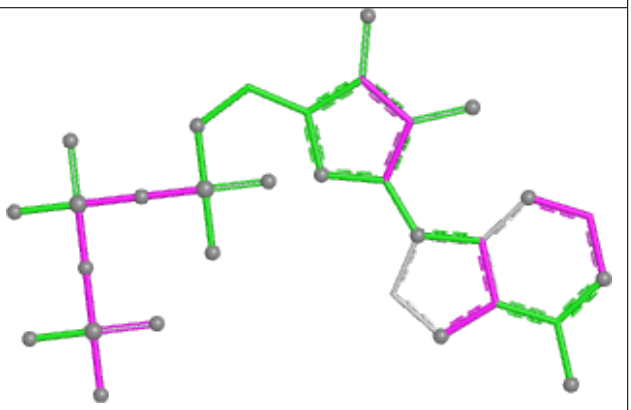
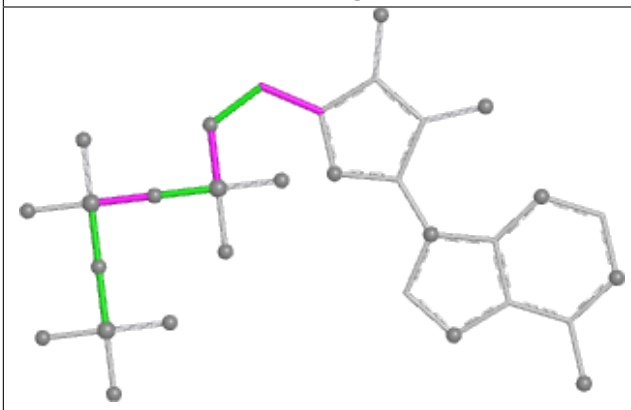
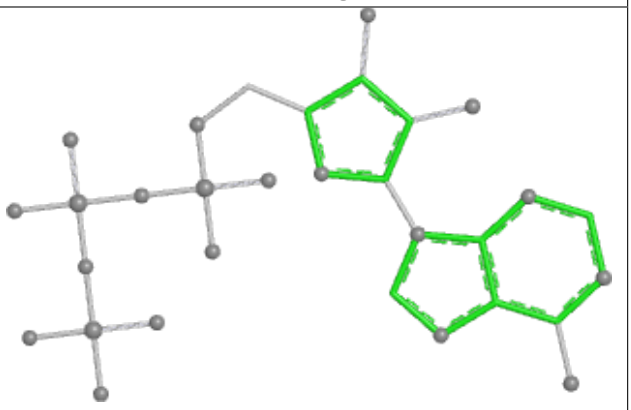


Torsions



Rings

Ligand ADP G 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP H 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	O	3
8	P	3
9	R	2
9	Q	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

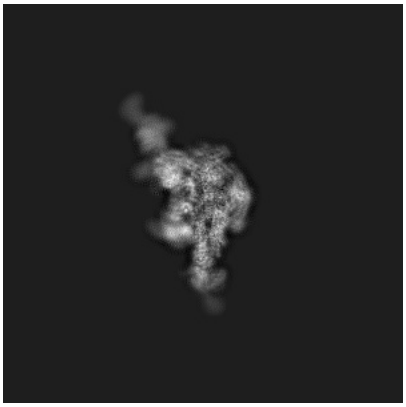
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4168. These allow visual inspection of the internal detail of the map and identification of artifacts.

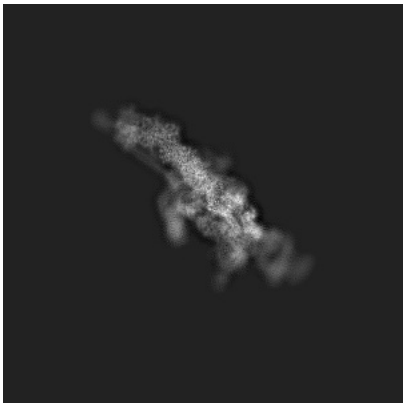
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

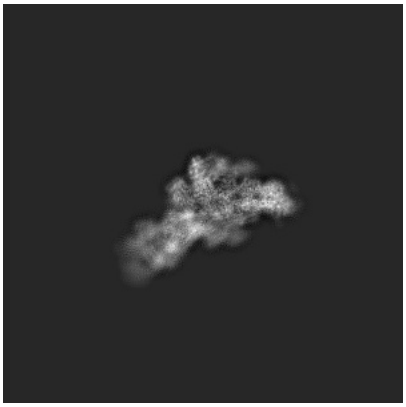
6.1.1 Primary map



X



Y

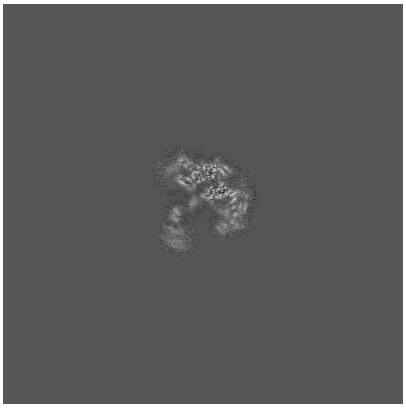


Z

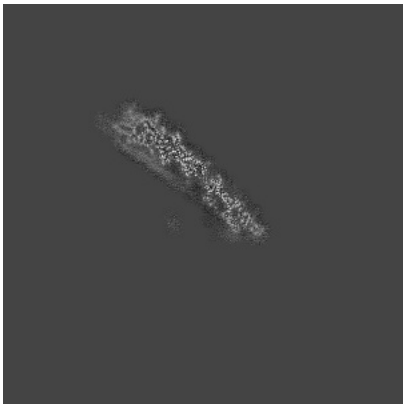
The images above show the map projected in three orthogonal directions.

6.2 Central slices

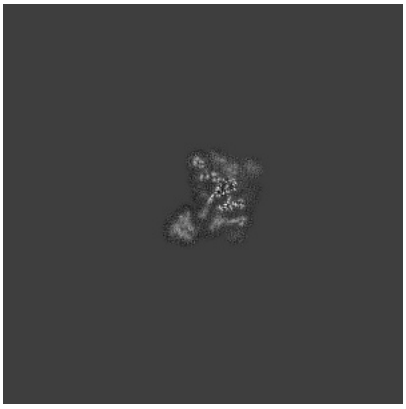
6.2.1 Primary map



X Index: 300



Y Index: 300

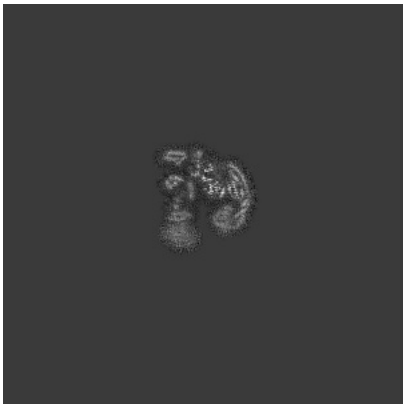


Z Index: 300

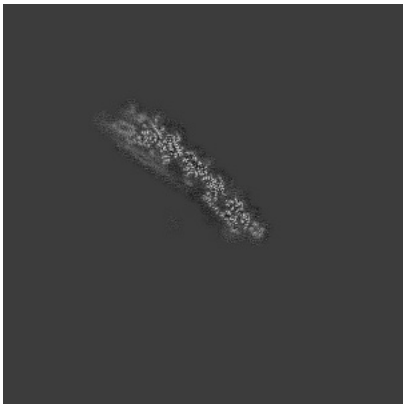
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

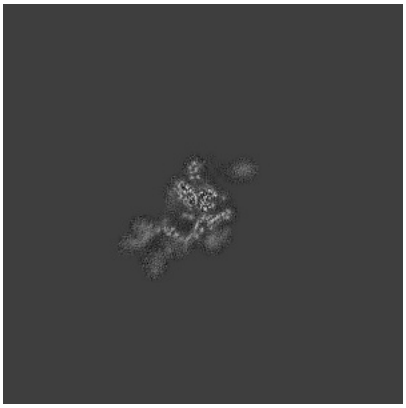
6.3.1 Primary map



X Index: 288



Y Index: 302

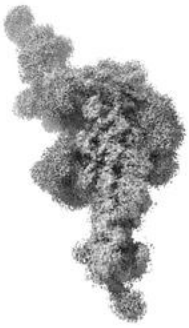


Z Index: 336

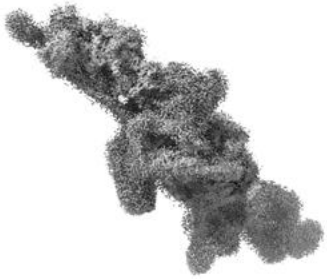
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

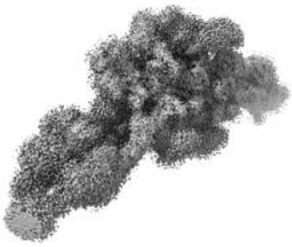
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.046. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

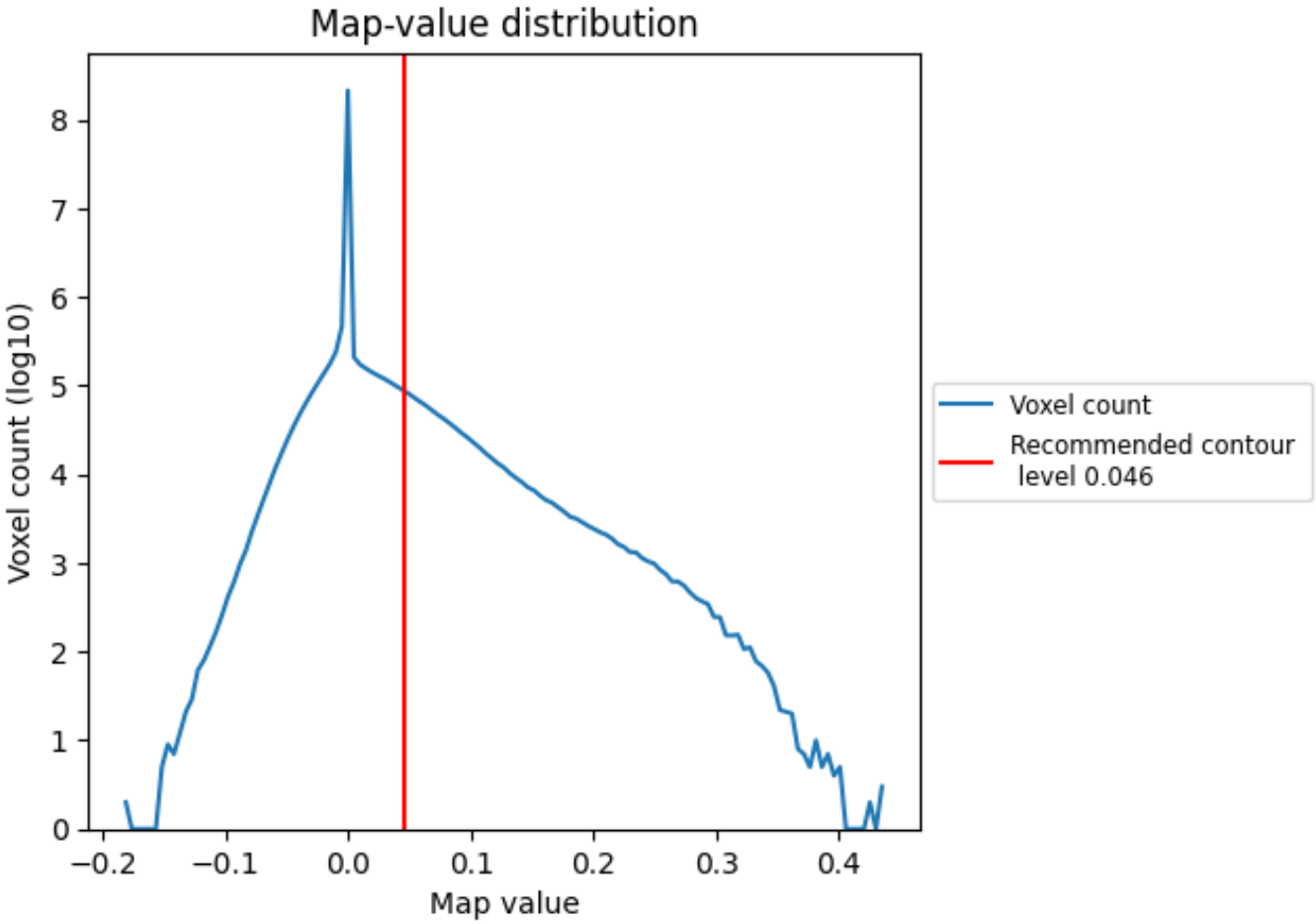
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

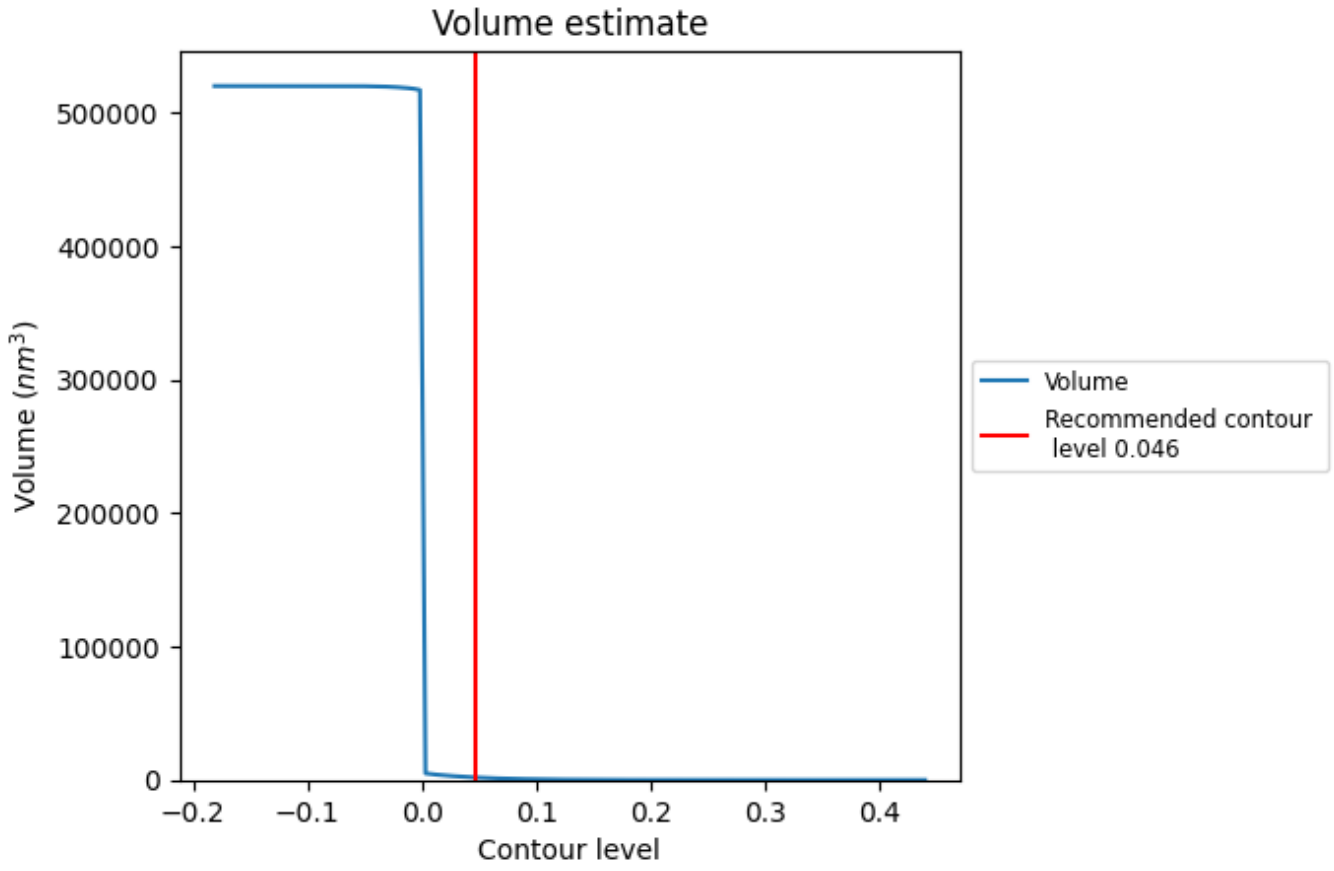
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

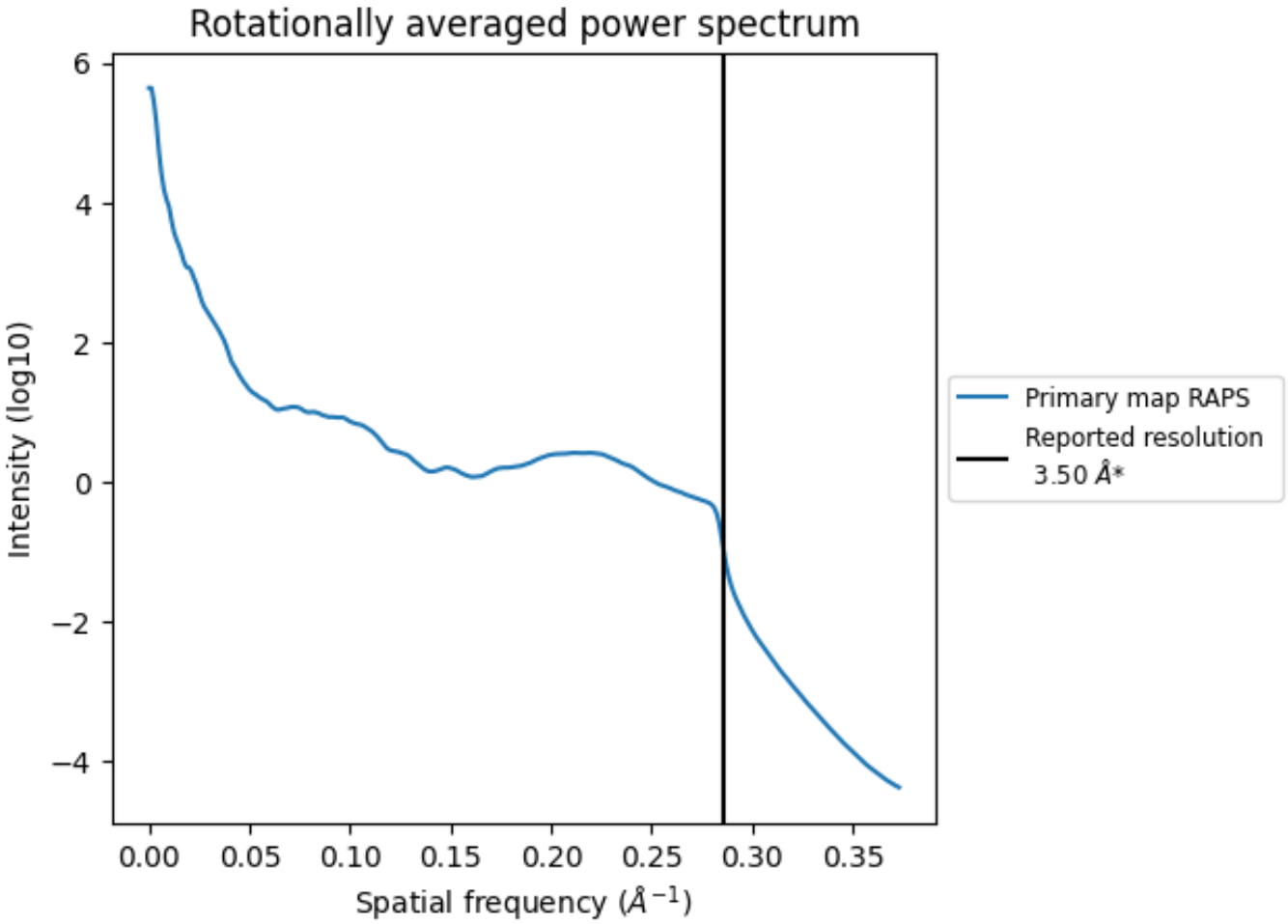
7.2 Volume estimate



The volume at the recommended contour level is 1916 nm^3; this corresponds to an approximate mass of 1731 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

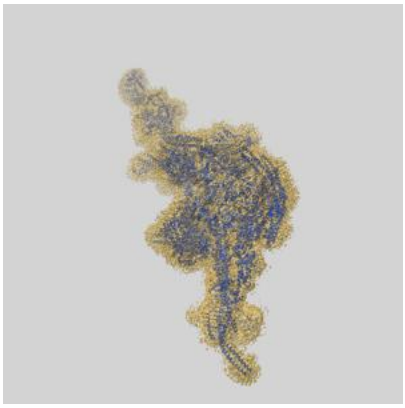
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

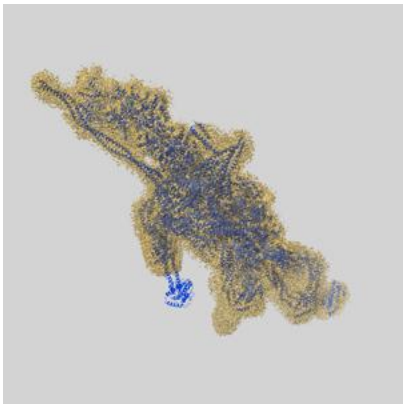
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4168 and PDB model 6F1T. Per-residue inclusion information can be found in section 3 on page 12.

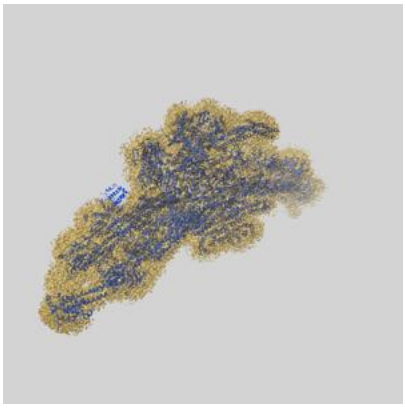
9.1 Map-model overlay



X



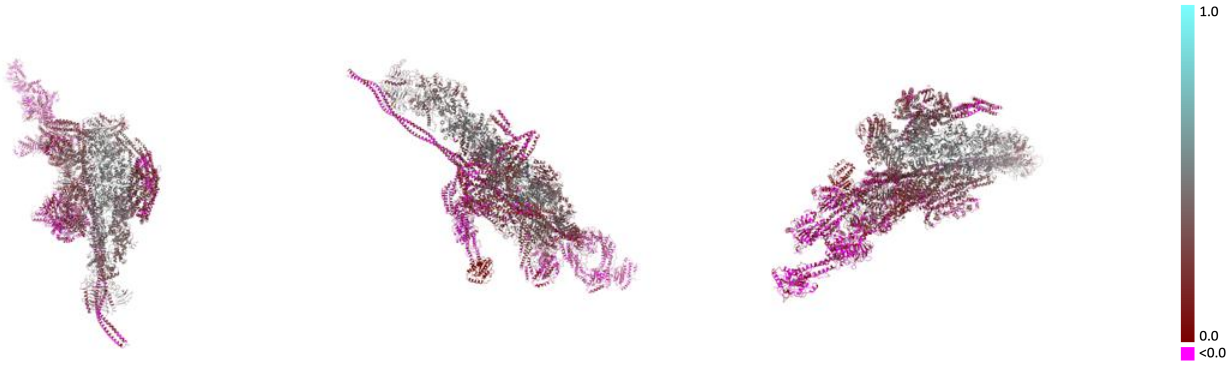
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.046 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

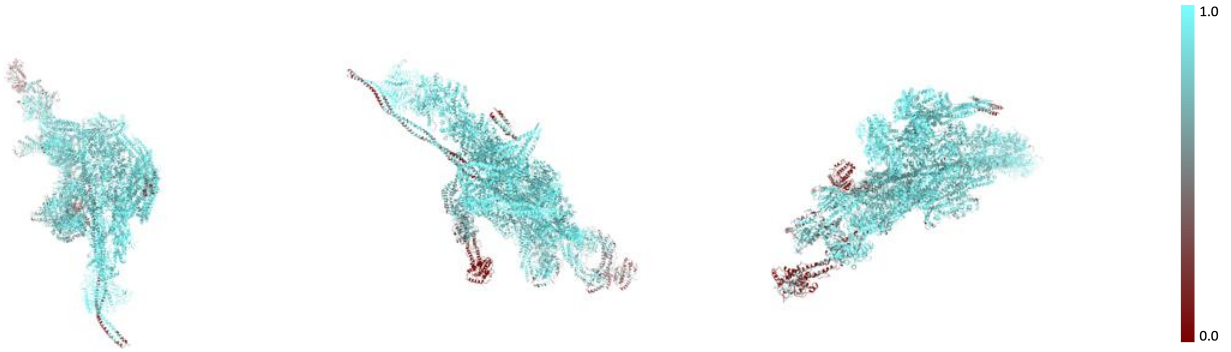
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

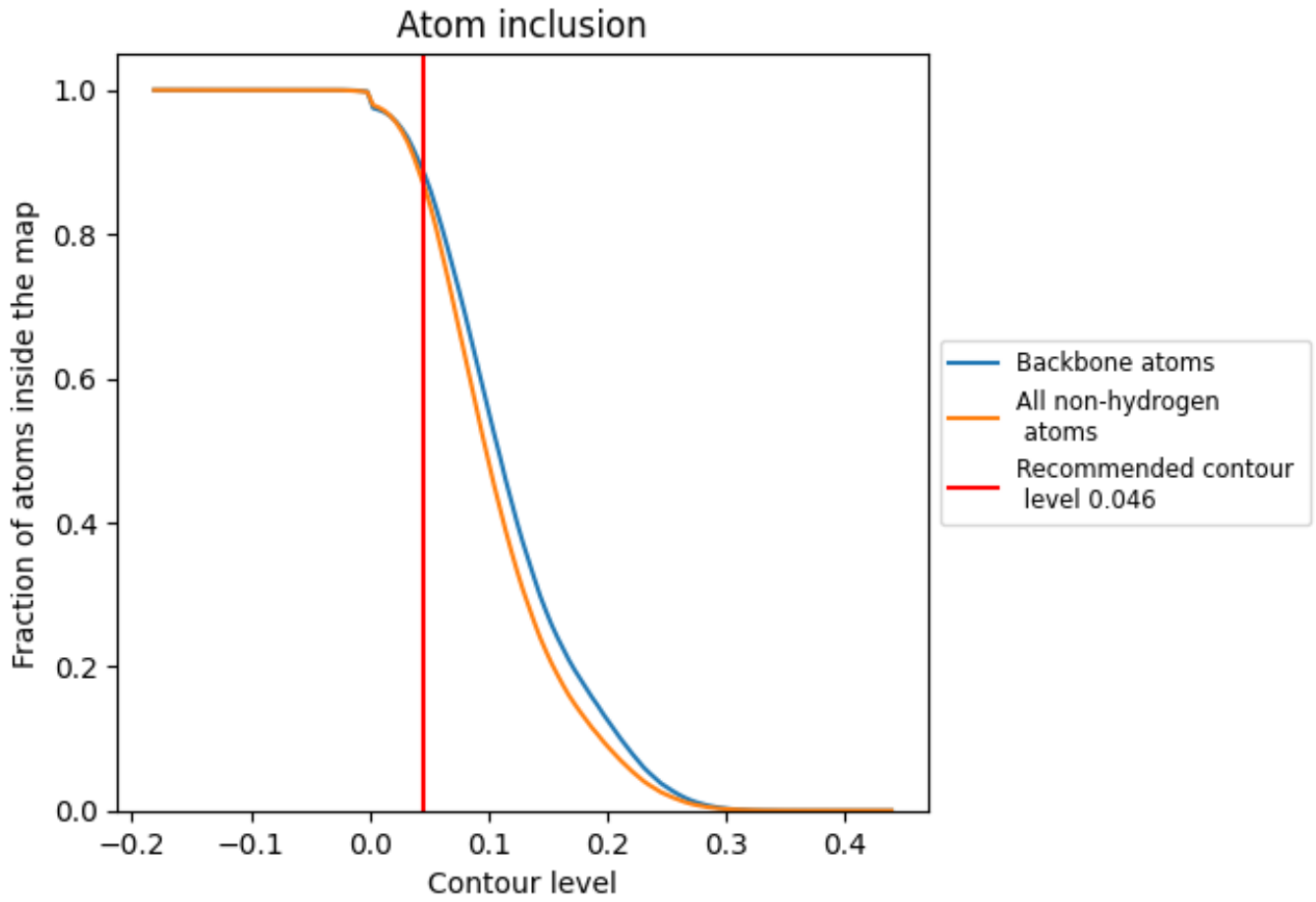
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.046).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.046) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.2690
A	0.9403	0.4110
B	0.9626	0.4730
C	0.9461	0.4780
D	0.9602	0.4650
E	0.9523	0.4730
F	0.9571	0.4600
G	0.9599	0.4500
H	0.9616	0.4520
I	0.9461	0.3910
J	0.9489	0.3890
K	0.9482	0.2900
L	0.9414	0.3630
M	0.9642	0.1830
N	0.9718	0.2050
O	0.9907	0.1940
P	0.9876	0.2470
Q	0.4943	0.1760
R	0.9931	0.4040
U	0.9620	0.3030
V	0.9988	0.3820
X	0.7123	0.1100
Y	0.9878	0.3960
Z	0.9923	0.3400
a	0.9250	0.4390
b	0.9319	0.4050
c	0.9444	0.4200
d	0.9130	0.3730
e	0.7293	0.1310
f	0.9010	0.2120
g	0.8225	0.0460
h	0.9155	0.2420
i	0.0234	-0.0000
j	0.8073	0.0720
k	0.6515	0.0120

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Chain	Atom inclusion	Q-score
l	0.6905	0.0350
m	0.8989	0.2480
n	0.7840	0.1680
o	0.9147	0.2180
p	0.8286	0.0500
q	0.6217	0.0260
r	0.2969	0.0000
s	0.7740	0.0320
t	0.7904	0.0600
x	0.6842	0.1050
z	0.9321	0.3110