



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 3LUE / pdb_00003lue
EMDB ID : EMD-5170
Title : Model of alpha-actinin CH1 bound to F-actin
Authors : Galkin, V.E.; Orlova, A.; Salmazo, A.; Djinovic-Carugo, K.; Egelman, E.H.
Deposited on : 2010-02-17
Resolution : 15.00 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

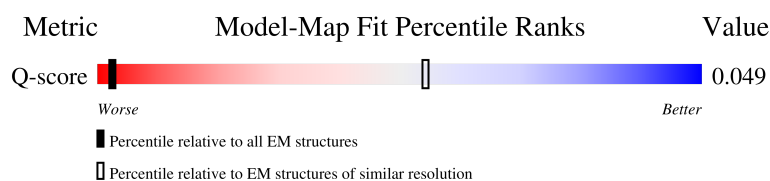
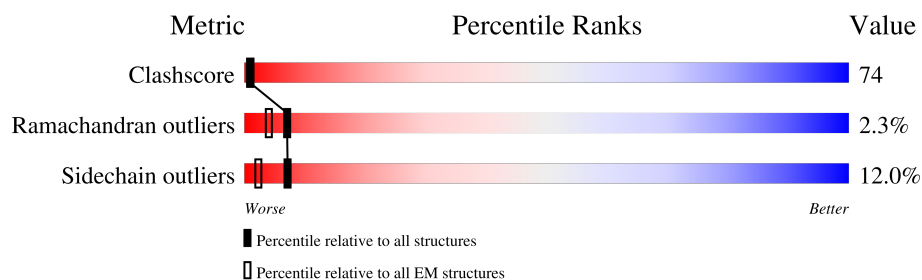
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	37 (14.50 - 15.50)

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 $\leq 5\%$. 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	374	31% 34% 44% 18% •
1	B	374	• 34% 44% 18% •
1	C	374	7% 31% 46% 19% •
1	D	374	5% 32% 45% 19% •

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Mol	Chain	Length	Quality of chain
1	E	374	
1	F	374	
1	G	374	
1	H	374	
1	I	374	
1	J	374	
2	K	109	
2	L	109	
2	M	109	
2	N	109	
2	O	109	
2	P	109	
2	Q	109	
2	R	109	
2	S	109	
2	T	109	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 37910 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 Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	B	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	C	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	D	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	E	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	F	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	G	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	H	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	I	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
1	J	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		

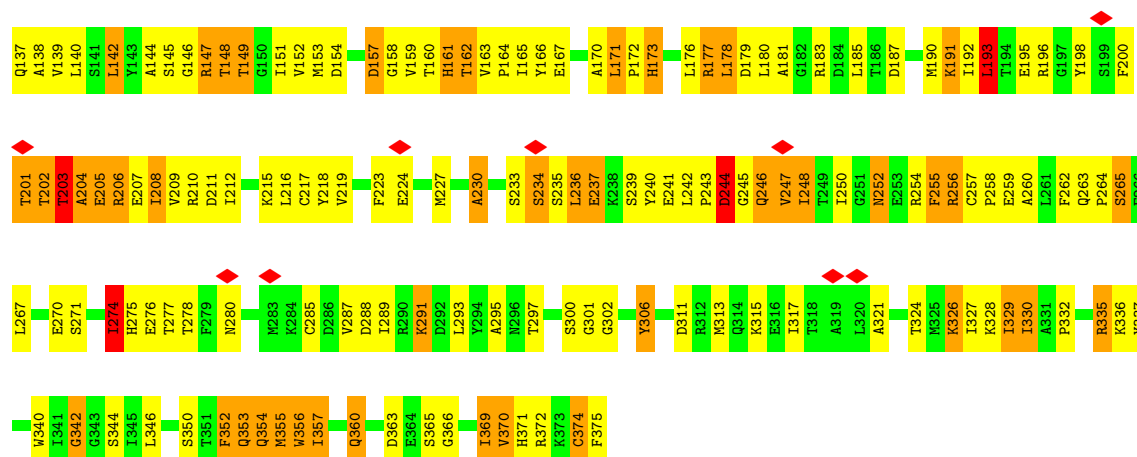
- Molecule 2 is a protein called Alpha-actinin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	109	Total	C	N	O	S	0	0
			874	561	157	151	5		
2	M	109	Total	C	N	O	S	0	0
			874	561	157	151	5		
2	L	109	Total	C	N	O	S	0	0
			874	561	157	151	5		
2	O	109	Total	C	N	O	S	0	0
			874	561	157	151	5		
2	N	109	Total	C	N	O	S	0	0
			874	561	157	151	5		

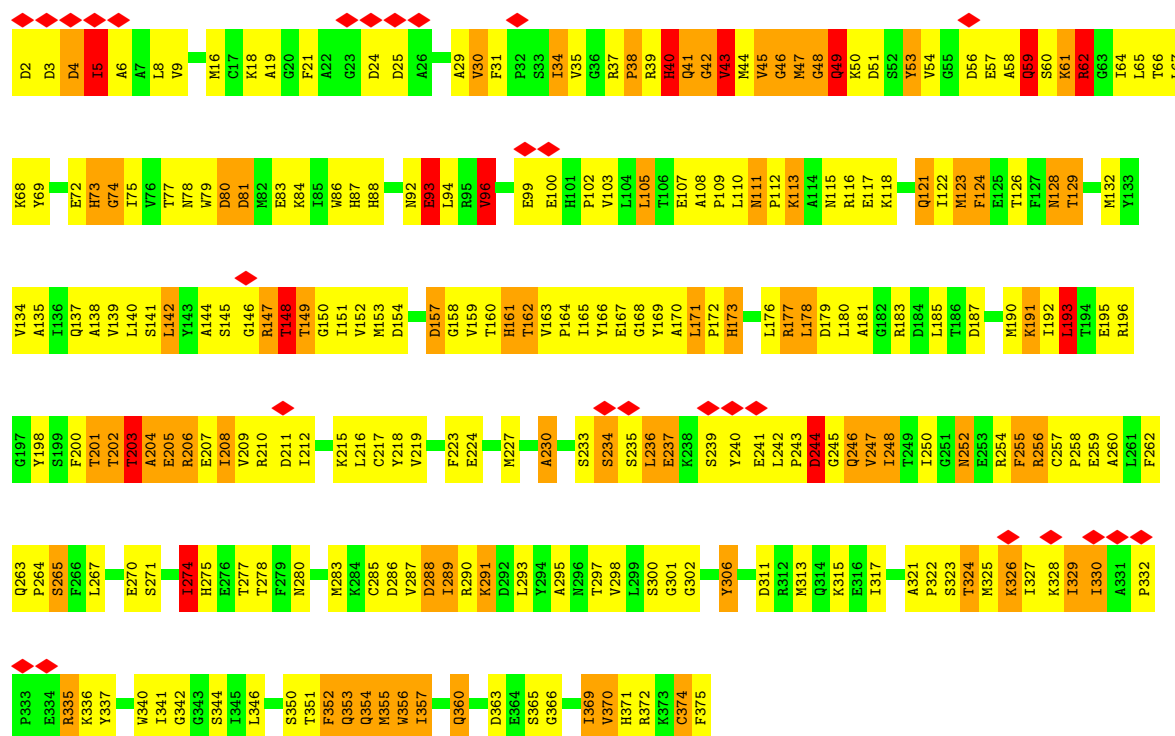
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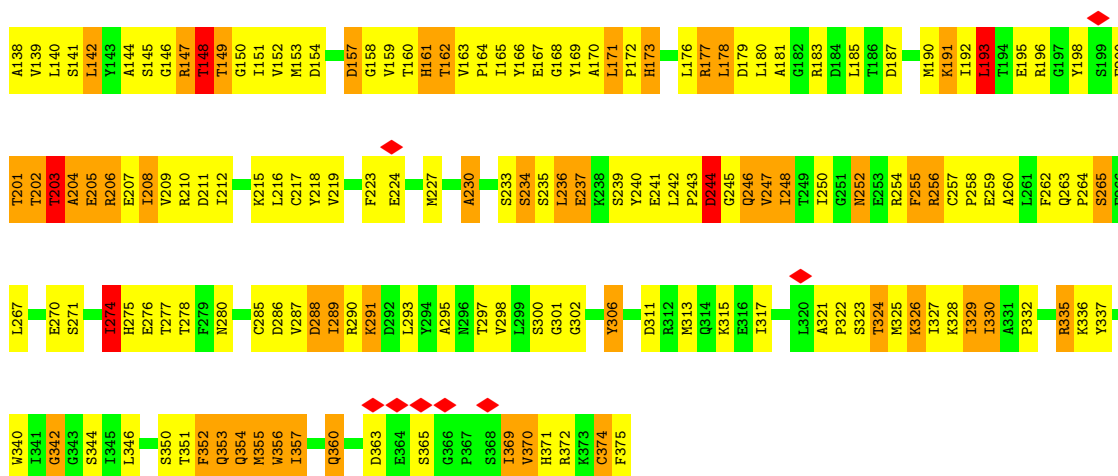
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	109	Total 874	C 561	N 157	O 151	S 5	0	0
2	P	109	Total 874	C 561	N 157	O 151	S 5	0	0
2	S	109	Total 874	C 561	N 157	O 151	S 5	0	0
2	R	109	Total 874	C 561	N 157	O 151	S 5	0	0
2	T	109	Total 874	C 561	N 157	O 151	S 5	0	0

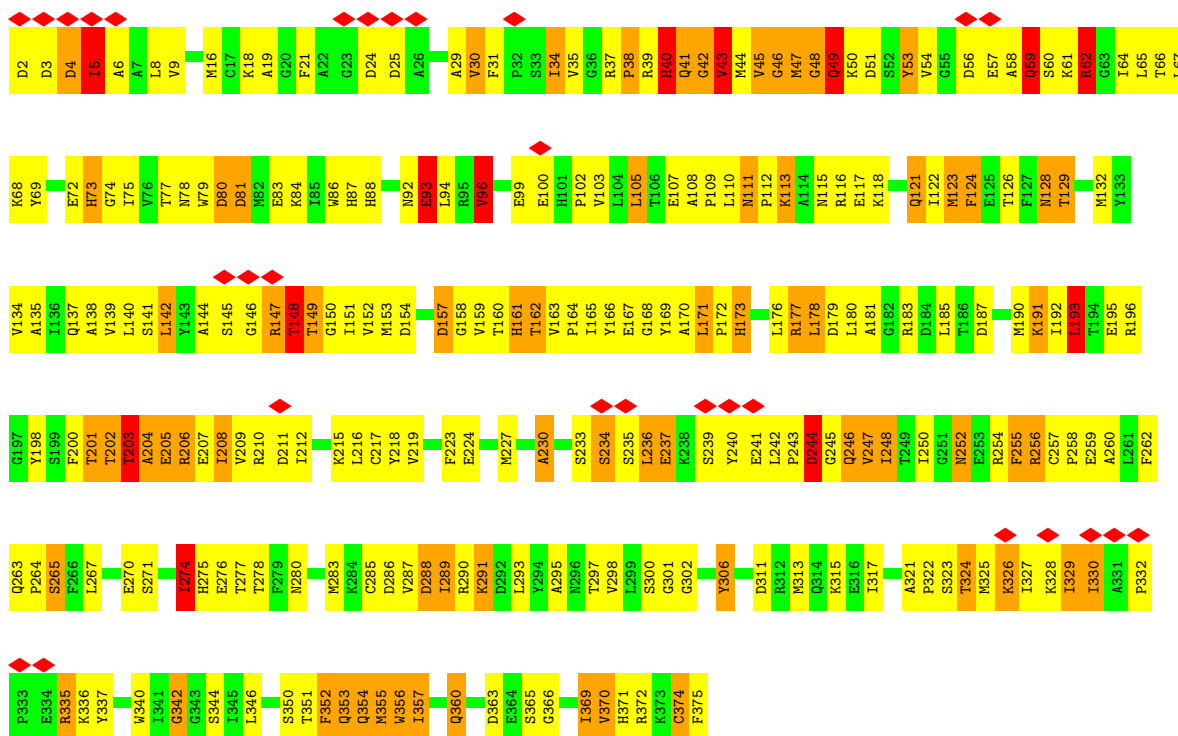


• Molecule 1: Actin, cytoplasmic 1



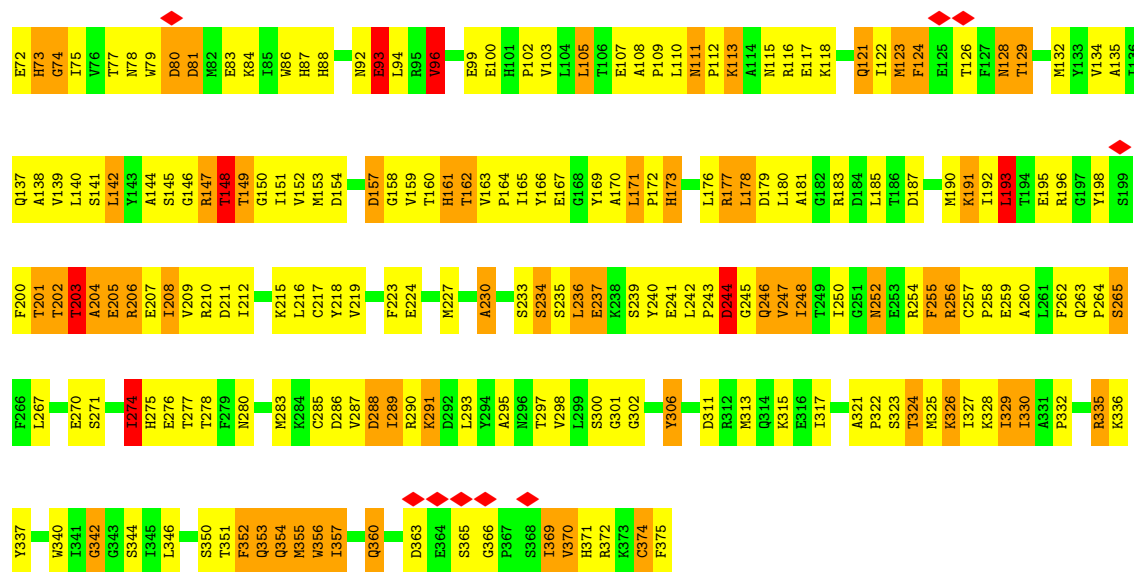


• Molecule 1: Actin, cytoplasmic 1

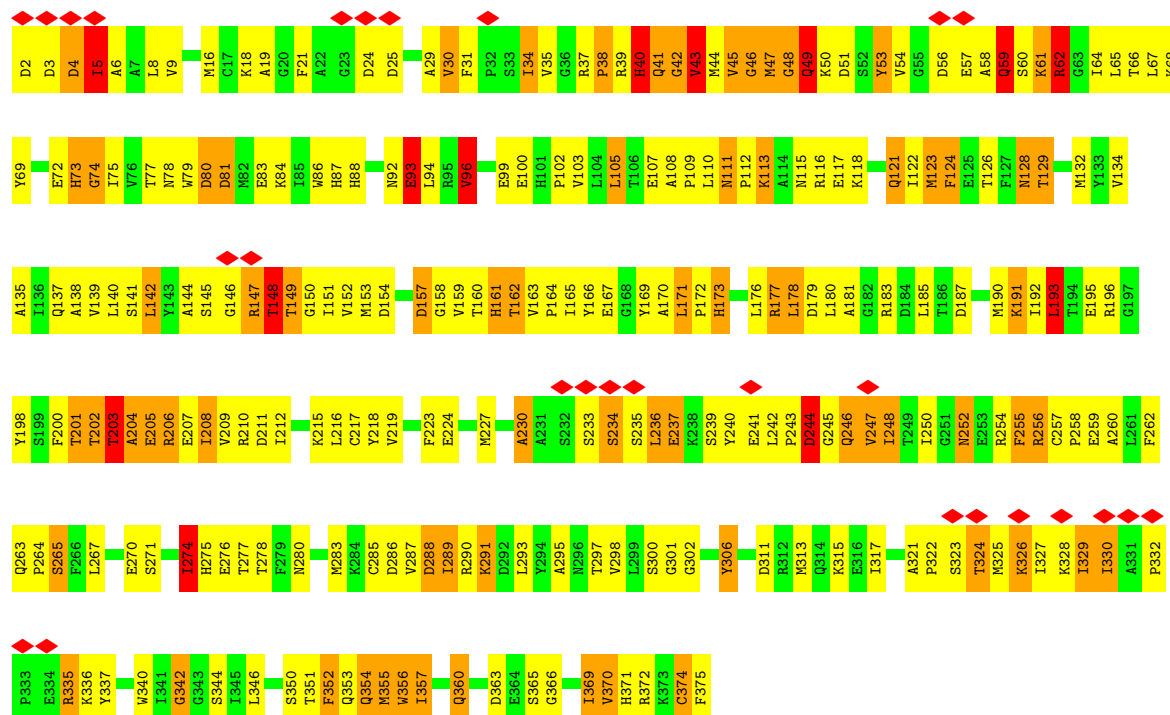


• Molecule 1: Actin, cytoplasmic 1

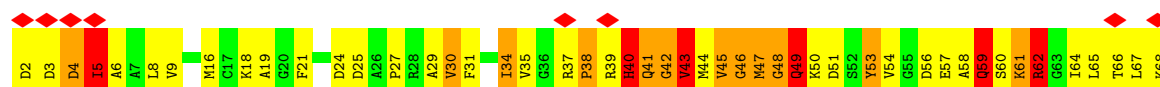


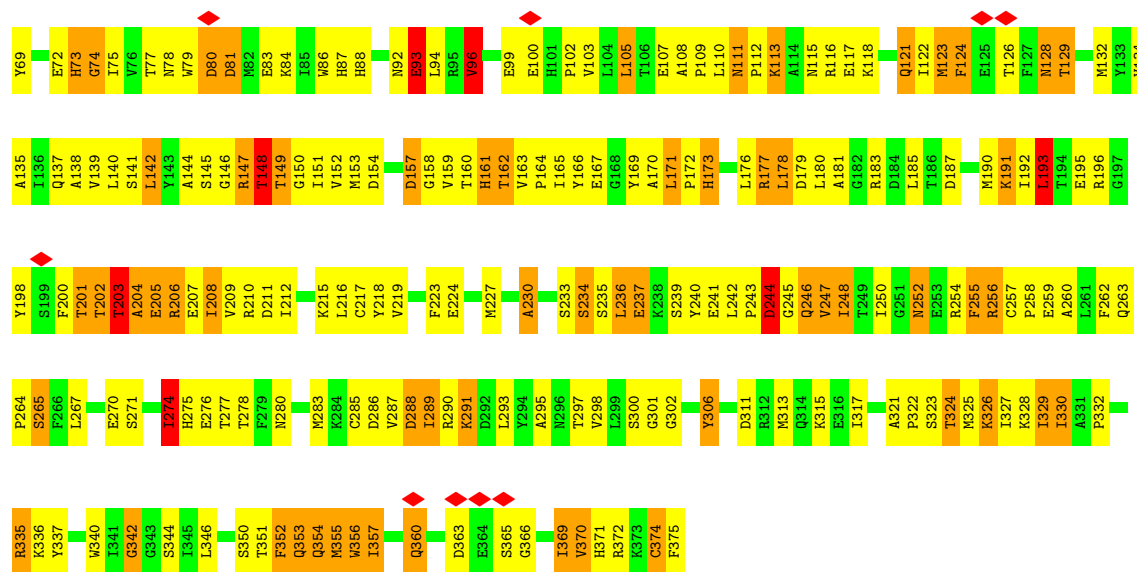


• Molecule 1: Actin, cytoplasmic 1

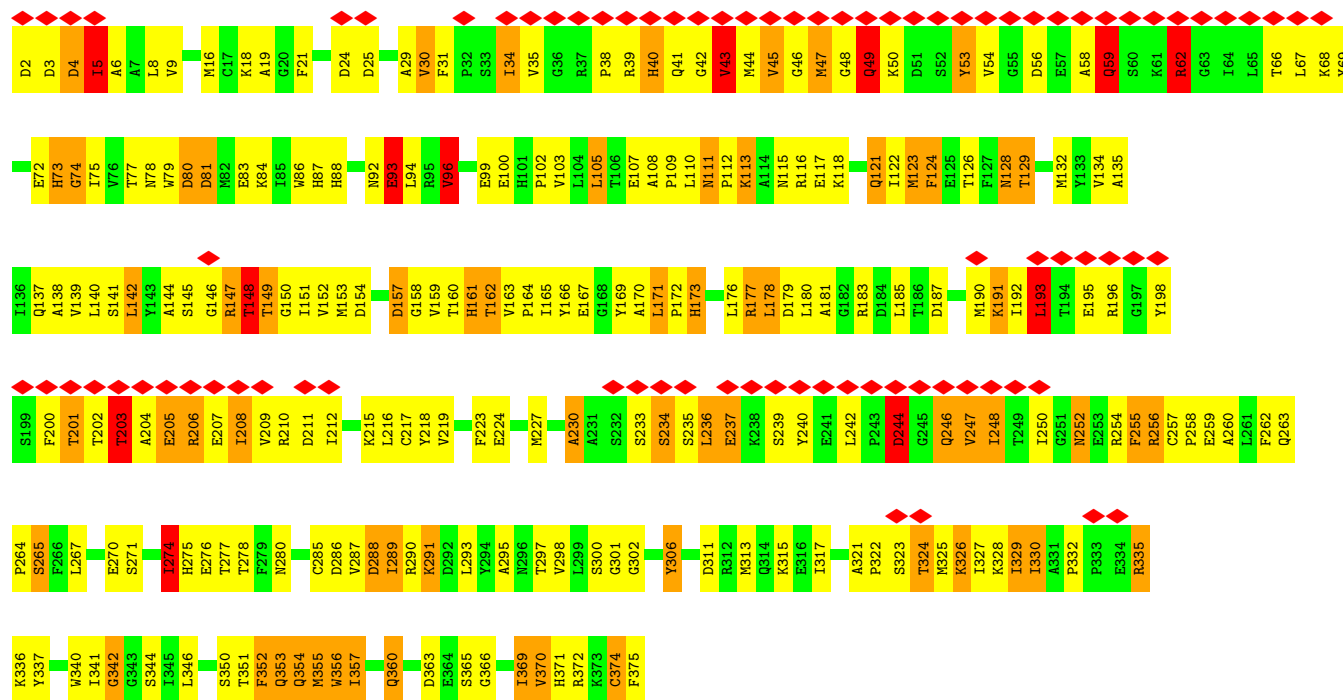


• Molecule 1: Actin, cytoplasmic 1

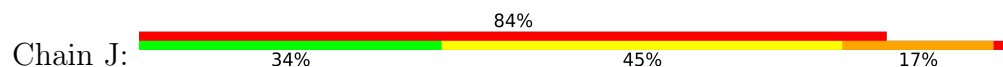


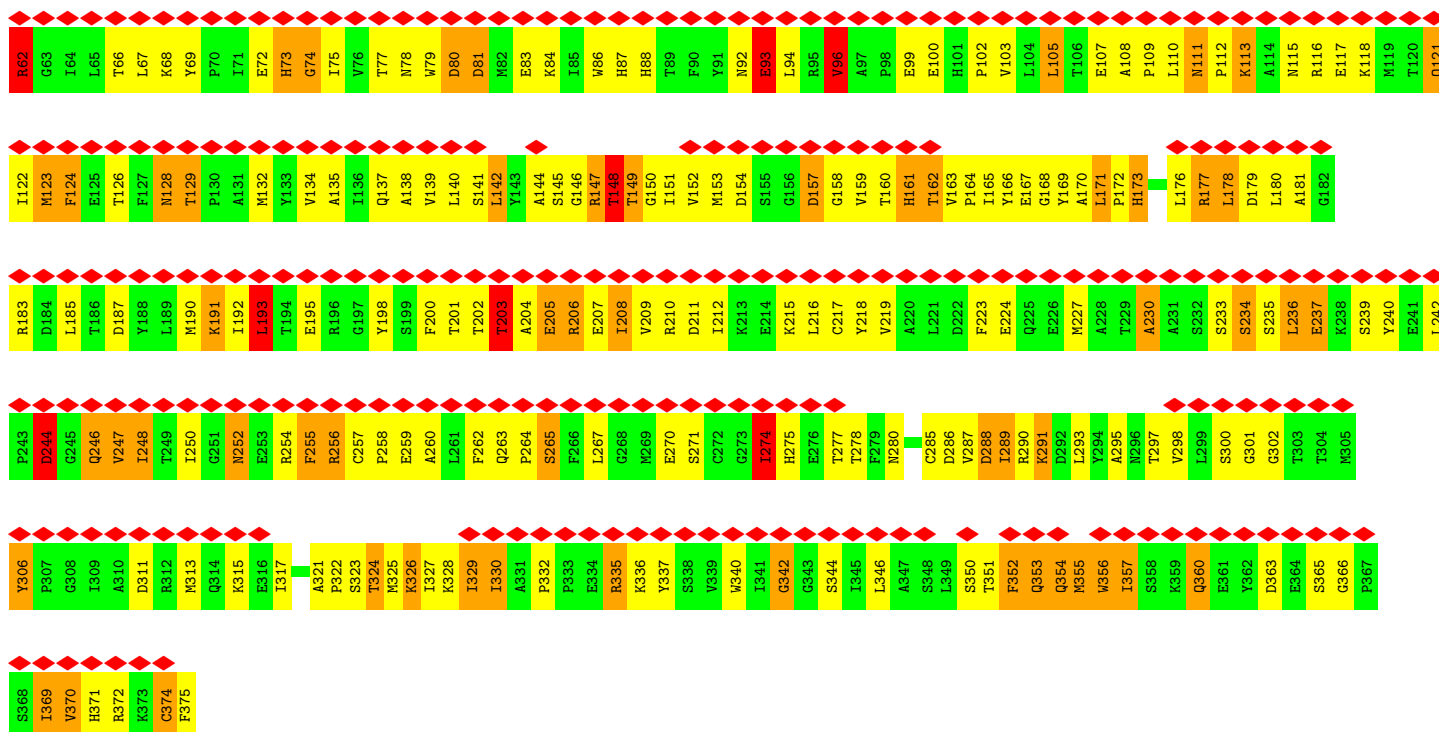


• Molecule 1: Actin, cytoplasmic 1

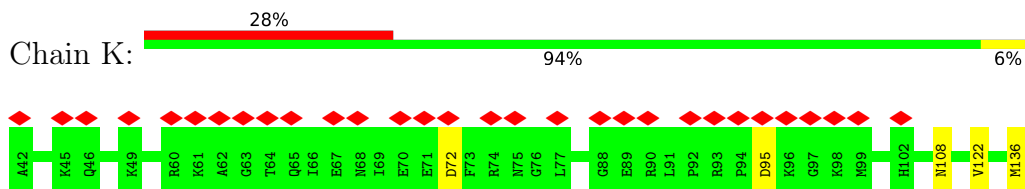


• Molecule 1: Actin, cytoplasmic 1

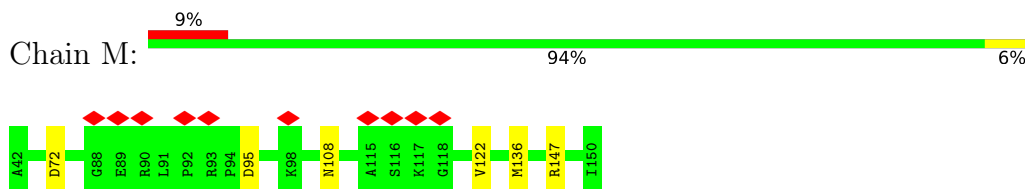




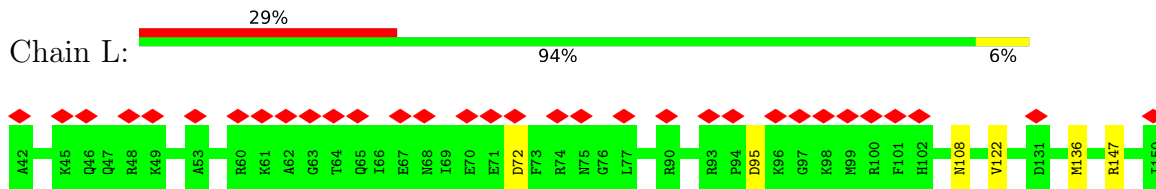
- Molecule 2: Alpha-actinin-3



- Molecule 2: Alpha-actinin-3

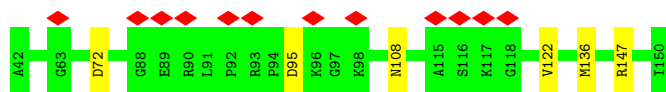


- Molecule 2: Alpha-actinin-3

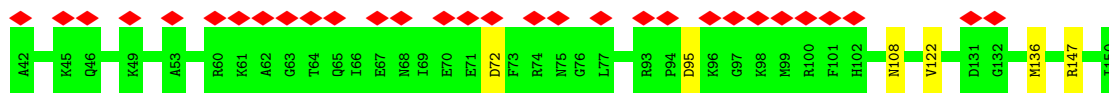


- Molecule 2: Alpha-actinin-3

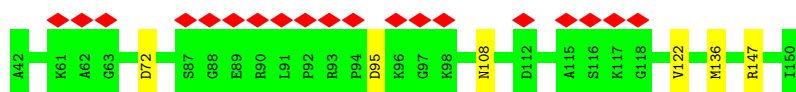




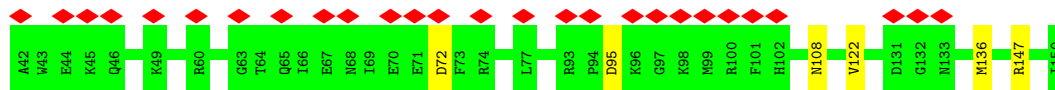
- Molecule 2: Alpha-actinin-3



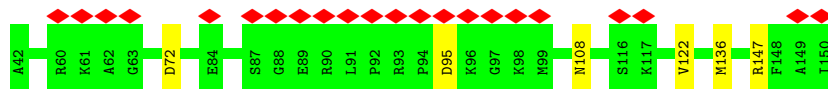
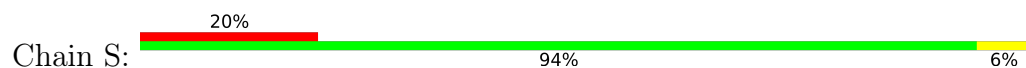
- Molecule 2: Alpha-actinin-3



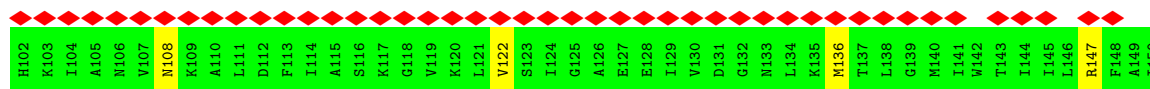
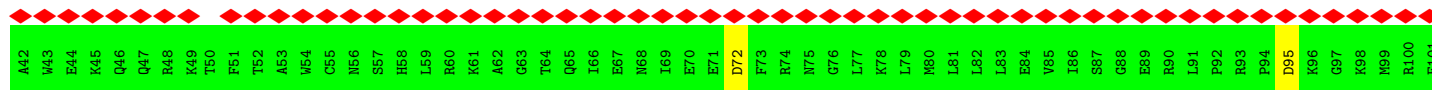
- Molecule 2: Alpha-actinin-3



- Molecule 2: Alpha-actinin-3



- Molecule 2: Alpha-actinin-3



- Molecule 2: Alpha-actinin-3



H102	K103	I104	A105	N106	V107	N108	K109	A110	L111	D112	F113	I114	A115	S116	K117	G118	V119	K120	L121	V122	S123	I124	G125	A126	E127	E128	I129	V130	D131	G132	N133	L134	K135	M136	T137	L138	G139	M140	I141	W142	T143	I144	I145	L146	R147	F148	A149	I150											
A42	W43	E44	K45	Q46	Q47	R48	K49	T50	F51	T52	A53	W54	C55	N56	S57	H58	L59	R60	K61	A62	G63	T64	Q65	I66	E67	N68	I69	E70	E71	D72	F73	R74	N75	G76	L77	K78	L79	M80	L81	L82	L83	E84	V85	I86	S87	G88	E89	R90	L91	P92	R93	P94	D95	K96	G97	K98	M99	R100	F101

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=166.8°, rise=27.7 Å, axial sym=C1	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Weiner filter	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	2.180	Depositor
Minimum map value	-0.684	Depositor
Average map value	0.077	Depositor
Map value standard deviation	0.294	Depositor
Recommended contour level	0.61	Depositor
Map size (Å)	238, 238, 238	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.38, 2.38, 2.38	Depositor

5 Model quality

5.1 Standard geometry

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	1.29	15/2974 (0.5%)	2.35	173/4016 (4.3%)
1	B	1.29	15/2974 (0.5%)	2.35	174/4016 (4.3%)
1	C	1.29	14/2974 (0.5%)	2.35	171/4016 (4.3%)
1	D	1.29	15/2974 (0.5%)	2.35	171/4016 (4.3%)
1	E	1.29	15/2974 (0.5%)	2.30	170/4016 (4.2%)
1	F	1.29	15/2974 (0.5%)	2.35	173/4016 (4.3%)
1	G	1.29	15/2974 (0.5%)	2.35	173/4016 (4.3%)
1	H	1.29	15/2974 (0.5%)	2.35	174/4016 (4.3%)
1	I	1.29	15/2974 (0.5%)	2.35	173/4016 (4.3%)
1	J	1.29	14/2974 (0.5%)	2.35	173/4016 (4.3%)
2	K	0.47	0/888	0.89	4/1190 (0.3%)
2	L	0.47	0/888	0.89	4/1190 (0.3%)
2	M	0.47	0/888	0.90	4/1190 (0.3%)
2	N	0.47	0/888	0.89	4/1190 (0.3%)
2	O	0.47	0/888	0.89	4/1190 (0.3%)
2	P	0.47	0/888	0.89	4/1190 (0.3%)
2	Q	0.47	0/888	0.89	4/1190 (0.3%)
2	R	0.47	0/888	0.89	4/1190 (0.3%)
2	S	0.47	0/888	0.89	4/1190 (0.3%)
2	T	0.47	0/888	0.89	4/1190 (0.3%)
All	All	1.16	148/38620 (0.4%)	2.10	1765/52060 (3.4%)

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
1	A	1	1
1	B	1	1
1	C	1	1
1	D	1	1
1	E	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	1	1
1	G	1	1
1	H	1	1
1	I	1	1
1	J	1	1
All	All	10	10

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	192	ILE	CA-CB	7.05	1.64	1.54
1	E	192	ILE	CA-CB	7.03	1.64	1.54
1	J	192	ILE	CA-CB	7.03	1.64	1.54
1	H	192	ILE	CA-CB	7.02	1.64	1.54
1	I	192	ILE	CA-CB	7.02	1.64	1.54

The worst 5 of 1765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	74	GLY	O-C-N	-20.62	90.01	123.00
1	B	74	GLY	O-C-N	-20.61	90.02	123.00
1	I	74	GLY	O-C-N	-20.61	90.03	123.00
1	A	74	GLY	O-C-N	-20.61	90.03	123.00
1	C	74	GLY	O-C-N	-20.60	90.03	123.00

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	73	HIS	CA
1	B	73	HIS	CA
1	C	73	HIS	CA
1	D	73	HIS	CA
1	E	73	HIS	CA

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ASP	Mainchain
1	B	4	ASP	Mainchain
1	C	4	ASP	Mainchain
1	D	4	ASP	Mainchain
1	E	4	ASP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2917	0	2851	479	0
1	B	2917	0	2851	481	0
1	C	2917	0	2847	726	0
1	D	2917	0	2847	725	0
1	E	2917	0	2847	727	0
1	F	2917	0	2847	725	0
1	G	2917	0	2847	724	0
1	H	2917	0	2847	726	0
1	I	2917	0	2857	481	0
1	J	2917	0	2857	476	0
2	K	874	0	917	0	0
2	L	874	0	917	0	0
2	M	874	0	917	0	0
2	N	874	0	917	0	0
2	O	874	0	917	0	0
2	P	874	0	917	0	0
2	Q	874	0	917	0	0
2	R	874	0	917	0	0
2	S	874	0	917	0	0
2	T	874	0	917	0	0
All	All	37910	0	37668	4256	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 74.

The worst 5 of 4256 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:LEU:HD13	1:H:152:VAL:CG2	1.18	1.62
1:A:69:TYR:CB	1:A:84:LYS:H	0.99	1.62
1:G:245:GLY:HA2	1:I:324:THR:CA	1.28	1.61
1:C:69:TYR:CB	1:C:84:LYS:H	0.99	1.60
1:C:142:LEU:HD13	1:C:152:VAL:CG2	1.18	1.60

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/374 (96%)	318 (88%)	32 (9%)	11 (3%)	3	23
1	B	361/374 (96%)	318 (88%)	33 (9%)	10 (3%)	4	24
1	C	361/374 (96%)	318 (88%)	32 (9%)	11 (3%)	3	23
1	D	361/374 (96%)	318 (88%)	32 (9%)	11 (3%)	3	23
1	E	361/374 (96%)	318 (88%)	33 (9%)	10 (3%)	4	24
1	F	361/374 (96%)	318 (88%)	32 (9%)	11 (3%)	3	23
1	G	361/374 (96%)	318 (88%)	32 (9%)	11 (3%)	3	23
1	H	361/374 (96%)	318 (88%)	32 (9%)	11 (3%)	3	23
1	I	361/374 (96%)	318 (88%)	33 (9%)	10 (3%)	4	24
1	J	361/374 (96%)	318 (88%)	32 (9%)	11 (3%)	3	23
2	K	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	L	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	M	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	N	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	O	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	P	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	Q	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	R	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	S	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
2	T	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
All	All	4680/4830 (97%)	4200 (90%)	373 (8%)	107 (2%)	7	28

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL

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Mol	Chain	Res	Type
1	A	203	THR
1	A	233	SER
1	A	355	MET
1	B	43	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	B	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	C	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	D	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	E	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	F	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	G	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	H	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	I	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	J	317/317 (100%)	271 (86%)	46 (14%)	3	13
2	K	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	L	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	M	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	N	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	O	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	P	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	Q	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	R	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	S	93/93 (100%)	90 (97%)	3 (3%)	34	56
2	T	93/93 (100%)	90 (97%)	3 (3%)	34	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4100/4100 (100%)	3610 (88%)	490 (12%)	7 17

5 of 490 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	18	LYS
1	J	246	GLN
1	G	80	ASP
1	J	208	ILE
2	N	108	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	353	GLN
1	I	353	GLN
1	H	41	GLN
1	H	353	GLN
1	J	87	HIS

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 ⓘ

There are no ligands in this entry.

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
1	A	6
1	B	6
1	C	6
1	G	6
1	I	6
1	D	6
1	E	6
1	F	6
1	H	6
1	J	6

The worst 5 of 60 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	69:TYR	C	70:PRO	N	11.23
1	B	69:TYR	C	70:PRO	N	11.23
1	C	69:TYR	C	70:PRO	N	11.23
1	G	69:TYR	C	70:PRO	N	11.23
1	I	69:TYR	C	70:PRO	N	11.23

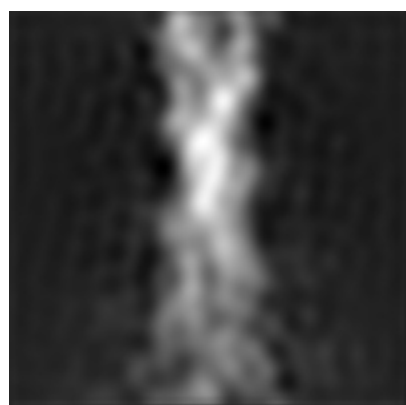
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5170. These allow visual inspection of the internal detail of the map and identification of artifacts.

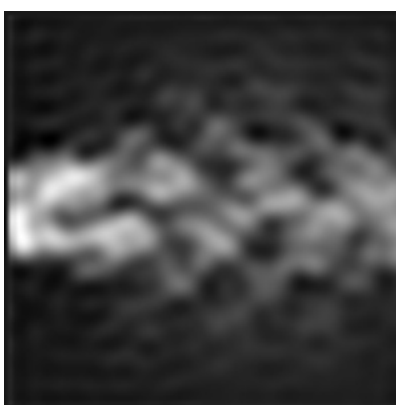
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

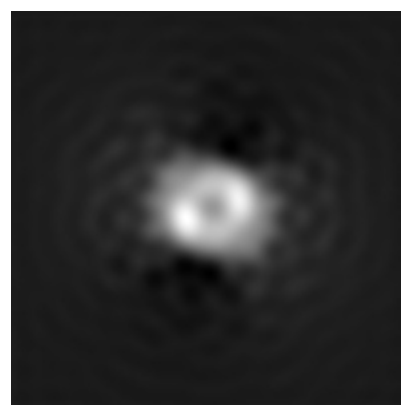
6.1.1 Primary map



X



Y

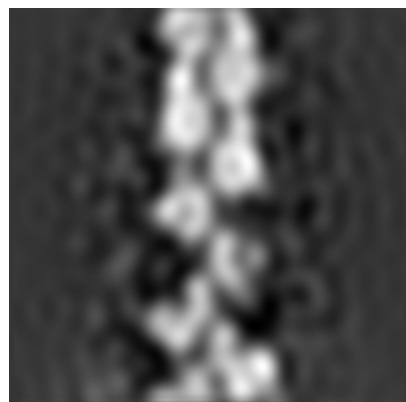


Z

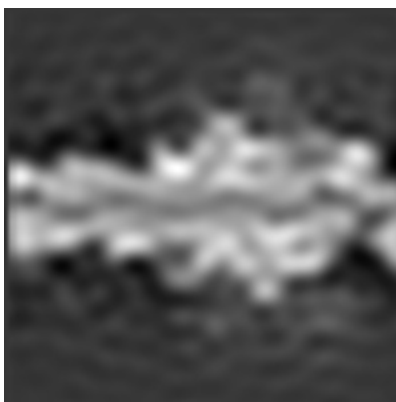
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

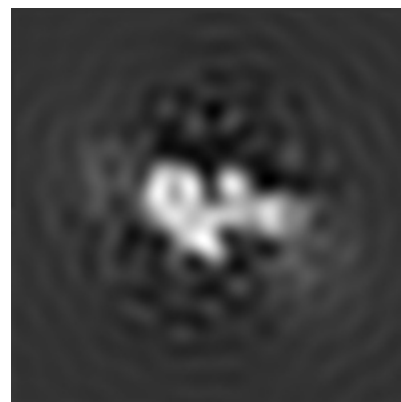
6.2.1 Primary map



X Index: 50



Y Index: 50

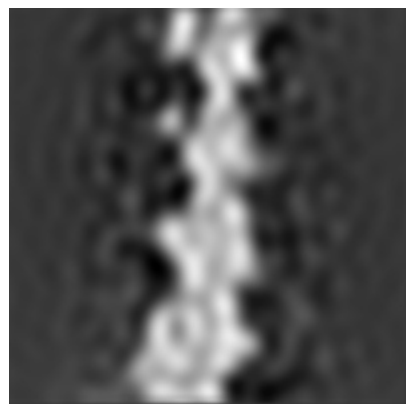


Z Index: 50

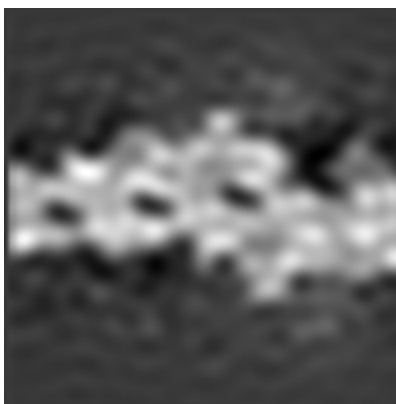
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

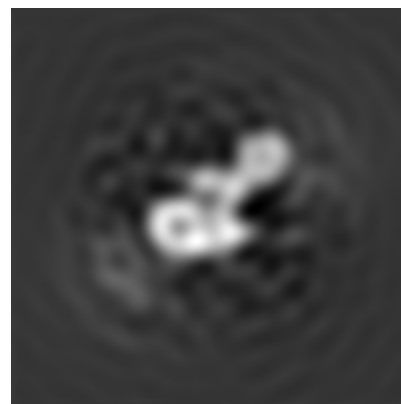
6.3.1 Primary map



X Index: 56



Y Index: 46

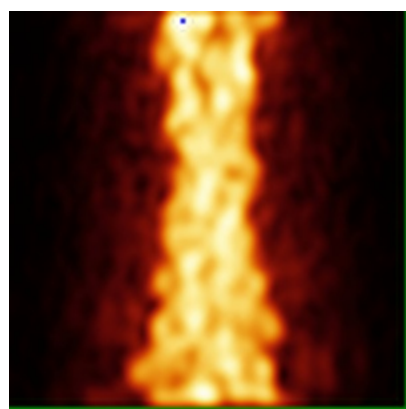


Z Index: 97

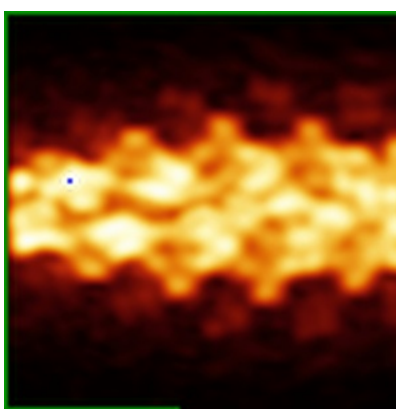
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

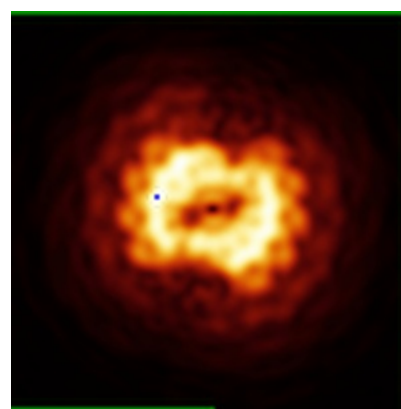
6.4.1 Primary map



X



Y

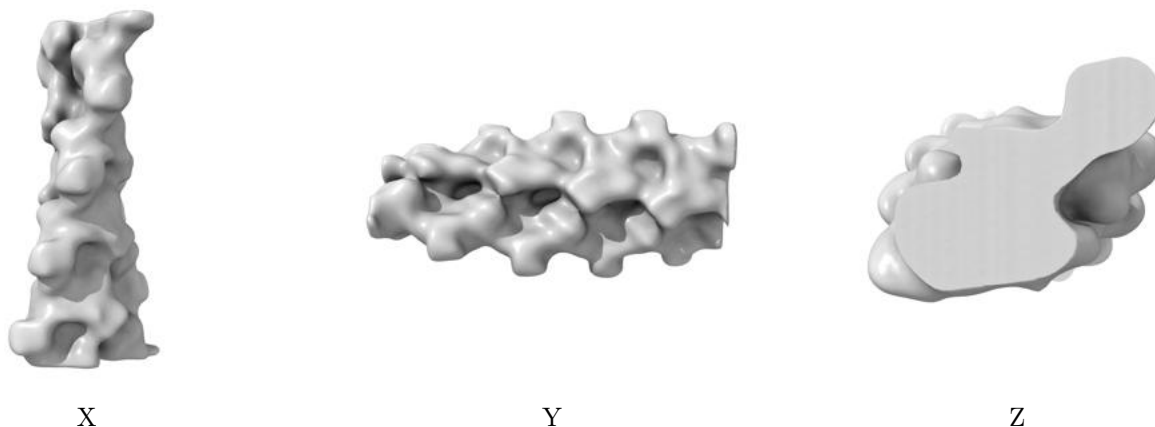


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.61. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

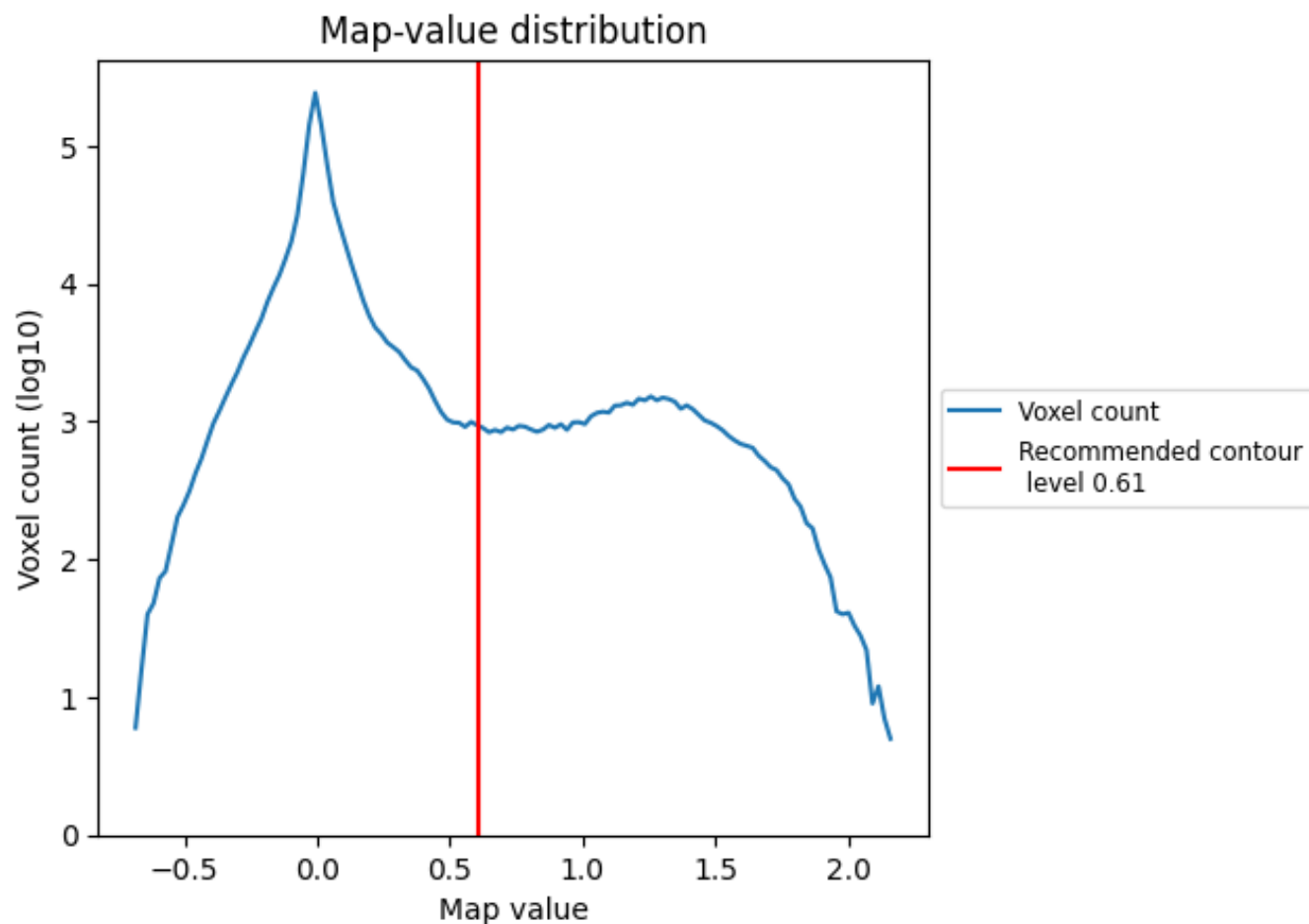
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

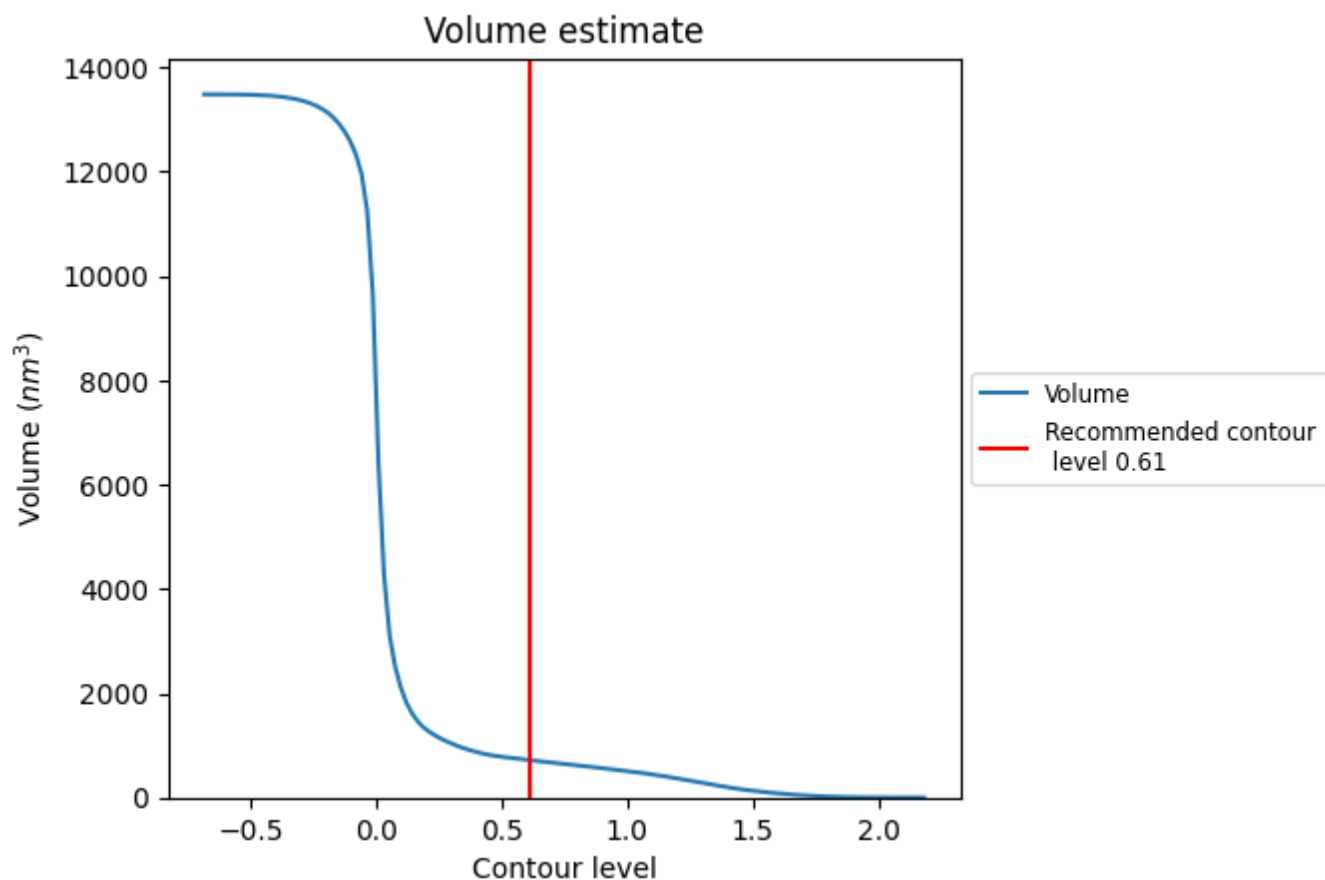
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

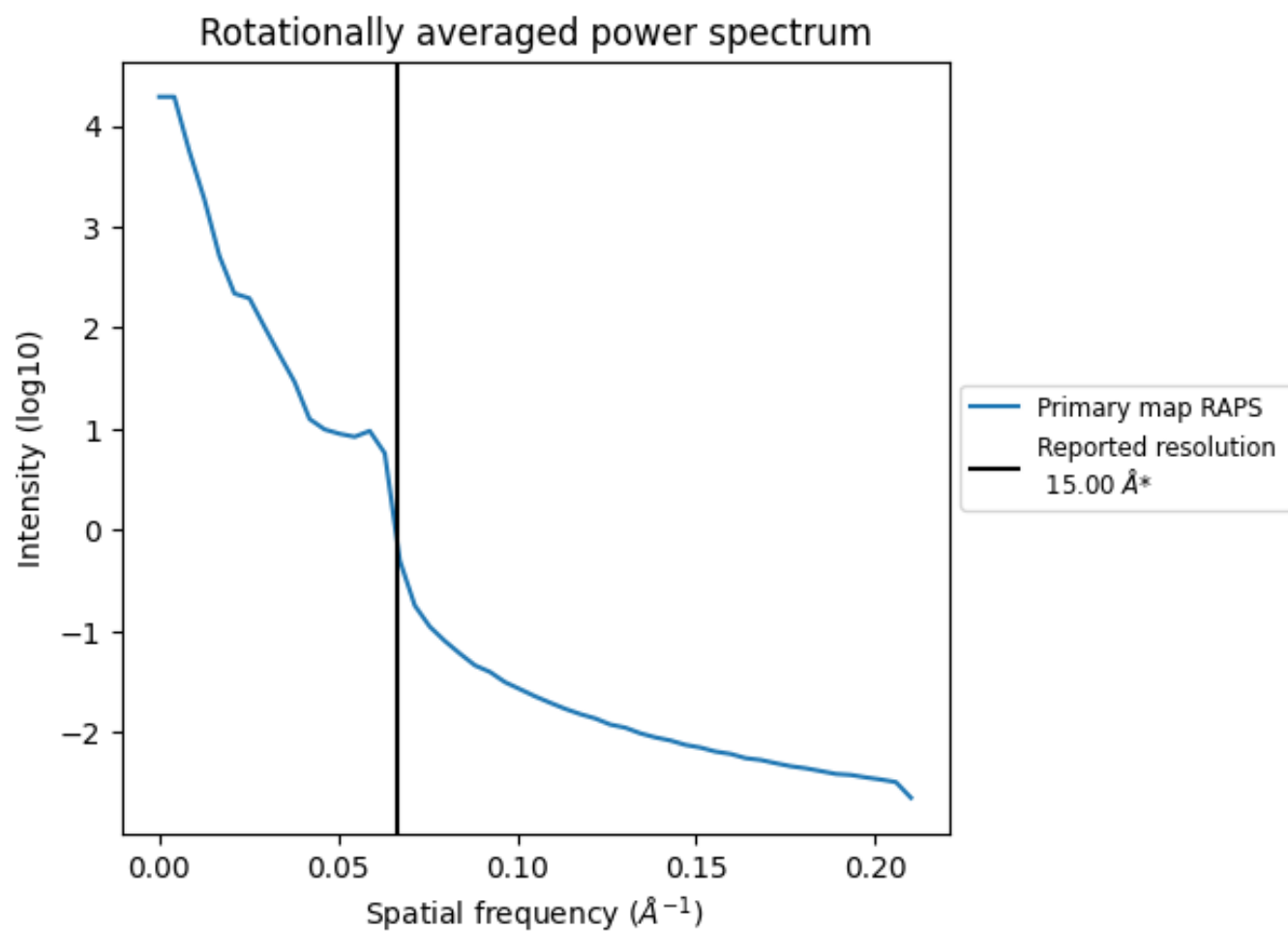
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 718 nm³; this corresponds to an approximate mass of 649 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.067 Å⁻¹

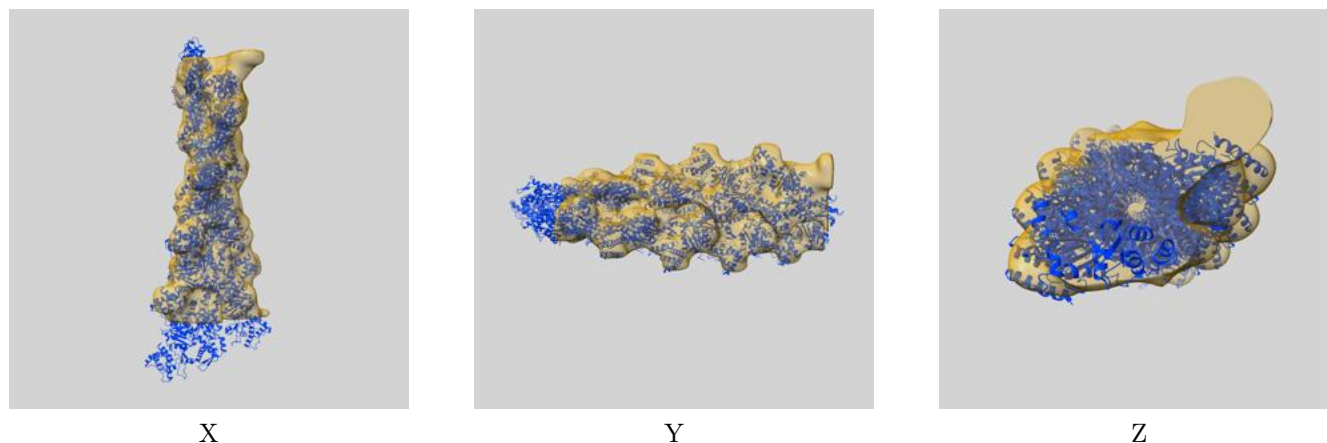
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

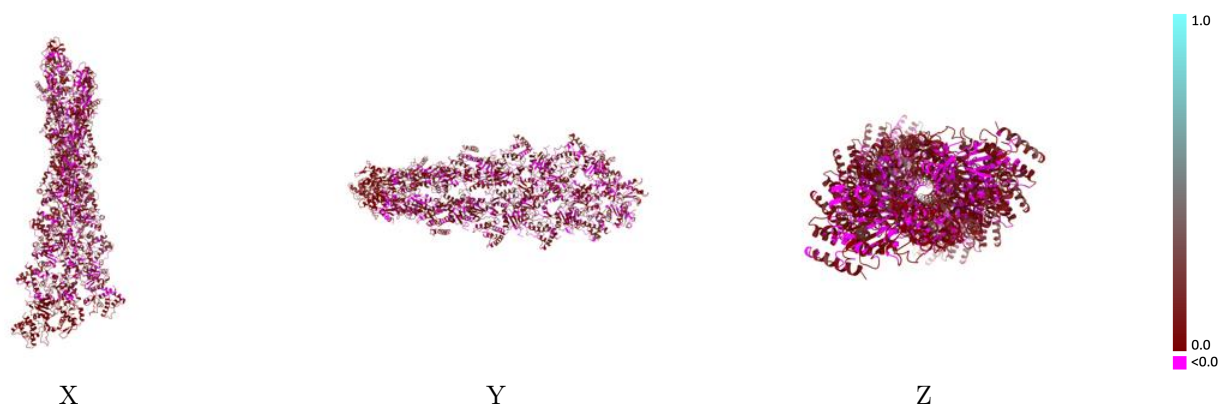
This section contains information regarding the fit between EMDB map EMD-5170 and PDB model 3LUE. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



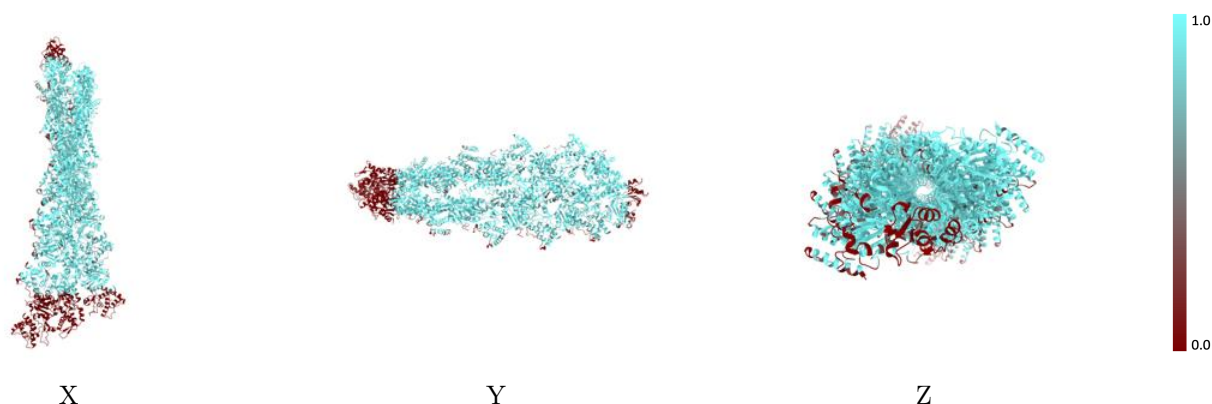
The images above show the 3D surface view of the map at the recommended contour level 0.61 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



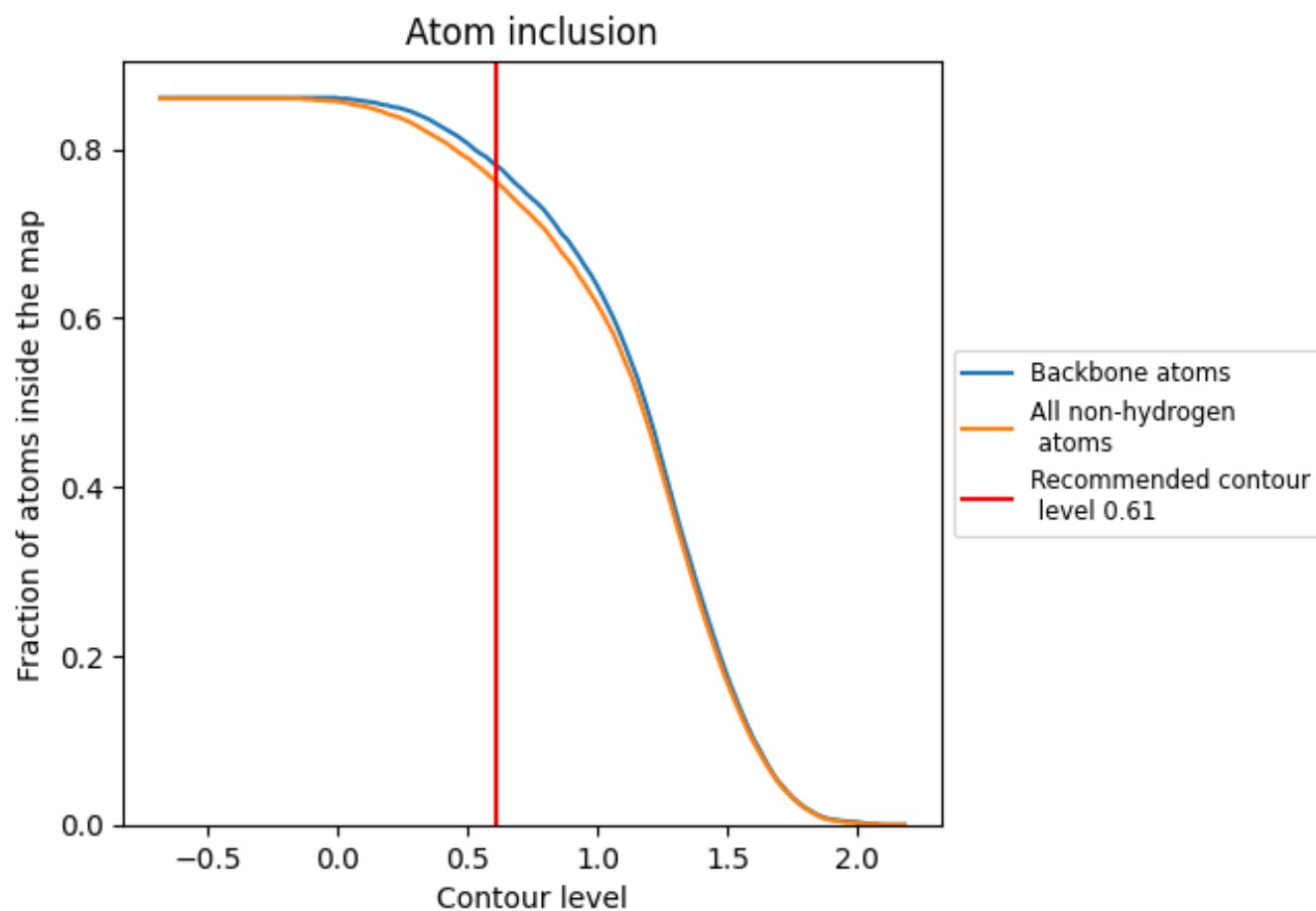
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.61).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.61) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7610	 0.0490
A	 0.6730	 0.0440
B	 0.9440	 0.0540
C	 0.9130	 0.0600
D	 0.9400	 0.0550
E	 0.9110	 0.0620
F	 0.9310	 0.0540
G	 0.9140	 0.0630
H	 0.9300	 0.0580
I	 0.7480	 0.0460
J	 0.1490	 0.0060
K	 0.6910	 0.0540
L	 0.6850	 0.0550
M	 0.8730	 0.0630
N	 0.6920	 0.0540
O	 0.8680	 0.0640
P	 0.7250	 0.0570
Q	 0.8100	 0.0620
R	 0.0500	 -0.0190
S	 0.7490	 0.0560
T	 0.0000	 0.0000

