Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 03:03 am BST

PDB ID	:	6F1U / pdb_00006f1u
EMDB ID	:	EMD-4169
Title	:	N terminal region of dynein tail domains in complex with dynactin filament and BICDR-1
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	:	3.40 Å(reported)

This is a Full wwPDB EM Validation 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:

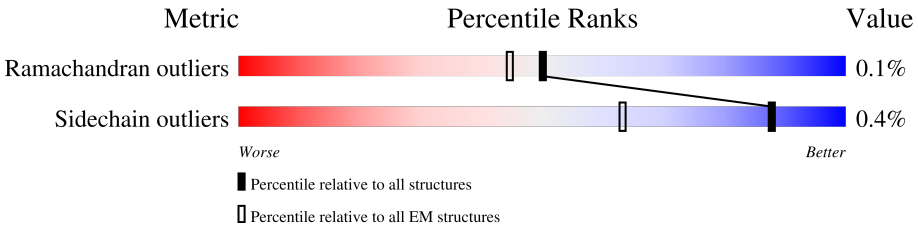
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.40 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	207382	16835
Sidechain outliers	206894	16415

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	B	376	97%
1	D	376	98%
1	F	376	97%
2	K	286	10% 96%
3	L	271	9% 99%
4	c	50	12% 74% 26%
5	d	26	19% 88% 8%
6	f	1186	8% 50% 50%
6	m	1186	32% 67%

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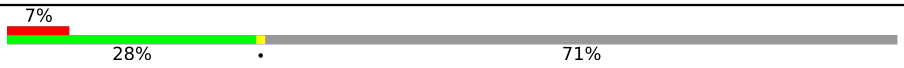
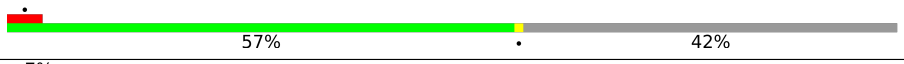
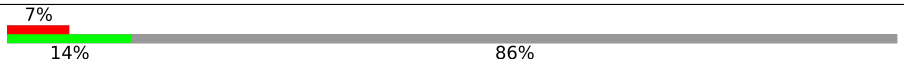
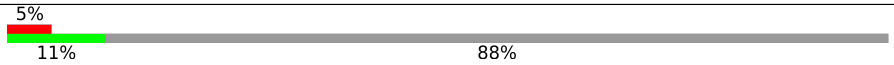
Mol	Chain	Length	Quality of chain
6	n	1186	
7	h	612	
8	X	577	
8	x	577	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28866 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	B	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	F	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		

- Molecule 2 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

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

- Molecule 3 is a protein called F-actin capping protein beta subunit.

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

- Molecule 4 is a protein called Dynactin subunit 2.

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

- Molecule 5 is a protein called Dynactin subunit 2.

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

- Molecule 6 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	596	Total	C	N	O	S	0	0
			4902	3107	894	886	15		
6	m	396	Total	C	N	O	S	0	0
			3288	2080	601	597	10		
6	n	341	Total	C	N	O	S	0	0
			2815	1777	512	517	9		

- Molecule 7 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	358	Total	C	N	O	S	0	0
			2801	1767	490	529	15		

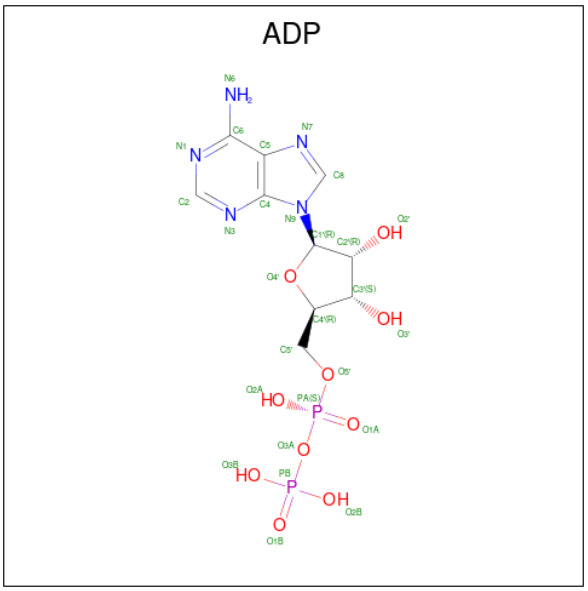
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 8 is a protein called BICD family-like cargo adapter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	79	Total	C	N	O	S	0	0
			688	413	134	140	1		
8	x	67	Total	C	N	O	S	0	0
			593	358	115	119	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



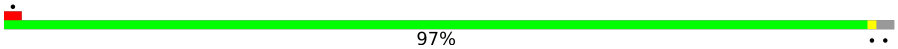
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

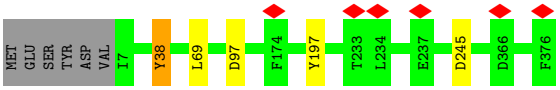
3 Residue-property plots (i)

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

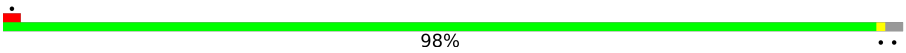
Chain B:

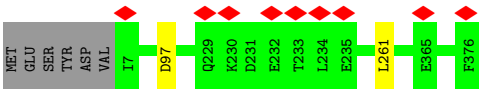




• Molecule 1: ARP1 actin related protein 1 homolog A

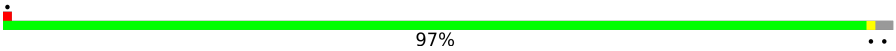
Chain D:





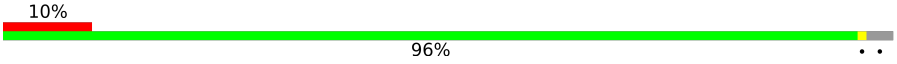
• Molecule 1: ARP1 actin related protein 1 homolog A

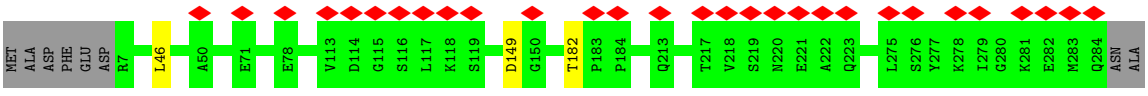
Chain F:



• Molecule 2: Capping protein (Actin filament) muscle Z-line, alpha 1

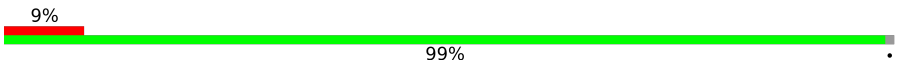
Chain K:

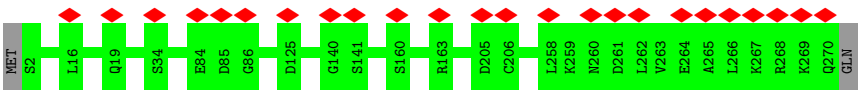




• Molecule 3: F-actin capping protein beta subunit

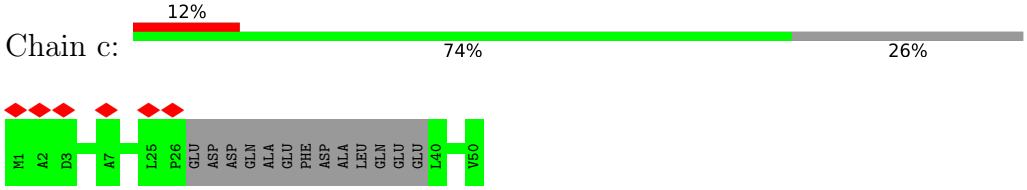
Chain L:





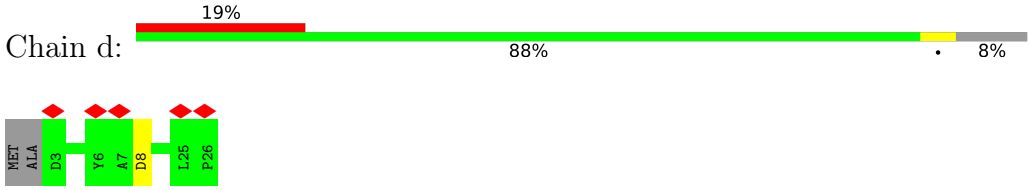
• Molecule 4: Dynactin subunit 2

Chain c:



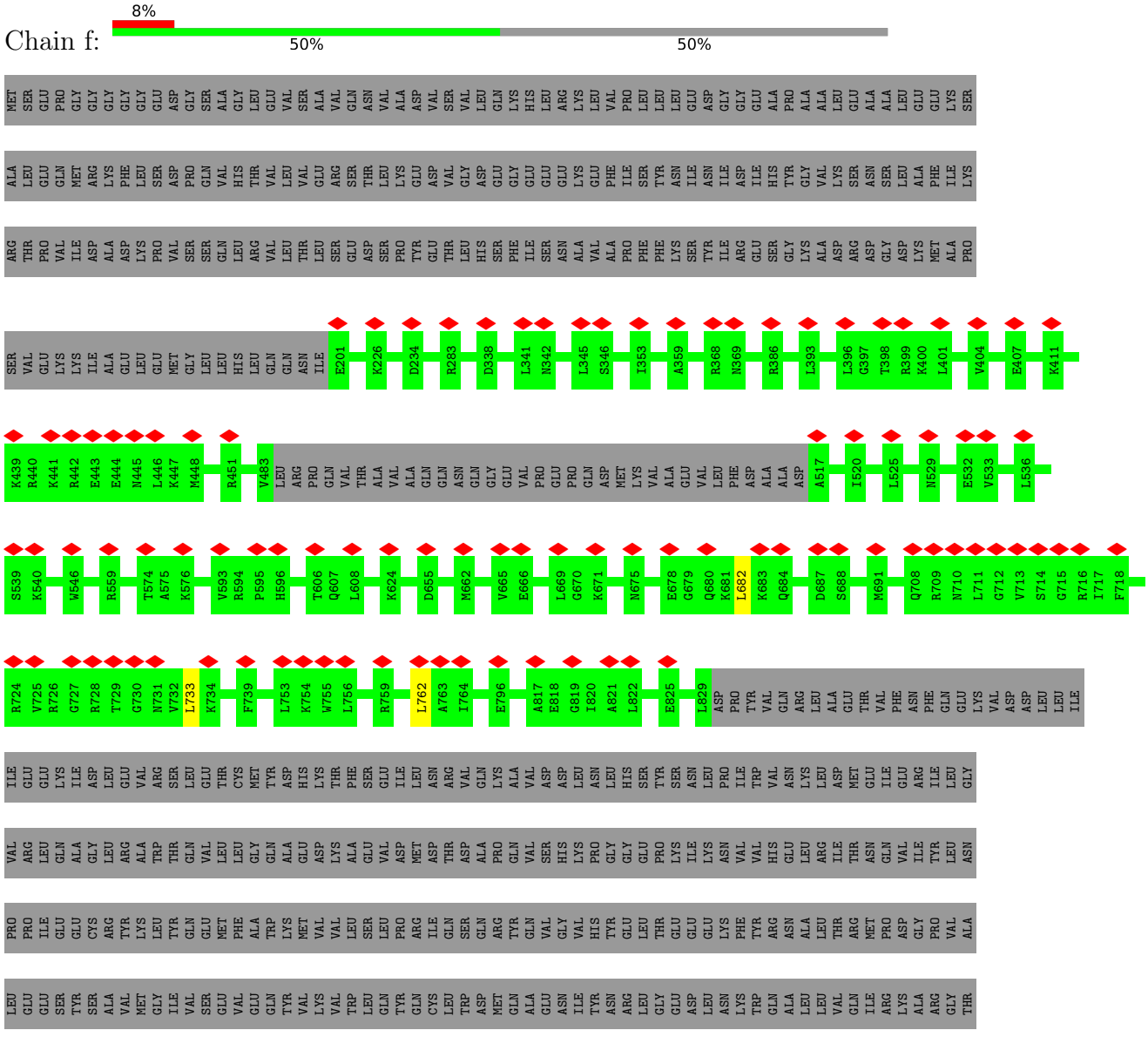
• Molecule 5: Dynactin subunit 2

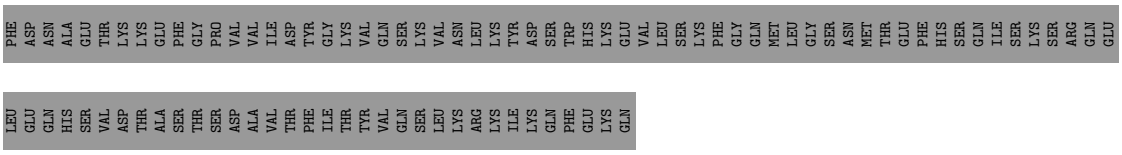
Chain d:



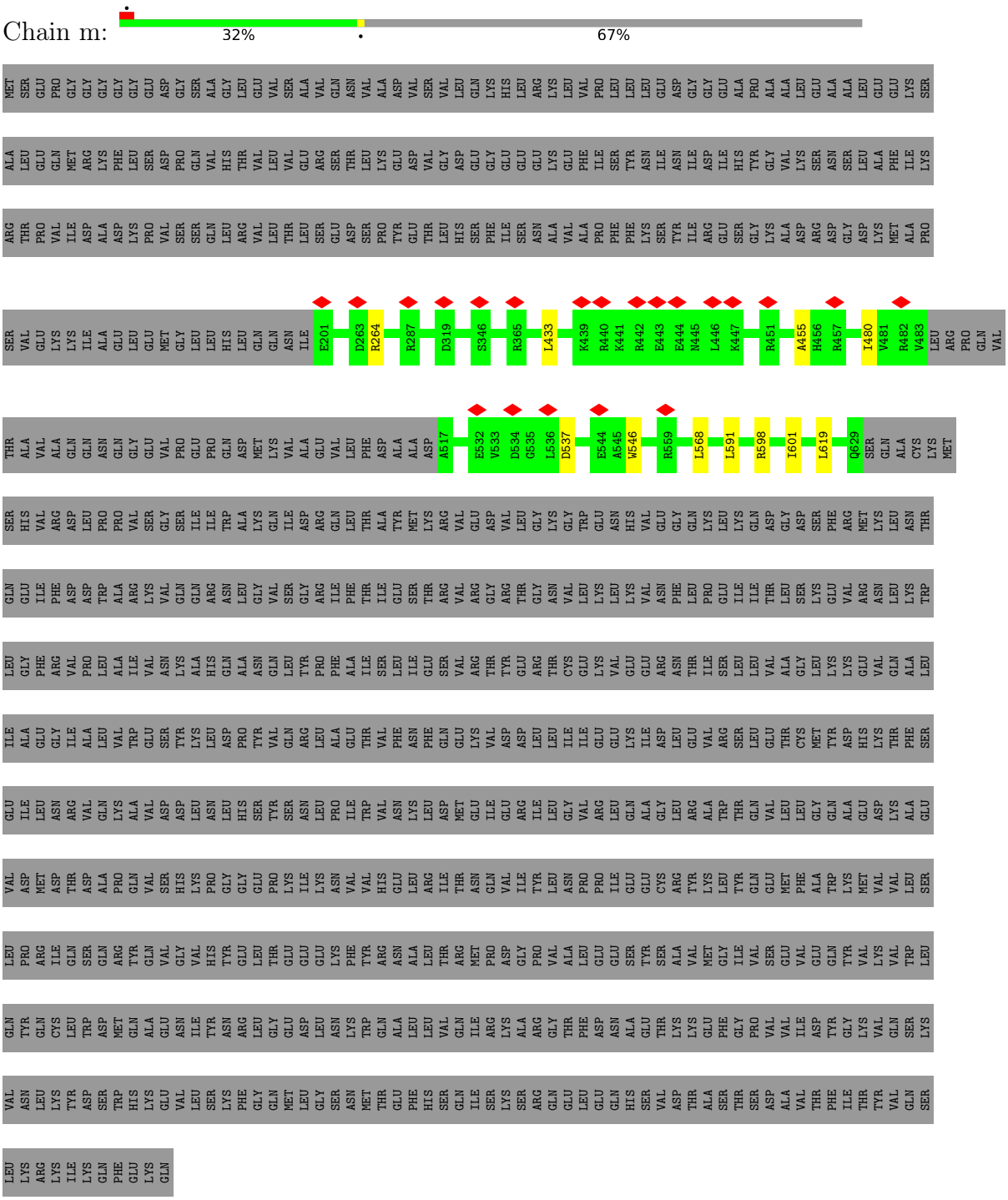
• Molecule 6: Cytoplasmic dynein 1 heavy chain 1

Chain f:

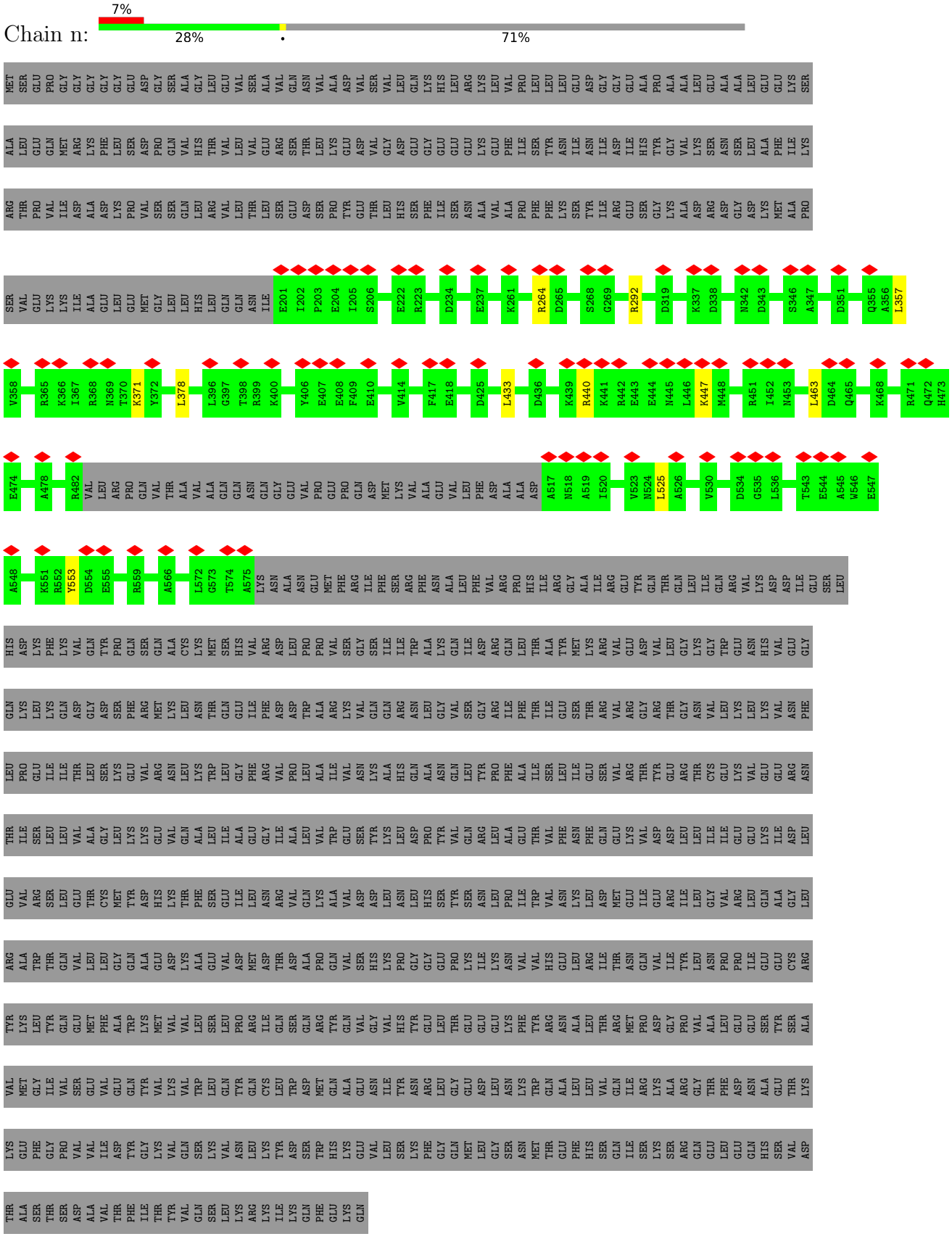




• Molecule 6: Cytoplasmic dynein 1 heavy chain 1

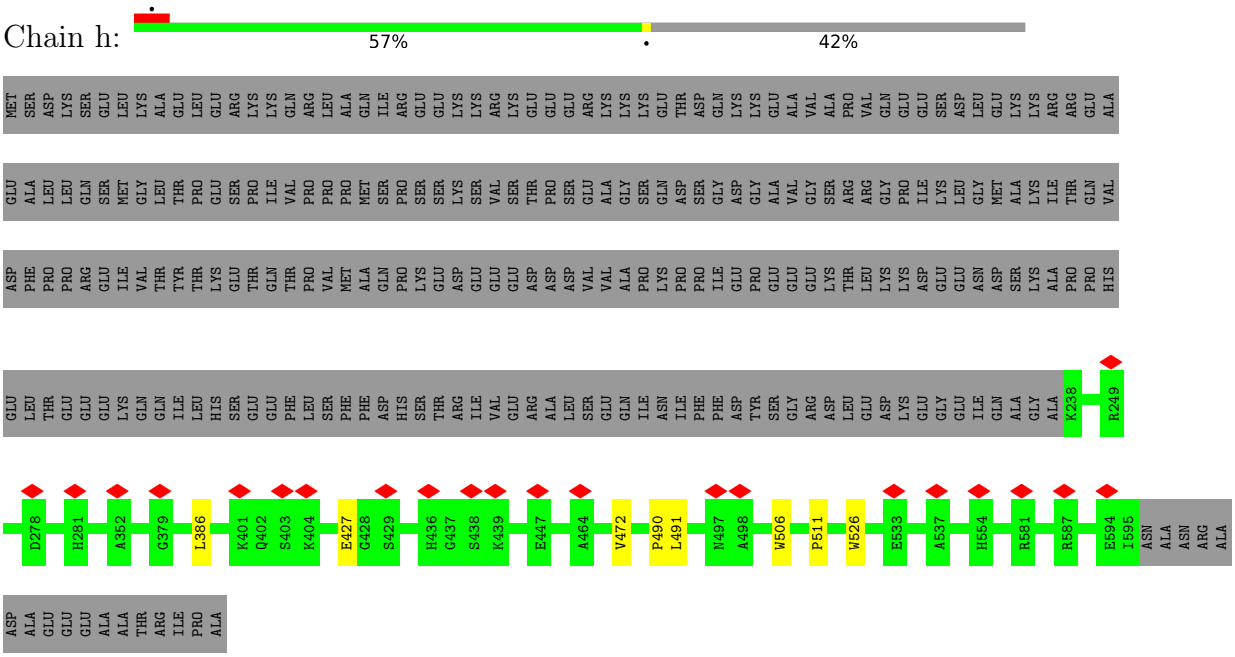


• Molecule 6: Cytoplasmic dynein 1 heavy chain 1



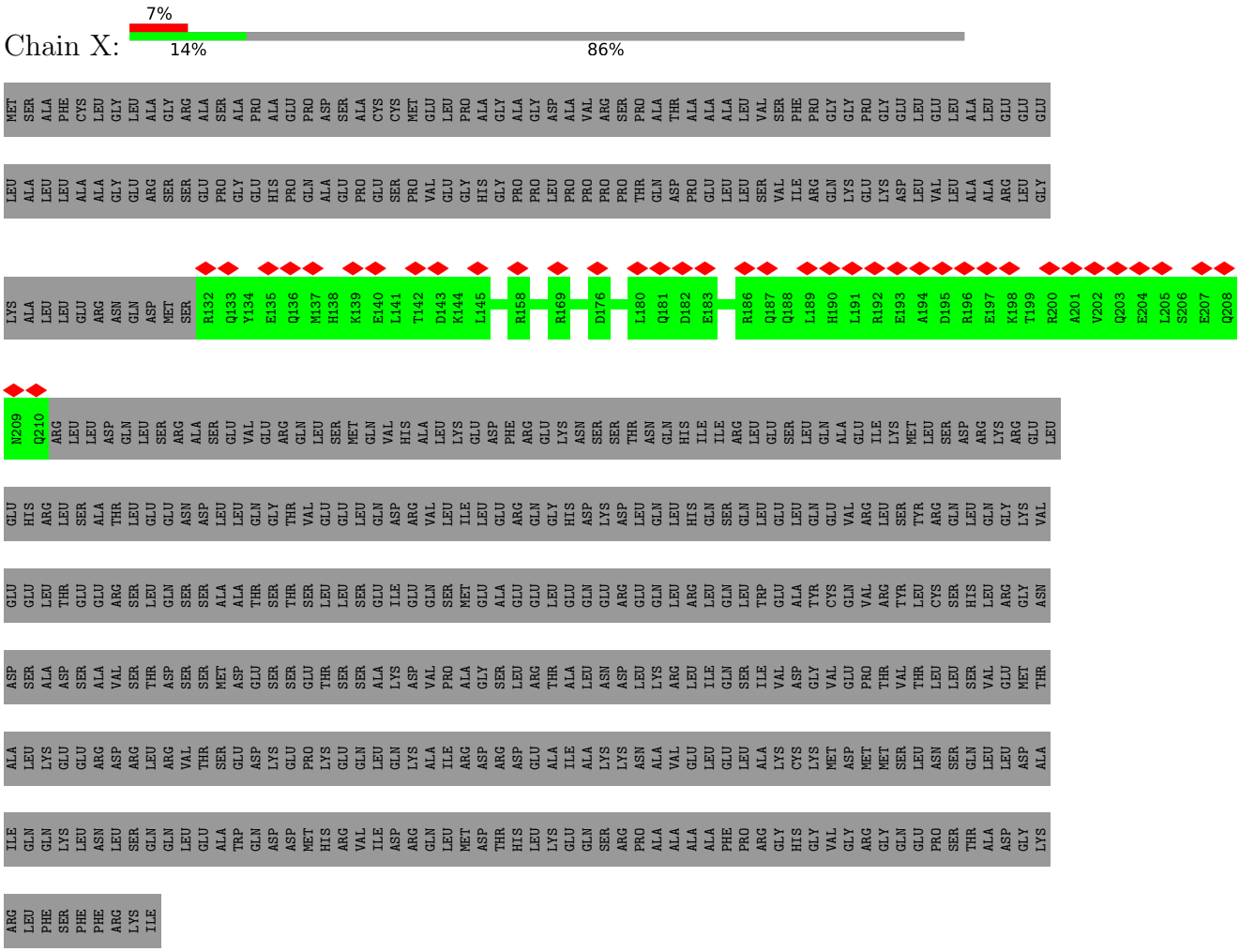
• Molecule 7: Cytoplasmic dynein 1 intermediate chain 2

Chain h:

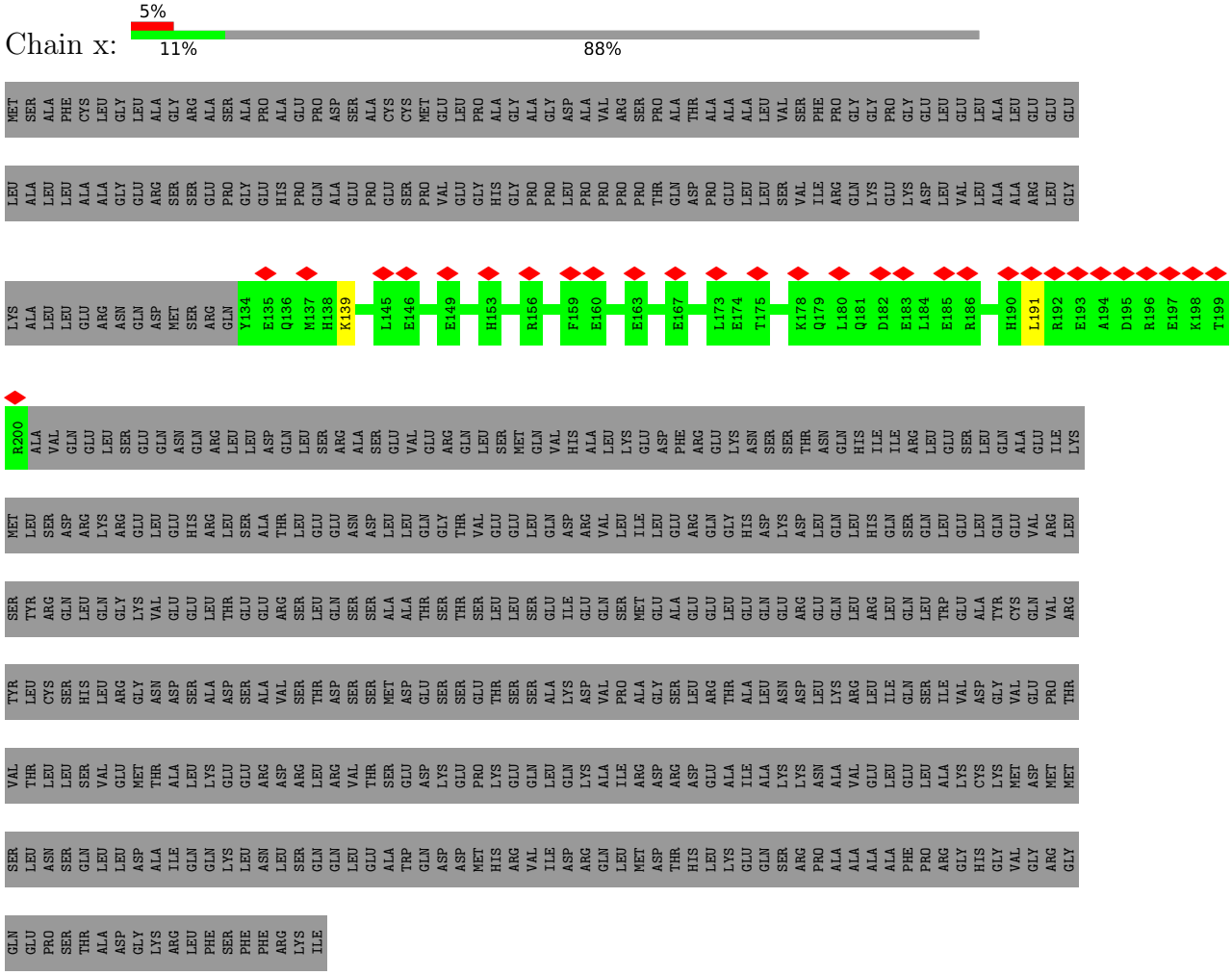


• Molecule 8: BICD family-like cargo adapter 1

Chain X:



• Molecule 8: BICD family-like cargo adapter 1



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	0.391	Depositor
Minimum map value	-0.145	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.09	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.82	0/3025	0.80	5/4085 (0.1%)
1	D	0.83	0/3025	0.79	2/4085 (0.0%)
1	F	0.89	1/3025 (0.0%)	0.84	3/4085 (0.1%)
2	K	0.64	0/2316	0.78	3/3135 (0.1%)
3	L	0.63	0/2156	0.77	0/2906
4	c	0.57	0/260	0.78	0/356
5	d	0.79	1/193 (0.5%)	0.74	0/265
6	f	0.55	0/4986	0.80	3/6718 (0.0%)
6	m	0.65	1/3344 (0.0%)	0.87	8/4504 (0.2%)
6	n	0.51	1/2860 (0.0%)	0.82	8/3854 (0.2%)
7	h	0.70	2/2880 (0.1%)	0.89	2/3927 (0.1%)
8	X	0.45	0/695	0.62	0/926
8	x	0.44	0/600	0.65	1/798 (0.1%)
All	All	0.69	6/29365 (0.0%)	0.81	35/39644 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	n	553	TYR	CD1-CE1	-7.94	1.27	1.39
6	m	546	TRP	CB-CG	-6.77	1.38	1.50
7	h	427	GLU	CG-CD	-5.82	1.43	1.51
7	h	506	TRP	CB-CG	-5.56	1.40	1.50
1	F	40	GLY	C-N	-5.46	1.21	1.34
5	d	8	ASP	C-N	-5.35	1.21	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	TYR	CB-CG-CD2	-9.14	115.51	121.00
6	m	601	ILE	CG1-CB-CG2	-8.35	93.04	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	TYR	CB-CG-CD1	7.48	125.49	121.00
6	m	480	ILE	CG1-CB-CG2	-6.89	96.25	111.40
6	n	553	TYR	CA-CB-CG	-6.81	100.46	113.40
2	K	182	THR	N-CA-C	-6.64	93.07	111.00
6	f	762	LEU	CA-CB-CG	-6.52	100.30	115.30
1	B	38	TYR	CA-CB-CG	6.38	125.52	113.40
1	D	261	LEU	CA-CB-CG	6.38	129.97	115.30
7	h	386	LEU	CA-CB-CG	-6.28	100.85	115.30
6	m	433	LEU	CB-CG-CD1	-6.17	100.52	111.00
6	n	433	LEU	CA-CB-CG	5.94	128.97	115.30
1	F	336	ARG	CB-CG-CD	-5.90	96.26	111.60
6	m	537	ASP	CB-CG-OD1	5.83	123.55	118.30
2	K	46	LEU	CA-CB-CG	5.80	128.63	115.30
6	f	733	LEU	CA-CB-CG	5.73	128.49	115.30
6	n	378	LEU	CA-CB-CG	-5.60	102.42	115.30
6	m	619	LEU	CA-CB-CG	-5.53	102.58	115.30
6	m	568	LEU	CA-CB-CG	-5.50	102.65	115.30
2	K	149	ASP	CB-CG-OD1	5.38	123.15	118.30
6	n	371	LYS	C-N-CA	-5.38	108.25	121.70
1	F	261	LEU	CB-CG-CD2	-5.38	101.86	111.00
8	x	191	LEU	CA-CB-CG	-5.34	103.01	115.30
6	n	463	LEU	CA-CB-CG	5.31	127.51	115.30
6	n	357	LEU	CA-CB-CG	5.30	127.49	115.30
6	n	553	TYR	CB-CG-CD1	-5.26	117.84	121.00
6	n	525	LEU	CA-CB-CG	5.24	127.36	115.30
1	F	97	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	97	ASP	CB-CG-OD2	5.22	123.00	118.30
6	m	591	LEU	CA-CB-CG	-5.18	103.38	115.30
1	B	97	ASP	CB-CG-OD2	5.17	122.95	118.30
6	m	598	ARG	NE-CZ-NH2	-5.09	117.75	120.30
7	h	506	TRP	CA-CB-CG	5.04	123.28	113.70
1	B	69	LEU	CA-CB-CG	-5.02	103.76	115.30
6	f	682	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	368/376 (98%)	338 (92%)	30 (8%)	0	100	100
1	D	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	F	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
2	K	276/286 (96%)	244 (88%)	32 (12%)	0	100	100
3	L	267/271 (98%)	233 (87%)	34 (13%)	0	100	100
4	c	33/50 (66%)	26 (79%)	7 (21%)	0	100	100
5	d	22/26 (85%)	16 (73%)	6 (27%)	0	100	100
6	f	592/1186 (50%)	538 (91%)	54 (9%)	0	100	100
6	m	392/1186 (33%)	361 (92%)	30 (8%)	1 (0%)	37	66
6	n	337/1186 (28%)	304 (90%)	33 (10%)	0	100	100
7	h	356/612 (58%)	299 (84%)	54 (15%)	3 (1%)	16	44
8	X	77/577 (13%)	74 (96%)	3 (4%)	0	100	100
8	x	65/577 (11%)	65 (100%)	0	0	100	100
All	All	3521/7085 (50%)	3162 (90%)	355 (10%)	4 (0%)	50	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	h	491	LEU
6	m	455	ALA
7	h	511	PRO
7	h	490	PRO

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	B	318/324 (98%)	315 (99%)	3 (1%)	75 86
1	D	318/324 (98%)	318 (100%)	0	100 100
1	F	318/324 (98%)	317 (100%)	1 (0%)	91 95
2	K	247/254 (97%)	247 (100%)	0	100 100
3	L	238/240 (99%)	238 (100%)	0	100 100
4	c	22/44 (50%)	22 (100%)	0	100 100
5	d	21/22 (96%)	21 (100%)	0	100 100
6	f	534/1056 (51%)	534 (100%)	0	100 100
6	m	358/1056 (34%)	357 (100%)	1 (0%)	91 95
6	n	307/1056 (29%)	303 (99%)	4 (1%)	65 78
7	h	307/531 (58%)	305 (99%)	2 (1%)	81 88
8	X	74/503 (15%)	74 (100%)	0	100 100
8	x	64/503 (13%)	63 (98%)	1 (2%)	58 75
All	All	3126/6237 (50%)	3114 (100%)	12 (0%)	88 93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	TYR
1	B	197	TYR
1	B	245	ASP
1	F	245	ASP
6	m	264	ARG
6	n	264	ARG
6	n	292	ARG
6	n	440	ARG
6	n	447	LYS
7	h	472	VAL
7	h	526	TRP
8	x	139	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	GLN

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Mol	Chain	Res	Type
1	B	133	ASN
1	D	10	GLN
1	D	133	ASN
1	F	9	ASN
1	F	44	HIS
1	F	297	ASN
3	L	20	GLN
6	f	215	ASN
6	f	311	HIS
6	f	421	GLN
6	f	653	GLN
6	f	708	GLN
6	f	731	ASN
6	f	773	GLN
6	m	280	ASN
6	m	311	HIS
6	m	391	GLN
6	m	472	GLN
6	m	529	ASN
6	m	589	ASN
6	n	472	GLN
6	n	473	HIS
7	h	306	GLN
7	h	345	GLN
8	X	161	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
9	ADP	D	800	-	24,29,29	1.24	3 (12%)	29,45,45	1.70	4 (13%)
9	ADP	F	800	1	24,29,29	1.17	1 (4%)	29,45,45	1.86	5 (17%)
9	ADP	B	800	-	24,29,29	1.17	2 (8%)	29,45,45	1.87	7 (24%)

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
9	ADP	D	800	-	-	4/12/32/32	0/3/3/3
9	ADP	F	800	1	-	4/12/32/32	0/3/3/3
9	ADP	B	800	-	-	3/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	800	ADP	C2'-C1'	-3.11	1.49	1.53
9	F	800	ADP	C2'-C1'	-2.83	1.49	1.53
9	D	800	ADP	C2'-C1'	-2.74	1.49	1.53
9	D	800	ADP	C4-N3	-2.40	1.32	1.35
9	B	800	ADP	C4-N3	-2.09	1.32	1.35
9	D	800	ADP	C5-N7	-2.02	1.32	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	800	ADP	PA-O3A-PB	-6.65	110.00	132.83
9	B	800	ADP	PA-O3A-PB	-5.71	113.24	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	800	ADP	PA-O3A-PB	-5.17	115.09	132.83
9	D	800	ADP	C3'-C2'-C1'	3.71	106.56	100.98
9	B	800	ADP	C3'-C2'-C1'	3.60	106.40	100.98
9	F	800	ADP	C4-C5-N7	-3.03	106.24	109.40
9	F	800	ADP	N3-C2-N1	-3.02	123.96	128.68
9	B	800	ADP	N3-C2-N1	-2.97	124.03	128.68
9	B	800	ADP	C4-C5-N7	-2.49	106.80	109.40
9	D	800	ADP	O2'-C2'-C3'	-2.48	103.79	111.82
9	B	800	ADP	O2A-PA-O1A	2.38	124.03	112.24
9	F	800	ADP	O3B-PB-O1B	2.28	119.61	110.68
9	B	800	ADP	C2'-C3'-C4'	2.24	107.00	102.64
9	D	800	ADP	O4'-C1'-C2'	-2.20	103.72	106.93
9	B	800	ADP	O3B-PB-O2B	2.08	115.59	107.64
9	F	800	ADP	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	800	ADP	C3'-C4'-C5'-O5'
9	D	800	ADP	C5'-O5'-PA-O1A
9	D	800	ADP	C5'-O5'-PA-O3A
9	F	800	ADP	C5'-O5'-PA-O3A
9	F	800	ADP	C3'-C4'-C5'-O5'
9	D	800	ADP	O4'-C4'-C5'-O5'
9	D	800	ADP	C3'-C4'-C5'-O5'
9	F	800	ADP	O4'-C4'-C5'-O5'
9	B	800	ADP	O4'-C4'-C5'-O5'
9	F	800	ADP	C5'-O5'-PA-O2A
9	B	800	ADP	C5'-O5'-PA-O1A

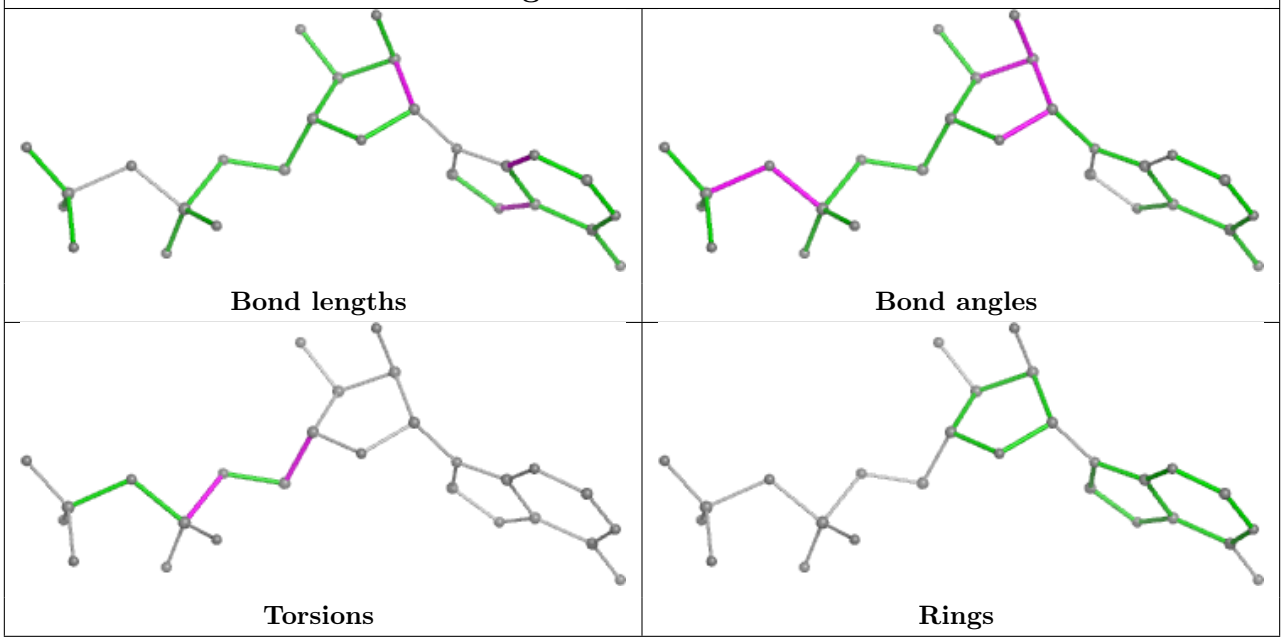
There are no ring outliers.

No monomer is involved in short contacts.

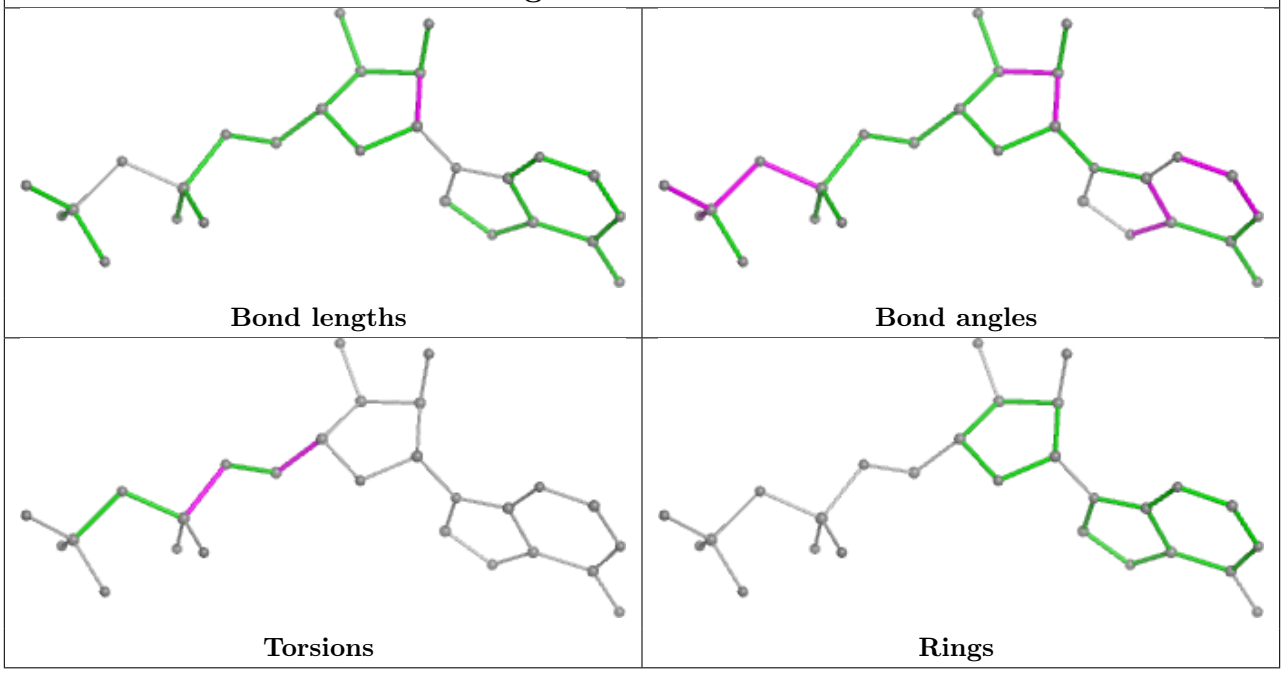
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

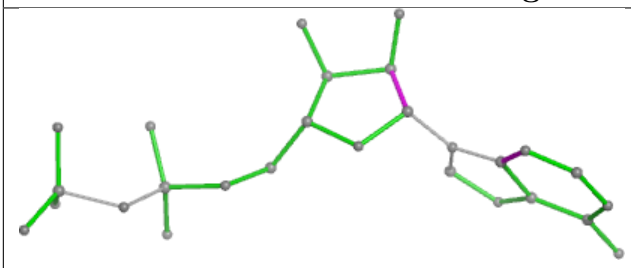
Ligand ADP D 800



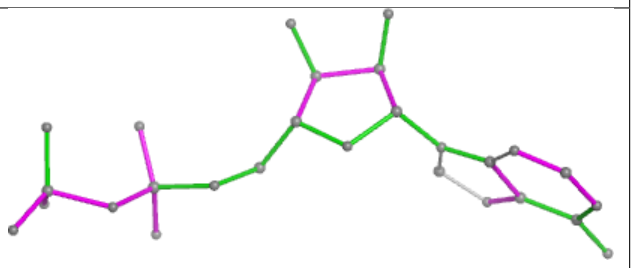
Ligand ADP F 800



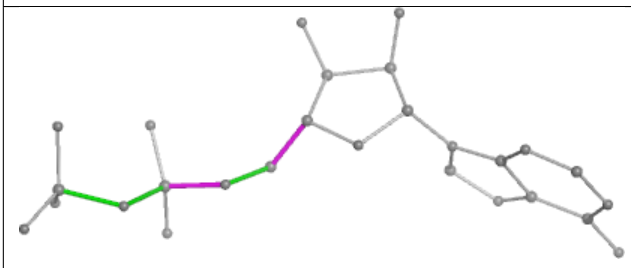
Ligand ADP B 800



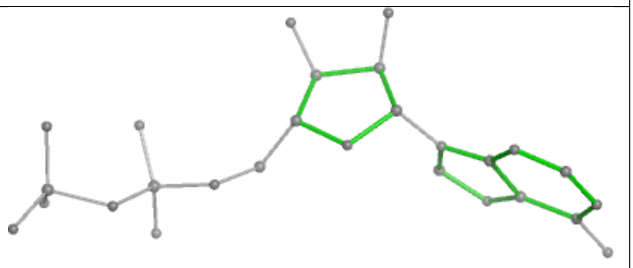
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

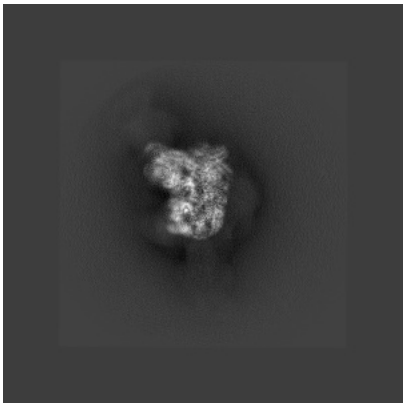
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4169. These allow visual inspection of the internal detail of the map and identification of artifacts.

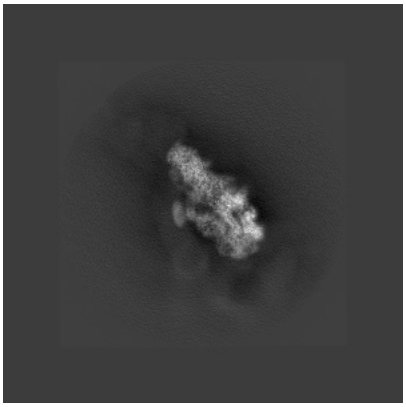
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

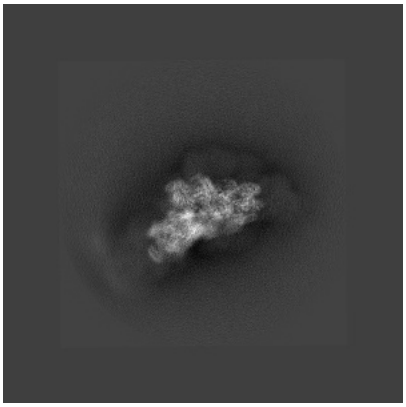
6.1.1 Primary map



X



Y

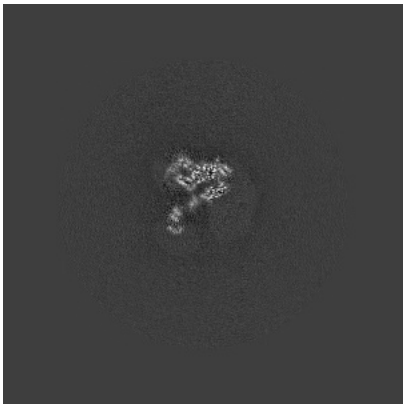


Z

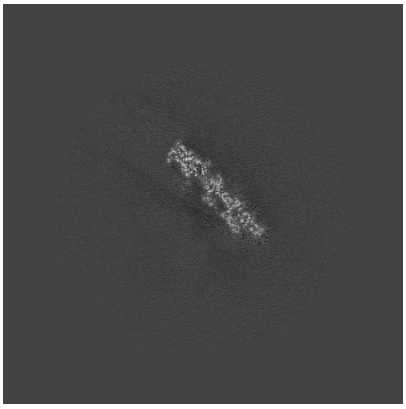
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 300



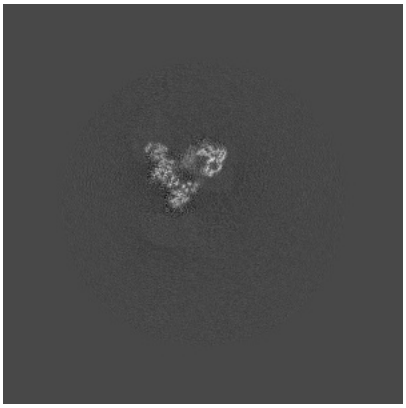
Y Index: 300

Z Index: 300

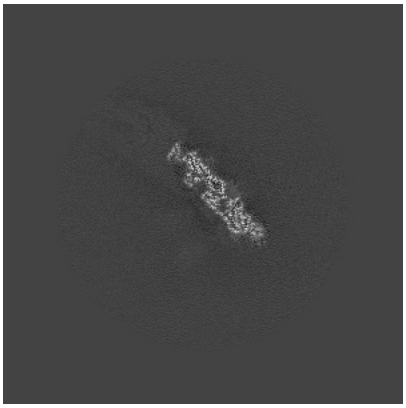
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

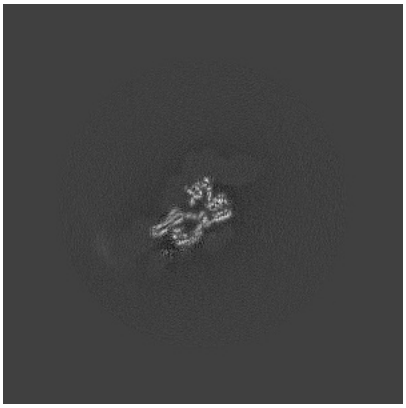
6.3.1 Primary map



X Index: 257



Y Index: 305

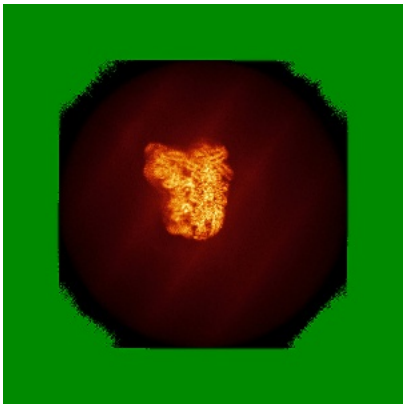


Z Index: 328

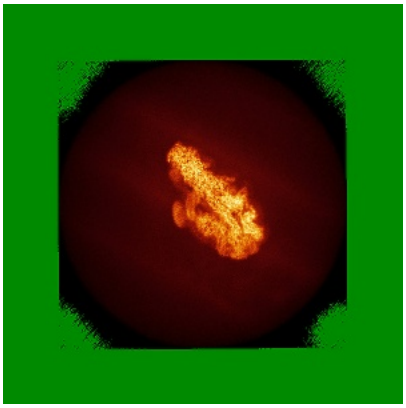
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

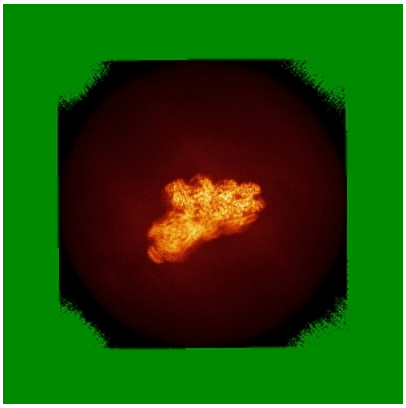
6.4.1 Primary map



X



Y

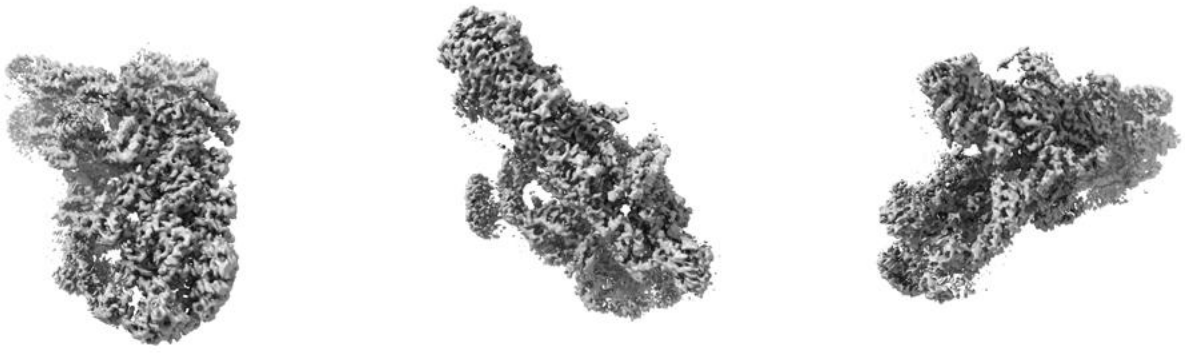


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

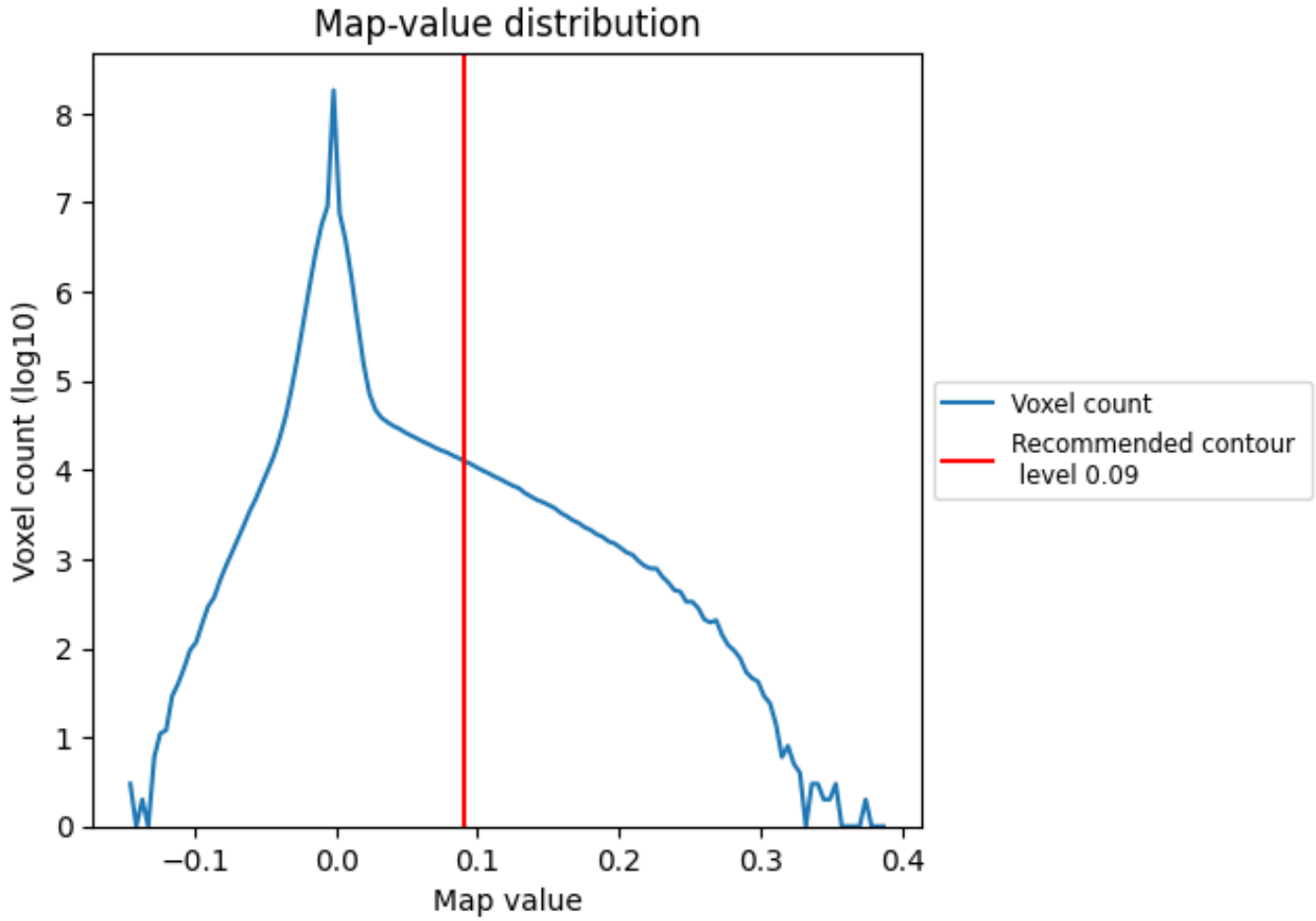
6.6 Mask visualisation (i)

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

7 Map analysis

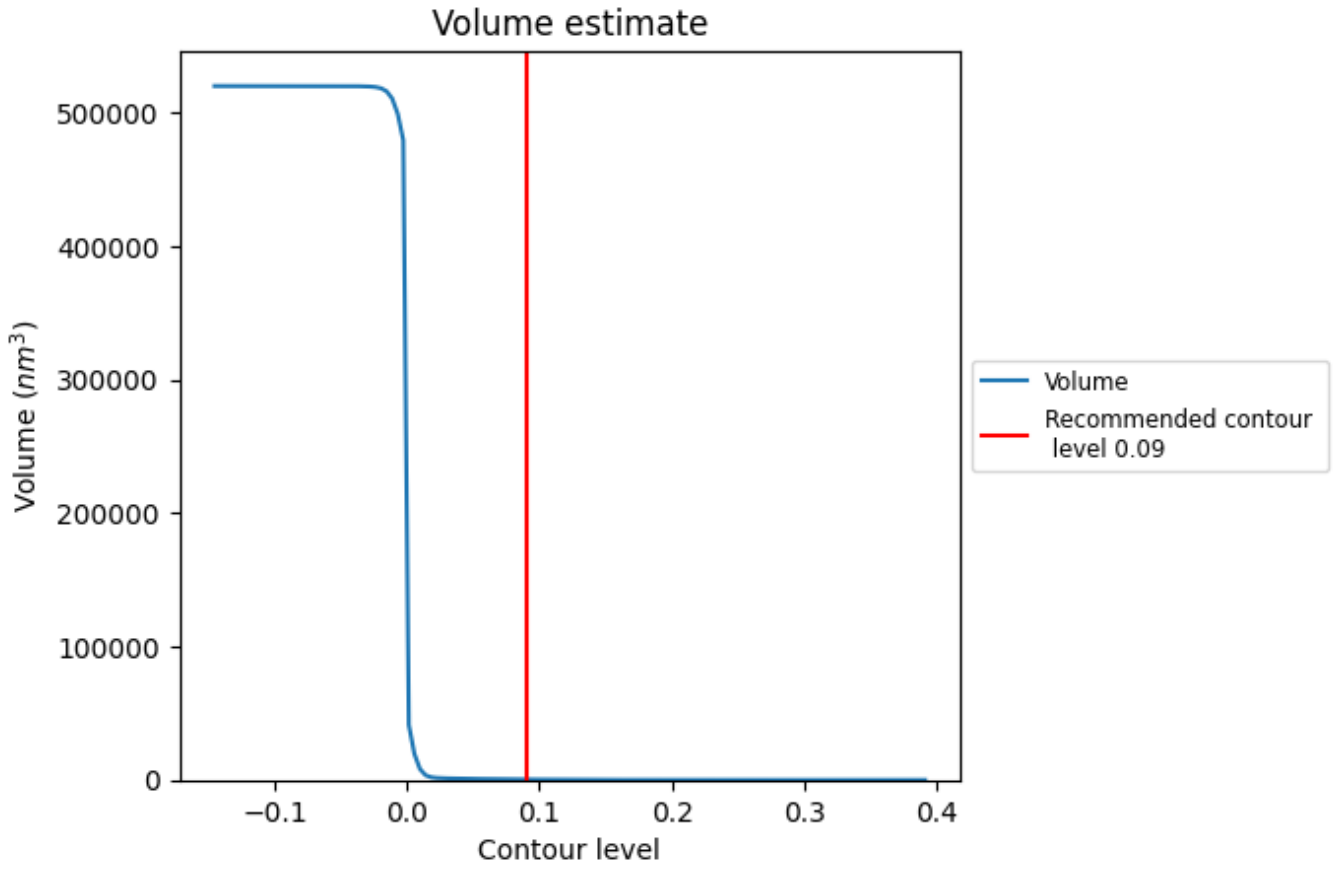
This section contains the results of statistical analysis of the map.

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.

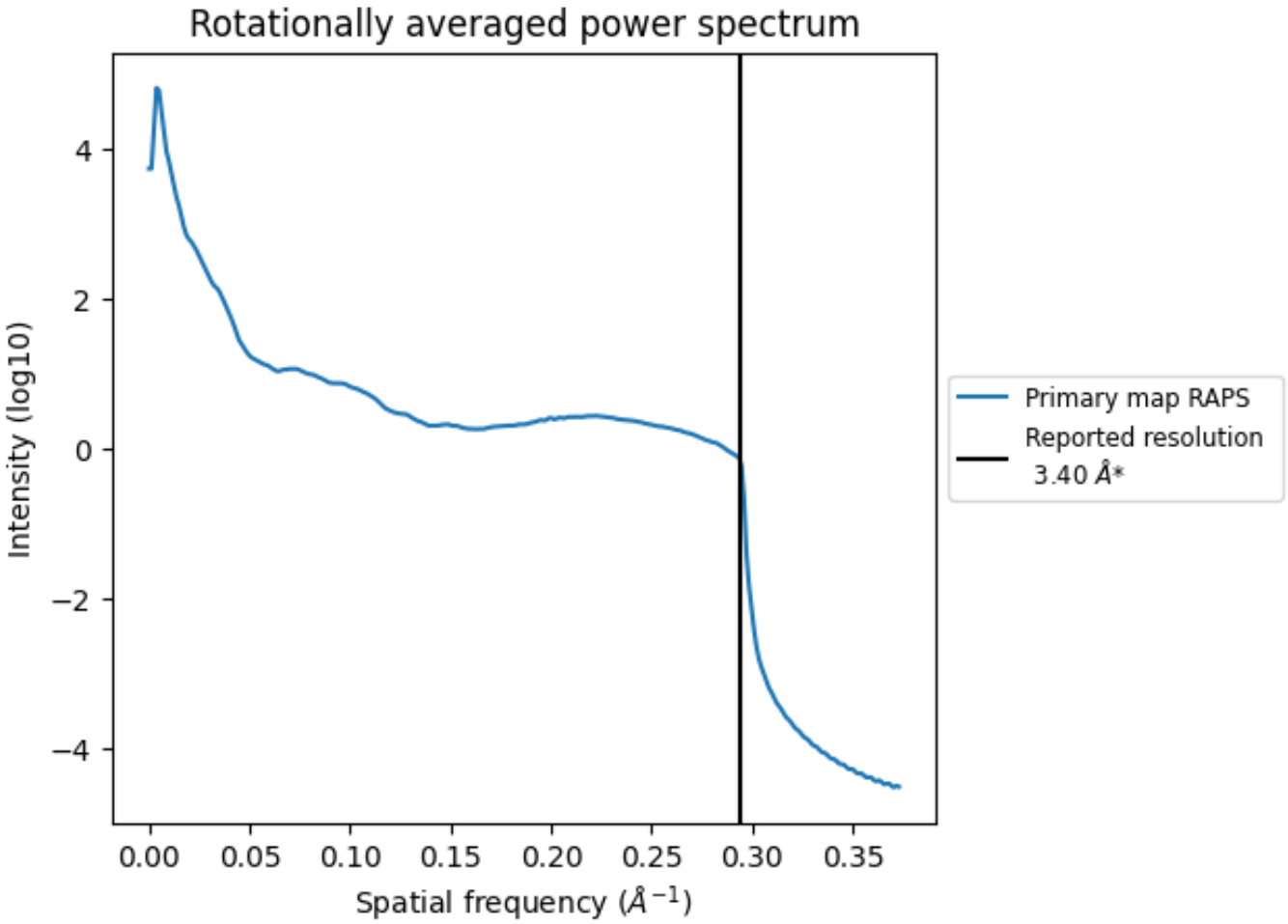
7.2 Volume estimate



The volume at the recommended contour level is 373 nm^3; this corresponds to an approximate mass of 337 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 0.294 Å^{-1}

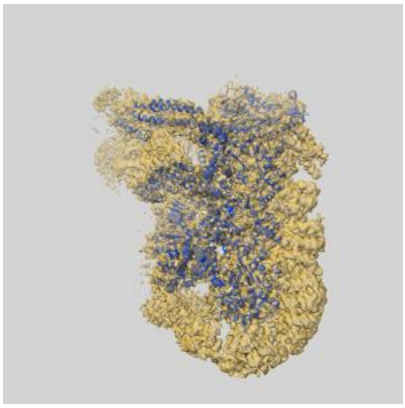
8 Fourier-Shell correlation

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

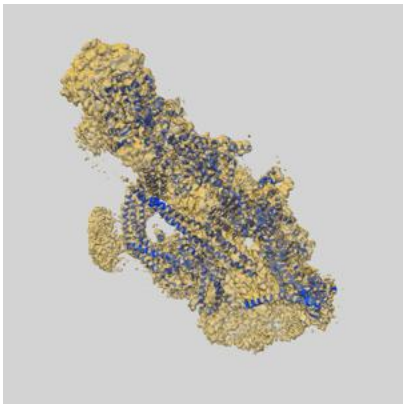
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4169 and PDB model 6F1U. Per-residue inclusion information can be found in section 3 on page 7.

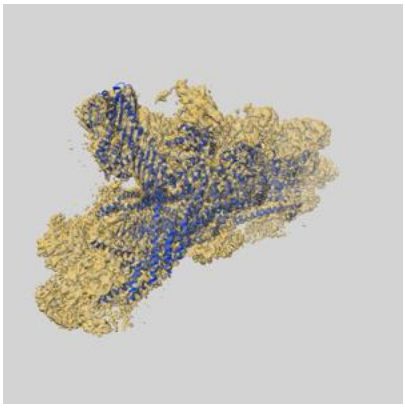
9.1 Map-model overlay



X



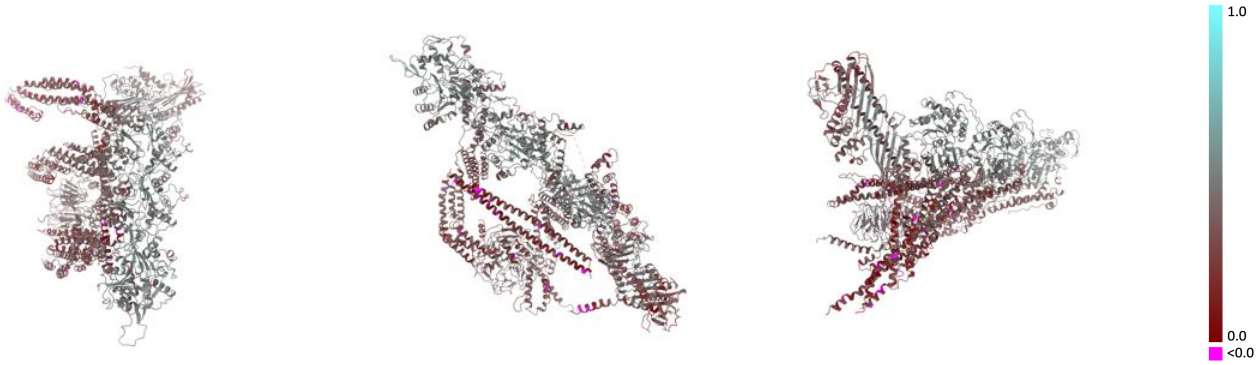
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

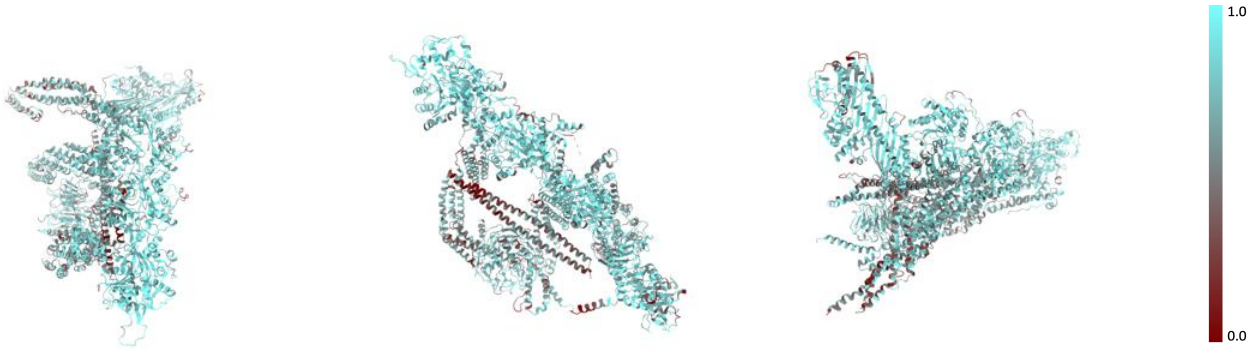
9.2 Q-score mapped to coordinate model (i)



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.

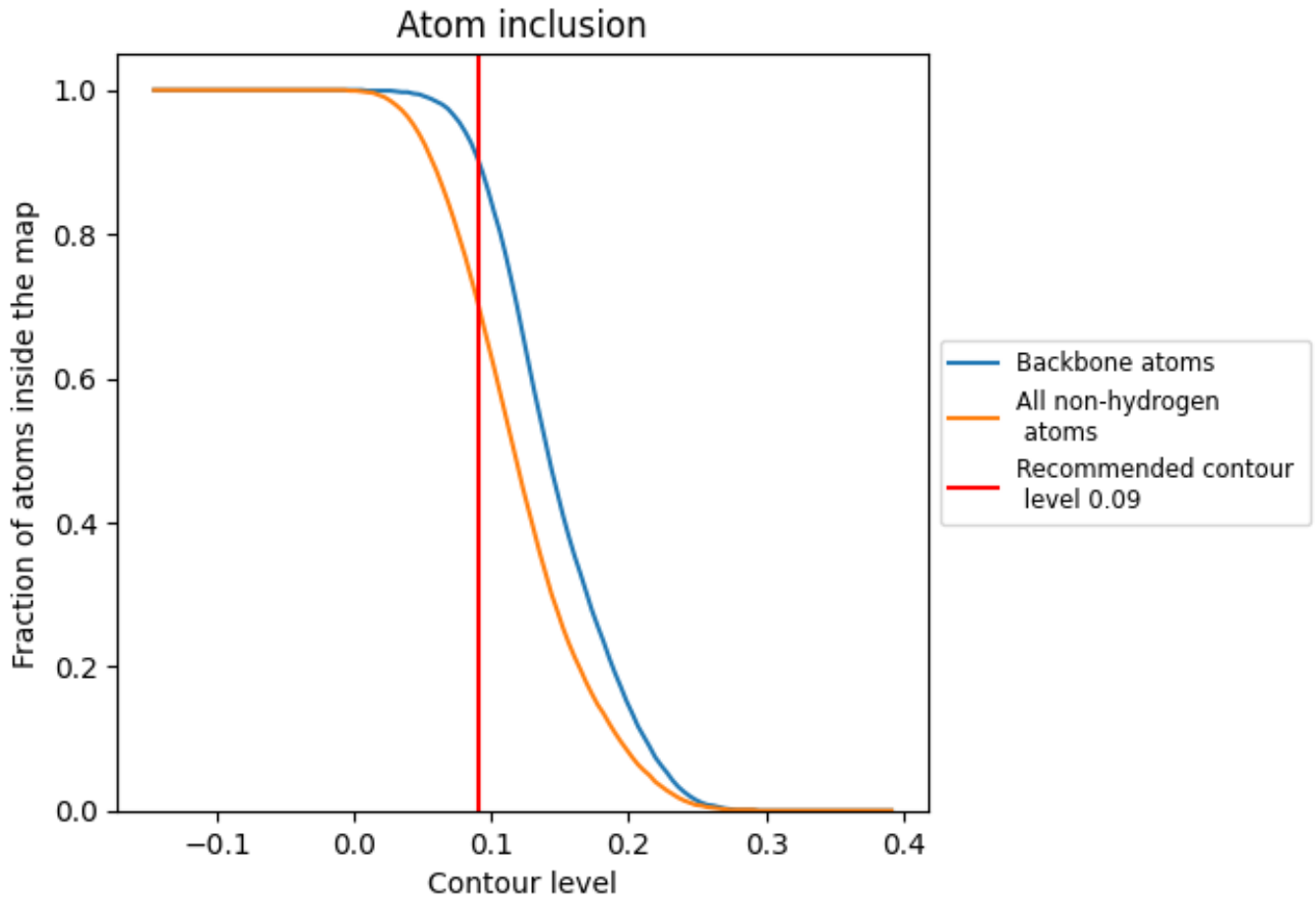
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 71% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7060	0.3740
B	0.8100	0.4770
D	0.8200	0.4800
F	0.8410	0.4820
K	0.7310	0.3700
L	0.7320	0.3990
X	0.3900	0.1670
c	0.6590	0.4530
d	0.6200	0.4340
f	0.6160	0.3080
h	0.7370	0.3720
m	0.7040	0.3490
n	0.5710	0.2440
x	0.4080	0.2140