



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 02:43 PM UTC

PDB ID : 9AZ6 / pdb_00009az6
EMDB ID : EMD-44013
Title : F-actin-Talin(R13-DD) complex
Authors : Biertumpfel, C.; Yamada, Y.; Mizuno, N.
Deposited on : 2024-03-10
Resolution : 2.98 Å(reported)
Based on initial models : 2jsw, 8a2t, 2qdq

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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

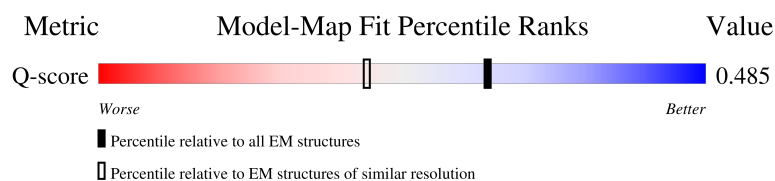
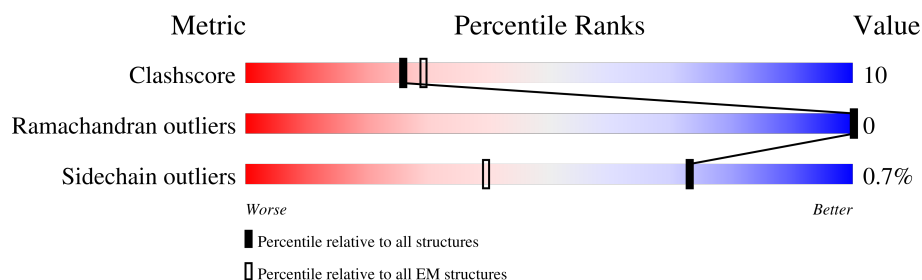
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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.

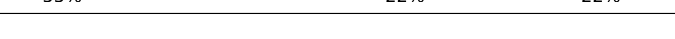
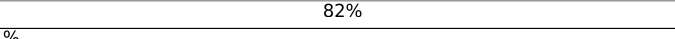
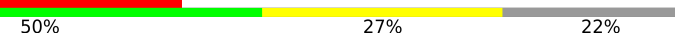
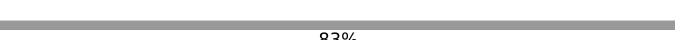
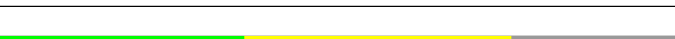
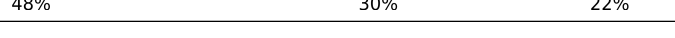
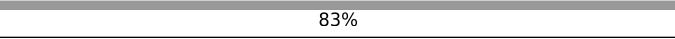


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13236 (2.48 - 3.48)

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	375	
1	B	375	
1	C	375	
1	D	375	

Continued on next page...

Mol	Chain	Length	Quality of chain
1	E	375	
2	F	246	
2	G	246	
2	H	246	
2	I	246	
2	J	246	
2	K	246	
2	L	246	
2	M	246	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21831 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, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	373	Total	C	N	O	S	0	0
			2916	1846	491	558	21		
1	B	373	Total	C	N	O	S	0	0
			2916	1846	491	558	21		
1	C	373	Total	C	N	O	S	0	0
			2916	1846	491	558	21		
1	D	373	Total	C	N	O	S	0	0
			2916	1846	491	558	21		
1	E	373	Total	C	N	O	S	0	0
			2916	1846	491	558	21		

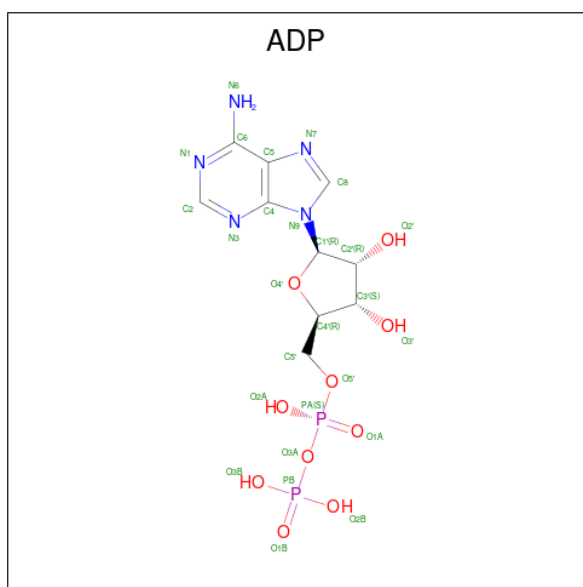
- Molecule 2 is a protein called Talin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	192	Total	C	N	O	S	0	0
			1422	874	262	280	6		
2	G	44	Total	C	N	O	S	0	0
			364	228	69	66	1		
2	H	192	Total	C	N	O	S	0	0
			1422	874	262	280	6		
2	I	42	Total	C	N	O	S	0	0
			353	221	67	64	1		
2	J	192	Total	C	N	O	S	0	0
			1422	874	262	280	6		
2	K	42	Total	C	N	O	S	0	0
			353	221	67	64	1		
2	L	192	Total	C	N	O	S	0	0
			1422	874	262	280	6		
2	M	42	Total	C	N	O	S	0	0
			353	221	67	64	1		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2296	GLY	-	expression tag	UNP P26039
F	2297	PRO	-	expression tag	UNP P26039
F	2298	ASP	-	expression tag	UNP P26039
F	2299	SER	-	expression tag	UNP P26039
F	2300	MET	-	expression tag	UNP P26039
G	2296	GLY	-	expression tag	UNP P26039
G	2297	PRO	-	expression tag	UNP P26039
G	2298	ASP	-	expression tag	UNP P26039
G	2299	SER	-	expression tag	UNP P26039
G	2300	MET	-	expression tag	UNP P26039
H	2296	GLY	-	expression tag	UNP P26039
H	2297	PRO	-	expression tag	UNP P26039
H	2298	ASP	-	expression tag	UNP P26039
H	2299	SER	-	expression tag	UNP P26039
H	2300	MET	-	expression tag	UNP P26039
I	2296	GLY	-	expression tag	UNP P26039
I	2297	PRO	-	expression tag	UNP P26039
I	2298	ASP	-	expression tag	UNP P26039
I	2299	SER	-	expression tag	UNP P26039
I	2300	MET	-	expression tag	UNP P26039
J	2296	GLY	-	expression tag	UNP P26039
J	2297	PRO	-	expression tag	UNP P26039
J	2298	ASP	-	expression tag	UNP P26039
J	2299	SER	-	expression tag	UNP P26039
J	2300	MET	-	expression tag	UNP P26039
K	2296	GLY	-	expression tag	UNP P26039
K	2297	PRO	-	expression tag	UNP P26039
K	2298	ASP	-	expression tag	UNP P26039
K	2299	SER	-	expression tag	UNP P26039
K	2300	MET	-	expression tag	UNP P26039
L	2296	GLY	-	expression tag	UNP P26039
L	2297	PRO	-	expression tag	UNP P26039
L	2298	ASP	-	expression tag	UNP P26039
L	2299	SER	-	expression tag	UNP P26039
L	2300	MET	-	expression tag	UNP P26039
M	2296	GLY	-	expression tag	UNP P26039
M	2297	PRO	-	expression tag	UNP P26039
M	2298	ASP	-	expression tag	UNP P26039
M	2299	SER	-	expression tag	UNP P26039
M	2300	MET	-	expression tag	UNP P26039

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

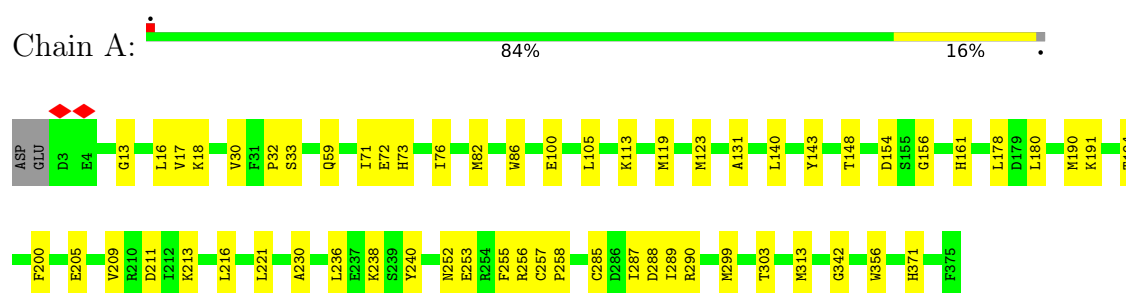
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	

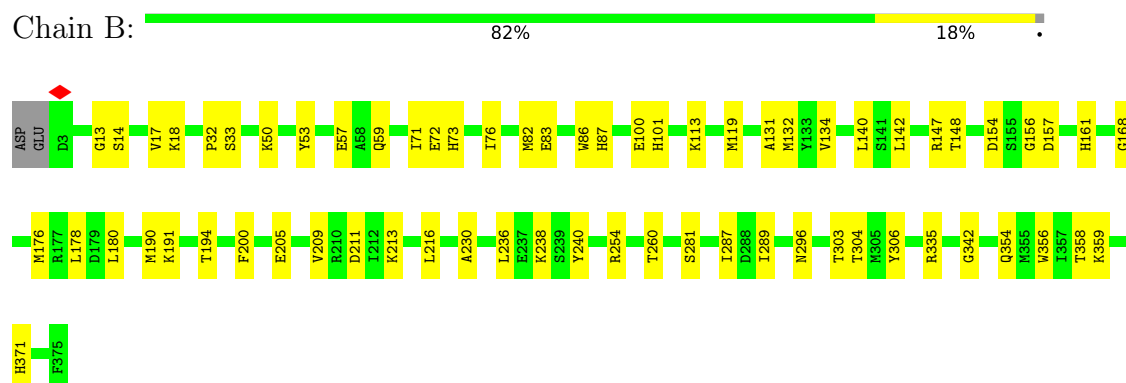
3 Residue-property plots

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.

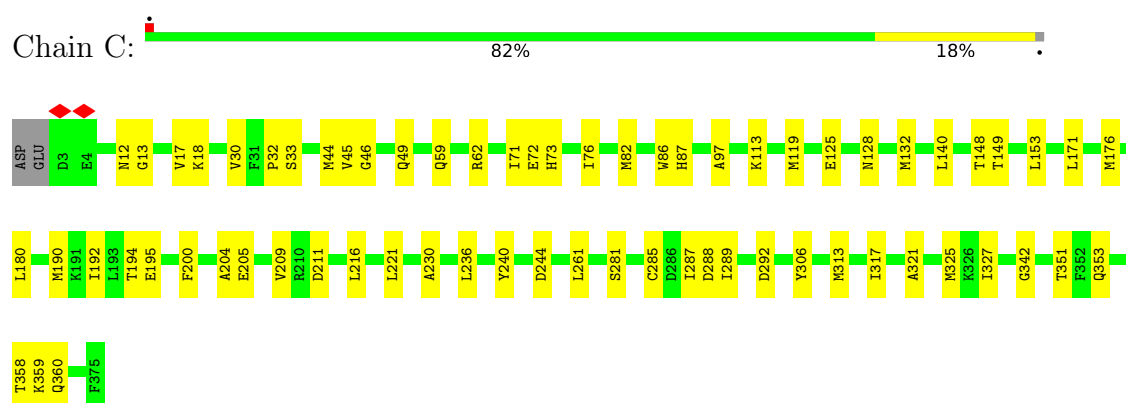
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



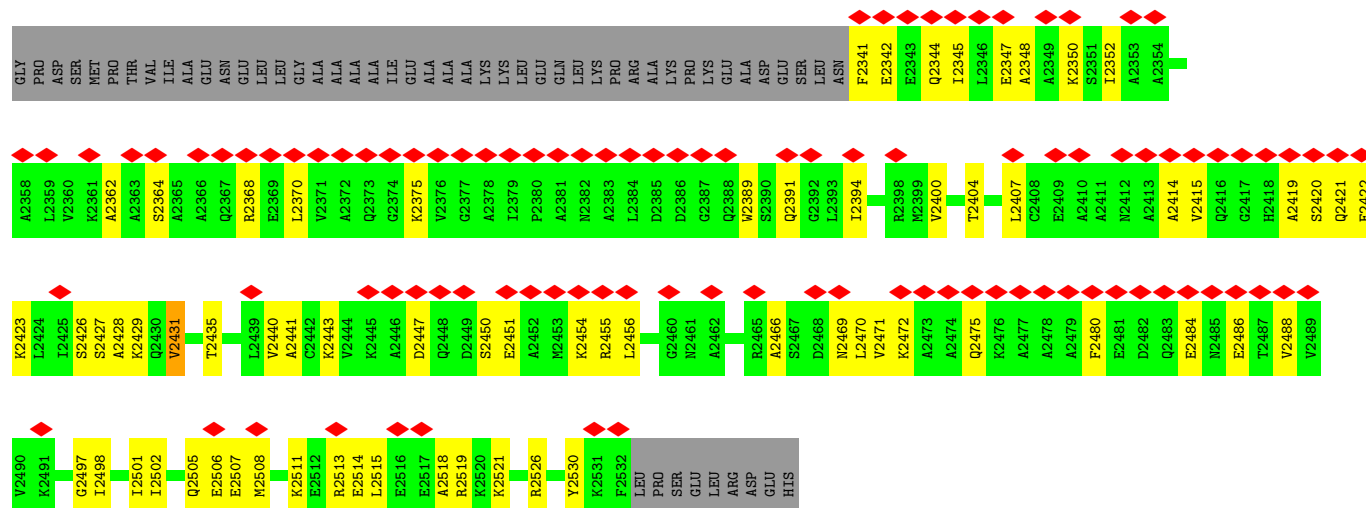
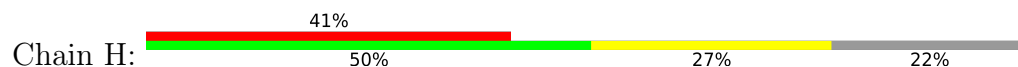
- Molecule 1: Actin, alpha skeletal muscle



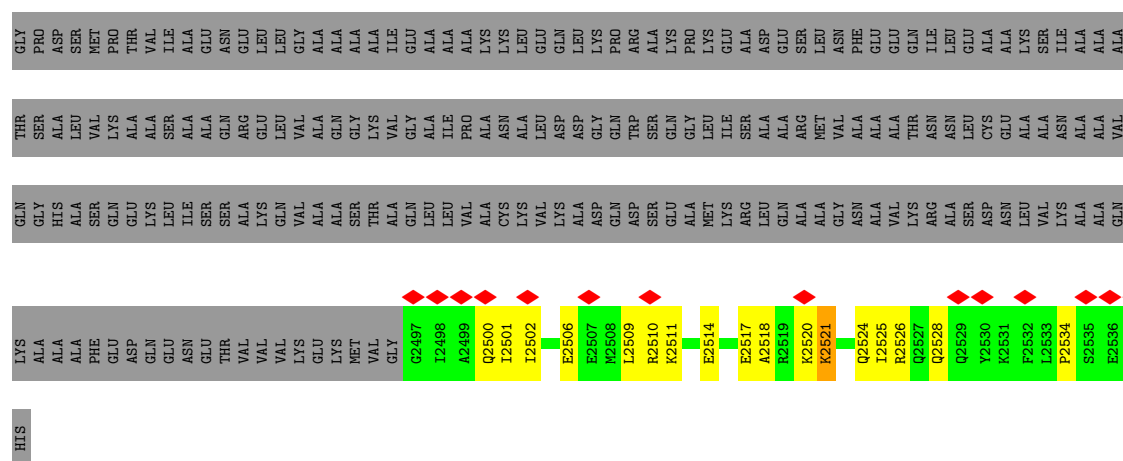
- [illegible]



• Molecule 2: Talin-1

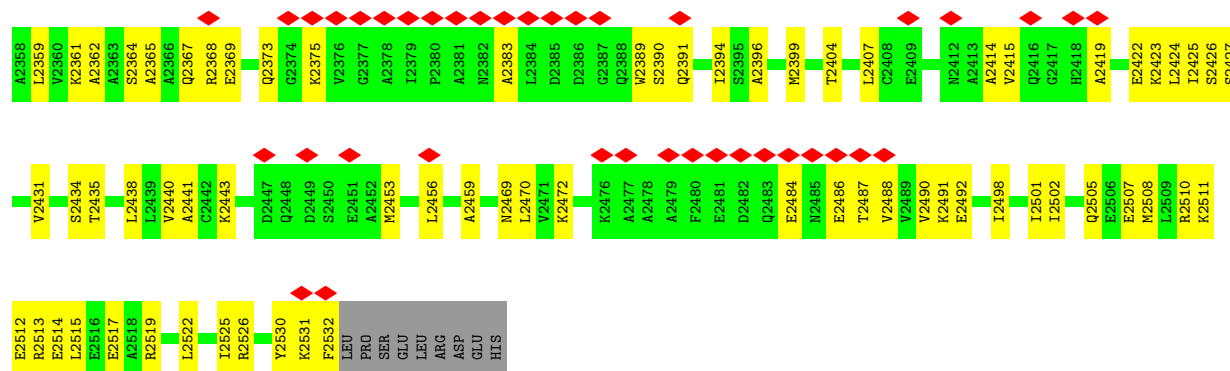


• Molecule 2: Talin-1



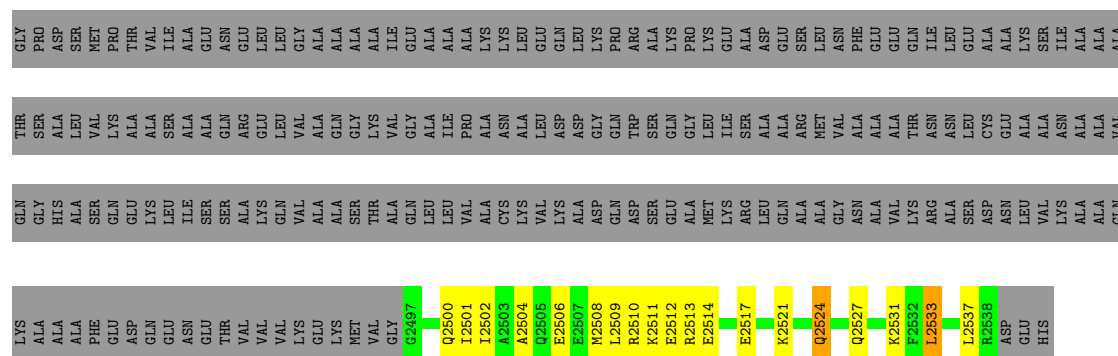
• Molecule 2: Talin-1





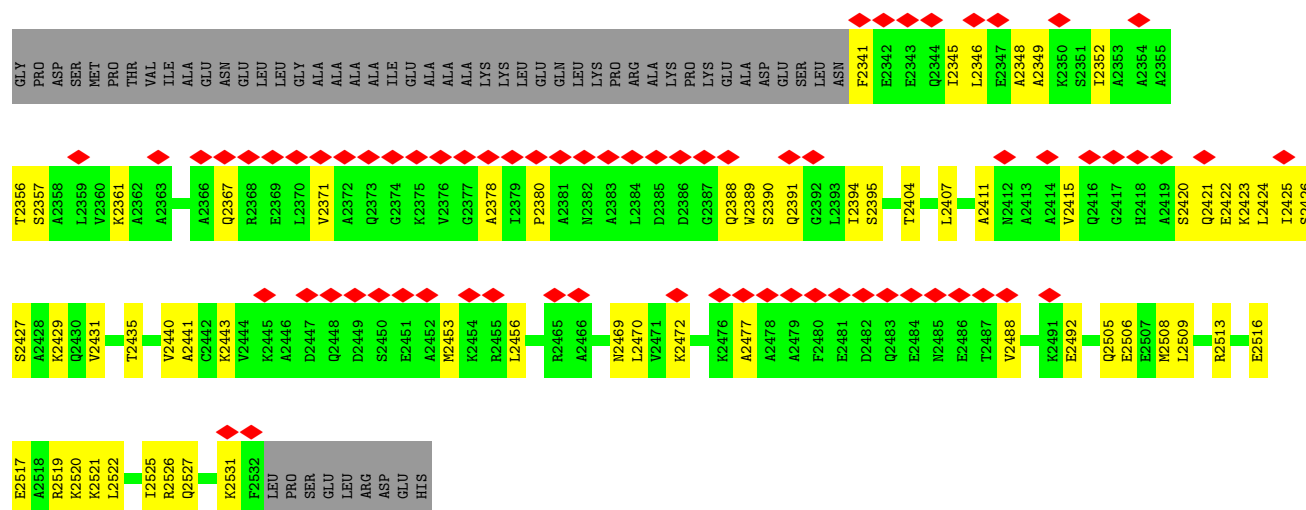
• Molecule 2: Talin-1

Chain K: 9% 7% . 83%



• Molecule 2: Talin-1

Chain L: 29% 54% 24% 22%



• Molecule 2: Talin-1

Chain M: 9% 7% . 83%

LYS	LYS	GLN	GLY	THR	GLY
ALA	ALA	GLY	ASP	SER	PRO
ALA	ALA	HIS	ALA	ALA	ASP
ALA	ALA	ALA	SER	LEU	SER
PHE	PHE	SER	VAL	VAL	MET
GLU	GLU	GLN	GLN	LYS	PRO
ASP	ASP	GLU	ALA	ALA	THR
GLN	GLN	LYS	LYS	ALA	VAL
GLU	GLU	LEU	LEU	SER	ILE
ASN	ASN	ILE	ILE	ALA	ALA
GLU	GLU	SER	SER	ALA	GLU
THR	THR	SER	ALA	ARG	ASN
VAL	VAL	ALA	ALA	GLU	GLU
VAL	VAL	LYS	LYS	LEU	LEU
LYS	LYS	VAL	VAL	VAL	GLY
GLU	GLU	ALA	ALA	ALA	ASN
LYS	LYS	ALA	ALA	GLN	ALA
MET	MET	SER	GLY	GLY	ALA
VAL	VAL	THR	THR	VAL	ILE
GLY	G2497	GLN	GLN	GLY	GLY
I2498	I2498	LEU	LEU	ILE	ALA
A2499	A2499	VAL	VAL	PRO	ALA
Q2500	Q2500	ALA	ALA	ASN	LYS
I2501	I2501	CYS	CYS	ASN	LYS
I2502	I2502	LYS	LYS	ALA	LEU
A2503	A2503	VAL	VAL	LEU	GLU
		LYS	LYS	ASP	GLN
E2506	E2506	ALA	ALA	ASP	LEU
		ASP	ASP	GLY	LYS
L2509	L2509	GLN	GLN	GLN	PRO
R2510	R2510	ASP	ASP	TRP	ARG
K2511	K2511	SER	SER	SER	LYS
		GLU	GLU	GLN	ALA
E2514	E2514	ALA	ALA	GLY	PRO
L2515	L2515	MET	MET	LEU	LYS
E2516	E2516	LYS	LYS	ILE	GLU
E2517	E2517	ARG	ARG	SER	ALA
A2518	A2518	LEU	LEU	ASP	ASP
R2519	R2519	GLN	GLN	ALA	GLU
K2520	K2520	ALA	ALA	ARG	SER
K2521	K2521	ALA	ALA	MET	LEU
		GLY	GLY	VAL	ASN
Q2524	Q2524	ASN	ASN	ALA	PHE
I2525	I2525	ALA	ALA	ALA	GLU
		VAL	VAL	ALA	GLU
		LYS	LYS	THR	GLN
Q2528	Q2528	ARG	ARG	ASN	ILE
Q2529	Q2529	ALA	ALA	ASN	LEU
Y2530	Y2530	SER	SER	LEU	GLU
K2531	K2531	ASP	ASP	CYS	ALA
F2532	F2532	ASN	ASN	GLU	ALA
		LEU	LEU	ALA	LYS
R2538	R2538	VAL	VAL	ALA	SER
ASP	ASP	LYS	LYS	ASN	ILE
GLU	GLU	ALA	ALA	ALA	ALA
HIS	HIS	GLN	GLN	VAL	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.66, -166.66°, rise=27.6, 27.6 Å, axial sym=C1, C1	Depositor
Number of segments used	206326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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, MG, HIC

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	0.19	0/2966	0.30	0/4017
1	B	0.20	0/2966	0.30	0/4017
1	C	0.20	0/2966	0.30	0/4017
1	D	0.19	0/2966	0.32	0/4017
1	E	0.18	0/2966	0.31	0/4017
2	F	0.16	0/1429	0.38	0/1919
2	G	0.24	0/366	0.62	0/485
2	H	0.15	0/1429	0.36	0/1919
2	I	0.23	0/355	0.55	0/470
2	J	0.16	0/1429	0.38	0/1919
2	K	0.22	0/355	0.58	0/470
2	L	0.14	0/1429	0.39	0/1919
2	M	0.20	0/355	0.52	0/470
All	All	0.18	0/21977	0.35	0/29656

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	2916	0	2882	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2916	0	2882	47	0
1	C	2916	0	2882	58	0
1	D	2916	0	2882	52	0
1	E	2916	0	2882	40	0
2	F	1422	0	1461	48	0
2	G	364	0	384	22	0
2	H	1422	0	1461	61	0
2	I	353	0	372	24	0
2	J	1422	0	1461	59	0
2	K	353	0	372	24	0
2	L	1422	0	1461	53	0
2	M	353	0	372	27	0
3	A	27	0	12	2	0
3	B	27	0	12	3	0
3	C	27	0	12	3	0
3	D	27	0	12	3	0
3	E	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	21831	0	21814	445	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 10.

The worst 5 of 445 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)
2:L:2356:THR:HG21	2:L:2404:THR:HG21	1.55	0.86
2:J:2356:THR:HG21	2:J:2404:THR:HG21	1.58	0.86
2:F:2505:GLN:O	2:F:2508:MET:HB2	1.76	0.85
2:F:2367:GLN:HG3	2:F:2394:ILE:HG23	1.63	0.80
2:F:2420:SER:OG	2:G:2510:ARG:NH2	2.14	0.79

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	370/375 (99%)	367 (99%)	3 (1%)	0	100	100
1	B	370/375 (99%)	366 (99%)	4 (1%)	0	100	100
1	C	370/375 (99%)	368 (100%)	2 (0%)	0	100	100
1	D	370/375 (99%)	369 (100%)	1 (0%)	0	100	100
1	E	370/375 (99%)	369 (100%)	1 (0%)	0	100	100
2	F	190/246 (77%)	186 (98%)	4 (2%)	0	100	100
2	G	42/246 (17%)	41 (98%)	1 (2%)	0	100	100
2	H	190/246 (77%)	188 (99%)	2 (1%)	0	100	100
2	I	40/246 (16%)	40 (100%)	0	0	100	100
2	J	190/246 (77%)	186 (98%)	4 (2%)	0	100	100
2	K	40/246 (16%)	40 (100%)	0	0	100	100
2	L	190/246 (77%)	187 (98%)	3 (2%)	0	100	100
2	M	40/246 (16%)	40 (100%)	0	0	100	100
All	All	2772/3843 (72%)	2747 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	315/317 (99%)	314 (100%)	1 (0%)	86	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	315/317 (99%)	315 (100%)	0	100	100
1	C	315/317 (99%)	314 (100%)	1 (0%)	86	91
1	D	315/317 (99%)	314 (100%)	1 (0%)	86	91
1	E	315/317 (99%)	315 (100%)	0	100	100
2	F	139/181 (77%)	137 (99%)	2 (1%)	59	80
2	G	37/181 (20%)	36 (97%)	1 (3%)	39	70
2	H	139/181 (77%)	138 (99%)	1 (1%)	76	87
2	I	36/181 (20%)	35 (97%)	1 (3%)	38	69
2	J	139/181 (77%)	136 (98%)	3 (2%)	45	73
2	K	36/181 (20%)	34 (94%)	2 (6%)	19	50
2	L	139/181 (77%)	137 (99%)	2 (1%)	59	80
2	M	36/181 (20%)	34 (94%)	2 (6%)	19	50
All	All	2276/3033 (75%)	2259 (99%)	17 (1%)	73	87

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	2456	LEU
2	M	2538	ARG
2	I	2521	LYS
2	J	2352	ILE
2	J	2490	VAL

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

Mol	Chain	Res	Type
2	J	2461	ASN
2	L	2469	ASN
2	J	2500	GLN
2	K	2528	GLN
2	M	2505	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	HIC	D	73	1	10,11,12	0.50	0	9,14,16	0.67	0
1	HIC	A	73	1	10,11,12	0.51	0	9,14,16	0.68	0
1	HIC	E	73	1	10,11,12	0.50	0	9,14,16	0.64	0
1	HIC	C	73	1	10,11,12	0.50	0	9,14,16	0.65	0
1	HIC	B	73	1	10,11,12	0.50	0	9,14,16	0.60	0

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
1	HIC	D	73	1	-	0/5/6/8	0/1/1/1
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1
1	HIC	E	73	1	-	0/5/6/8	0/1/1/1
1	HIC	C	73	1	-	0/5/6/8	0/1/1/1
1	HIC	B	73	1	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	73	HIC	1	0
1	A	73	HIC	1	0
1	E	73	HIC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	73	HIC	1	0
1	B	73	HIC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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
3	ADP	A	401	4	28,29,29	1.39	5 (17%)	43,45,45	1.84	10 (23%)
3	ADP	D	401	4	28,29,29	1.38	5 (17%)	43,45,45	1.84	8 (18%)
3	ADP	E	401	4	28,29,29	1.39	5 (17%)	43,45,45	1.84	10 (23%)
3	ADP	B	401	4	28,29,29	1.38	5 (17%)	43,45,45	1.84	10 (23%)
3	ADP	C	401	4	28,29,29	1.38	5 (17%)	43,45,45	1.84	10 (23%)

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
3	ADP	A	401	4	-	6/16/32/32	0/3/3/3
3	ADP	D	401	4	-	3/16/32/32	0/3/3/3
3	ADP	E	401	4	-	5/16/32/32	0/3/3/3
3	ADP	B	401	4	-	7/16/32/32	0/3/3/3
3	ADP	C	401	4	-	6/16/32/32	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	ADP	C5-C4	4.46	1.47	1.39
3	E	401	ADP	C5-C4	4.45	1.47	1.39
3	A	401	ADP	C5-C4	4.44	1.47	1.39
3	B	401	ADP	C5-C4	4.41	1.47	1.39
3	C	401	ADP	C5-C4	4.41	1.46	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	C5-C4-N3	-5.77	118.77	126.72
3	C	401	ADP	C5-C4-N3	-5.72	118.83	126.72
3	E	401	ADP	C5-C4-N3	-5.71	118.85	126.72
3	B	401	ADP	C5-C4-N3	-5.69	118.88	126.72
3	A	401	ADP	C5-C4-N3	-5.68	118.89	126.72

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ADP	PA-O3A-PB-O2B
3	A	401	ADP	C5'-O5'-PA-O1A
3	A	401	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	C5'-O5'-PA-O3A
3	B	401	ADP	PA-O3A-PB-O2B

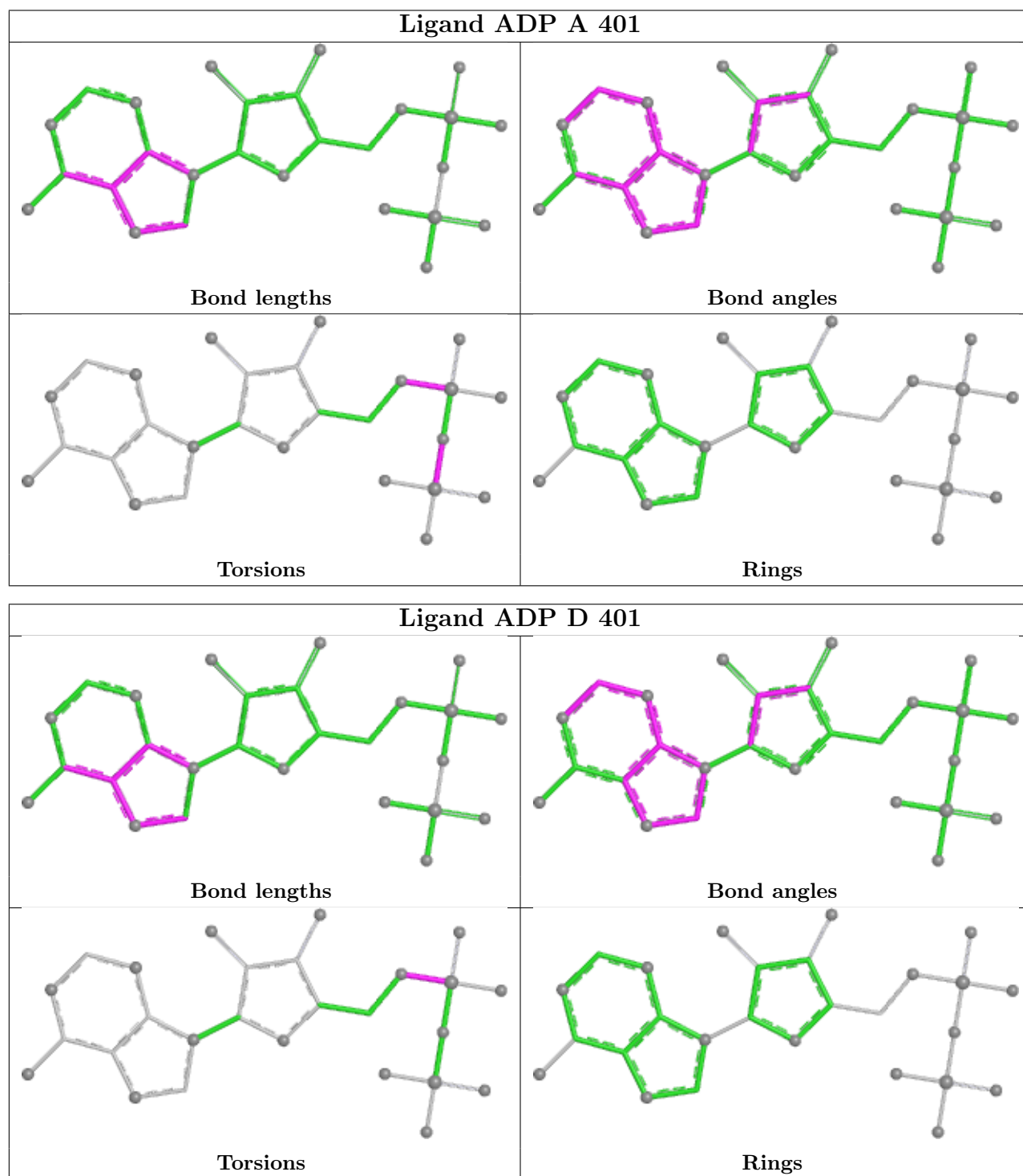
There are no ring outliers.

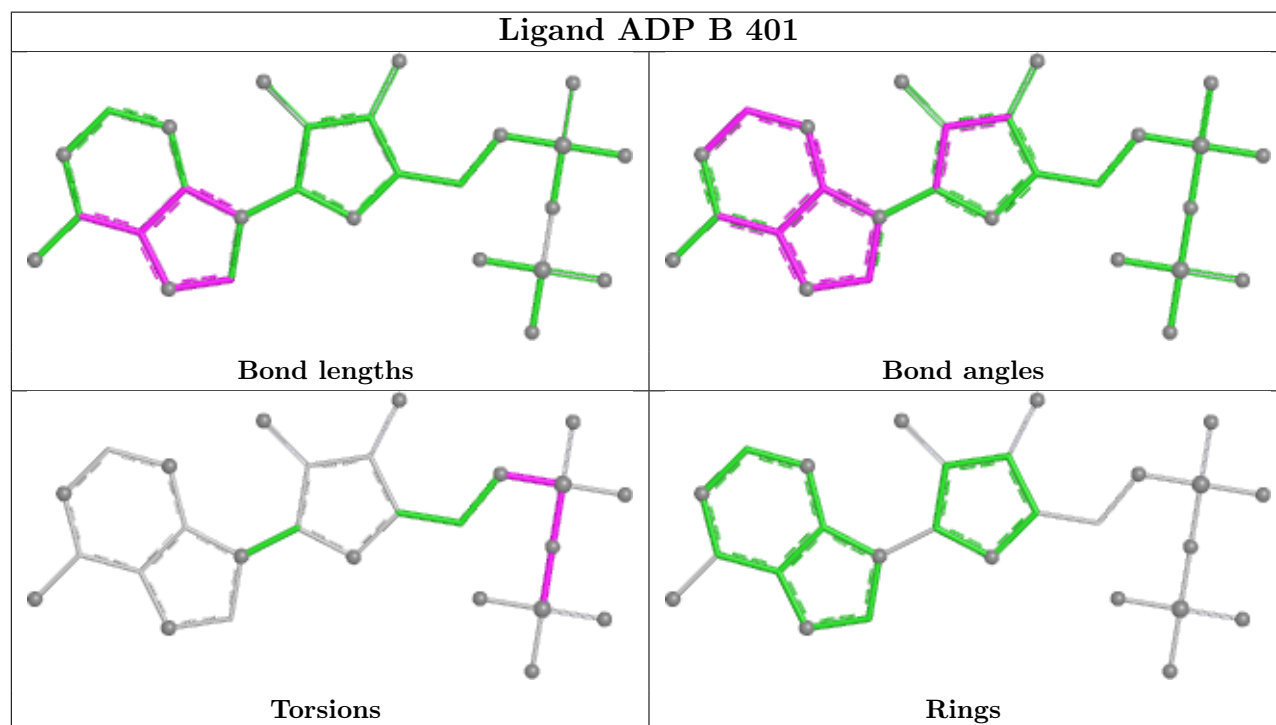
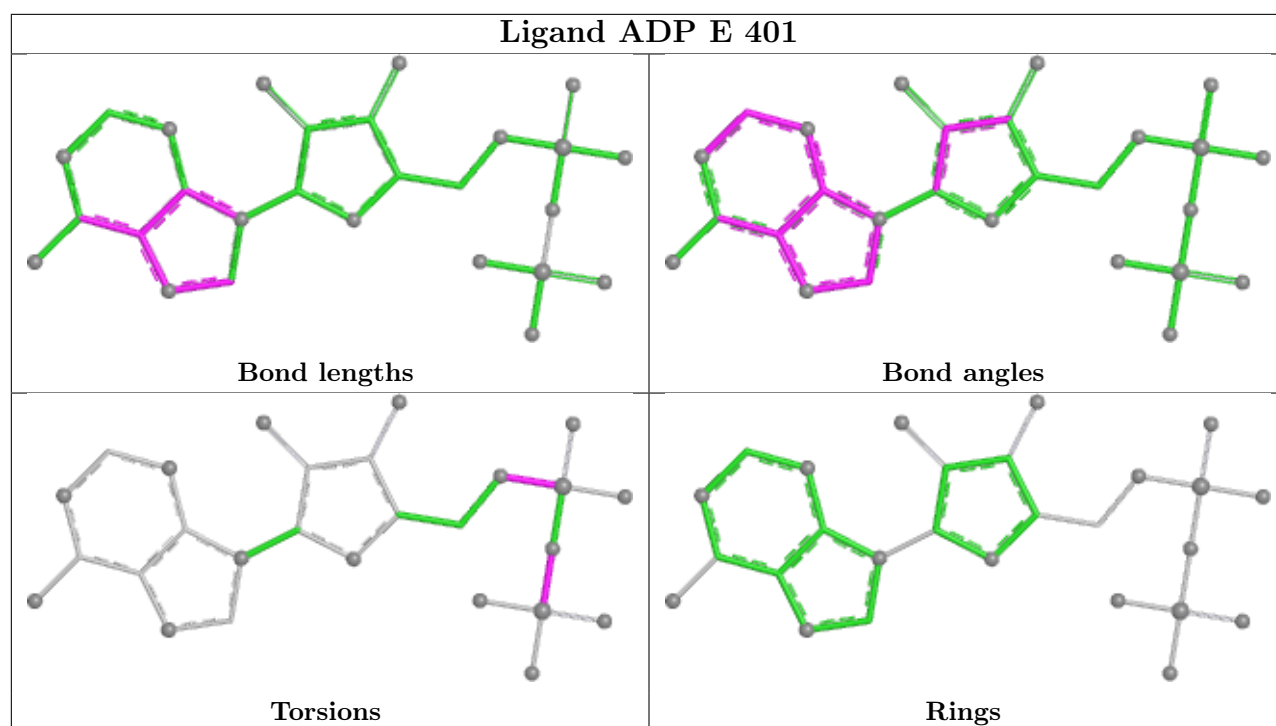
5 monomers are involved in 12 short contacts:

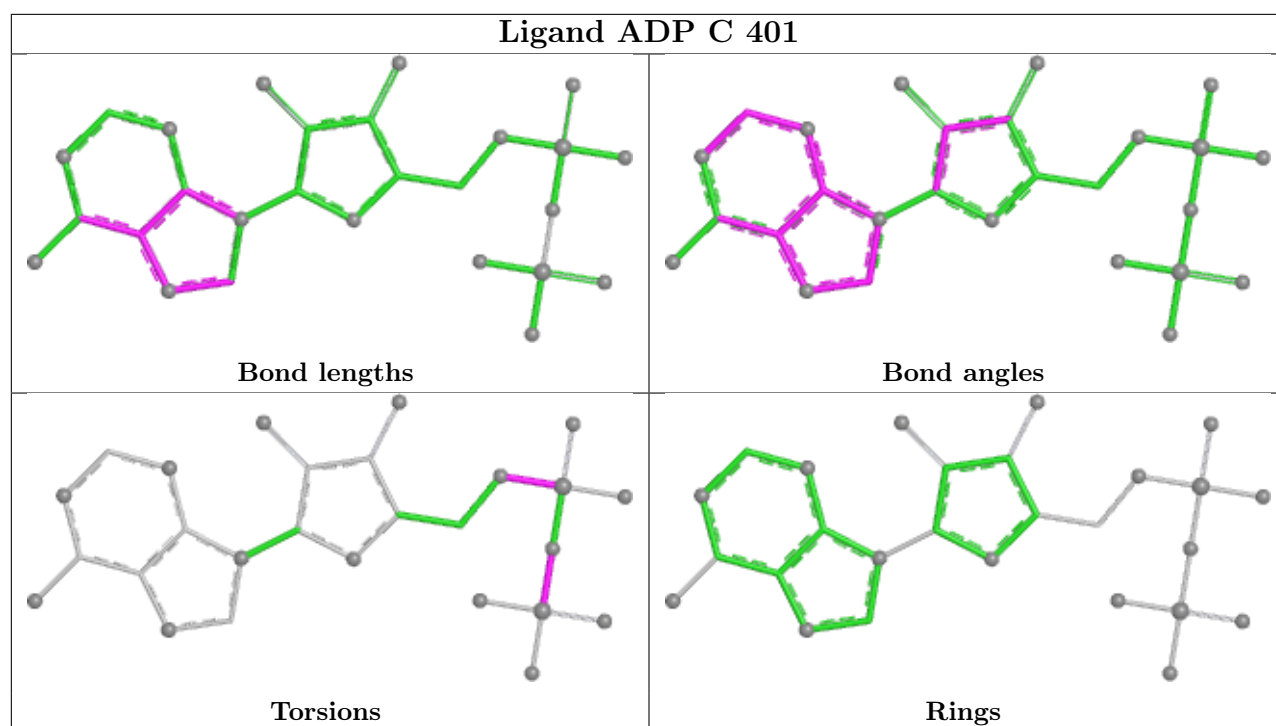
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	2	0
3	D	401	ADP	3	0
3	E	401	ADP	1	0
3	B	401	ADP	3	0
3	C	401	ADP	3	0

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 than 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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

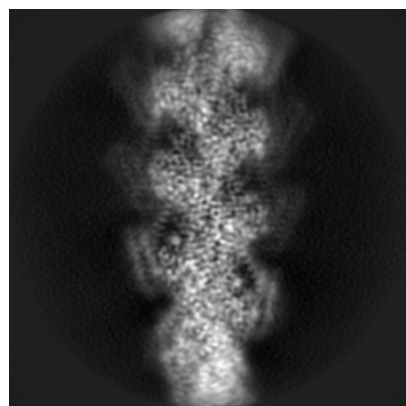
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44013. These allow visual inspection of the internal detail of the map and identification of artifacts.

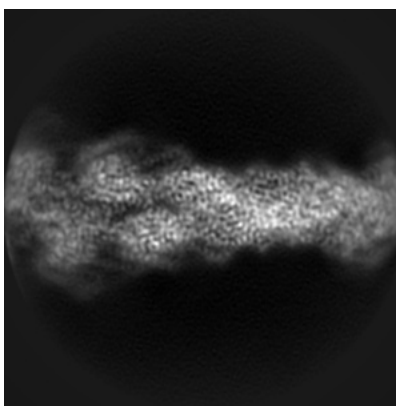
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

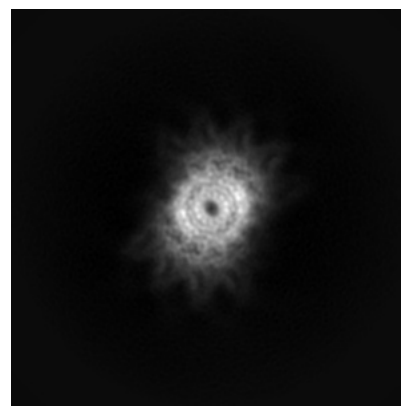
6.1.1 Primary map



X

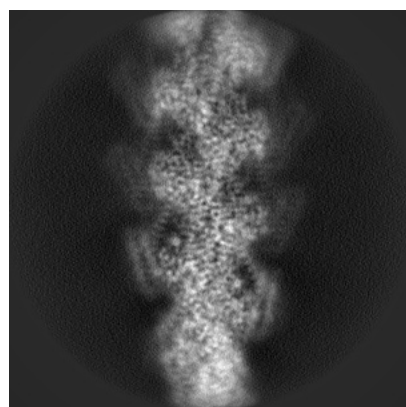


Y

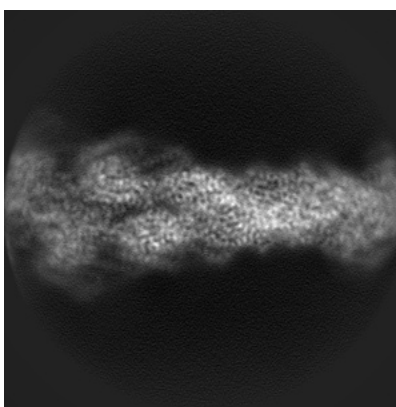


Z

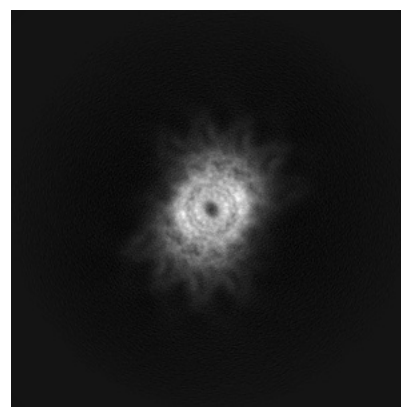
6.1.2 Raw map



X



Y

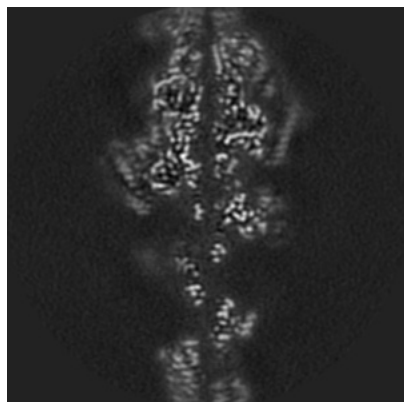


Z

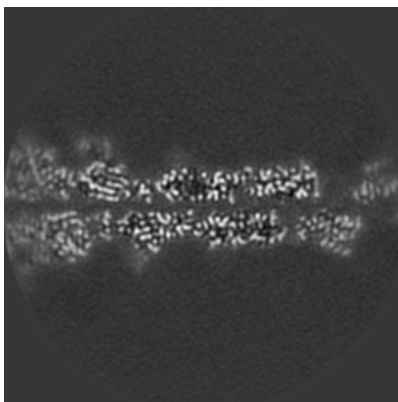
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

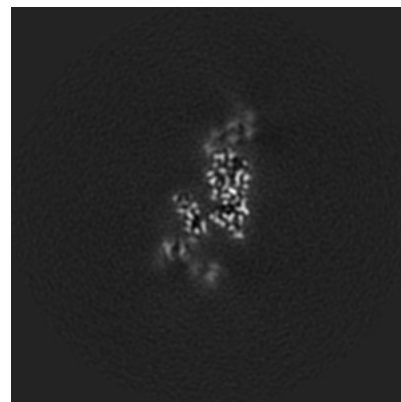
6.2.1 Primary map



X Index: 160

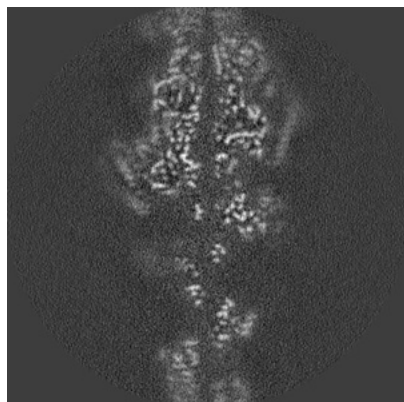


Y Index: 160

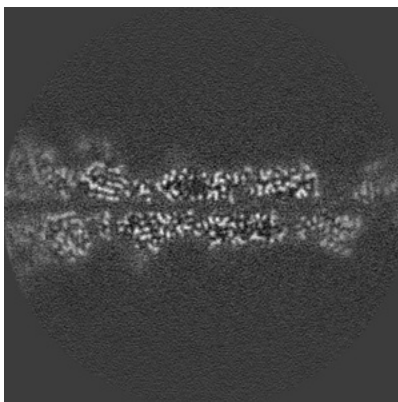


Z Index: 160

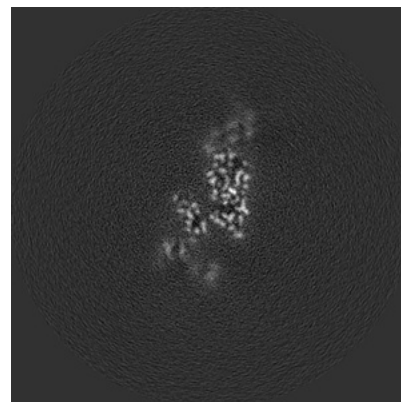
6.2.2 Raw map



X Index: 160



Y Index: 160

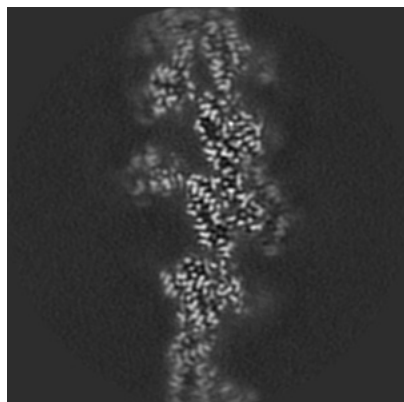


Z Index: 160

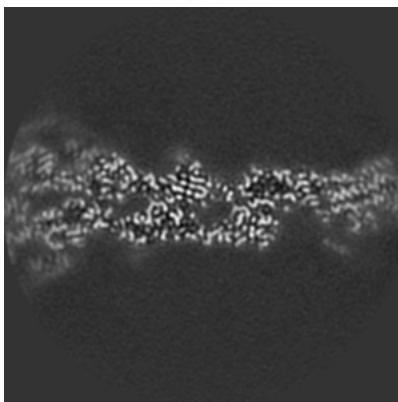
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

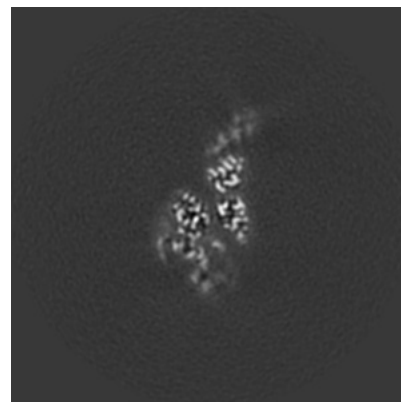
6.3.1 Primary map



X Index: 170

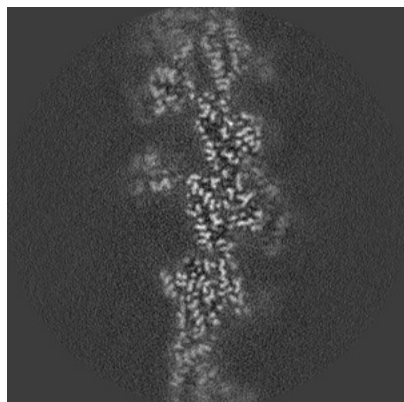


Y Index: 168

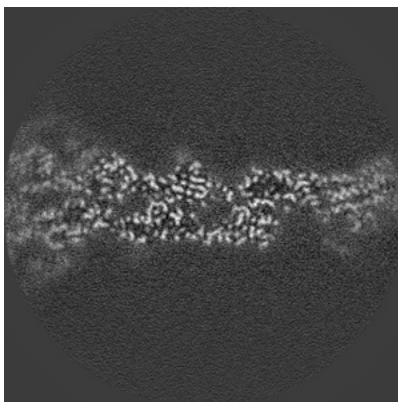


Z Index: 169

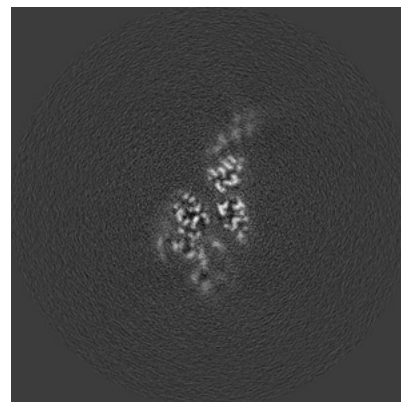
6.3.2 Raw map



X Index: 171



Y Index: 168

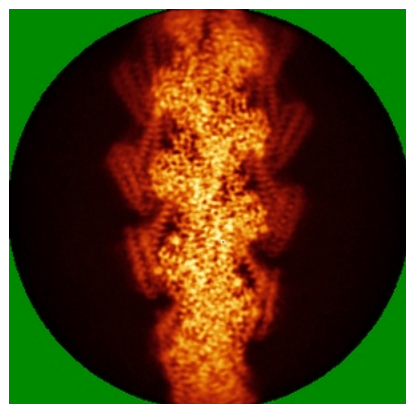


Z Index: 169

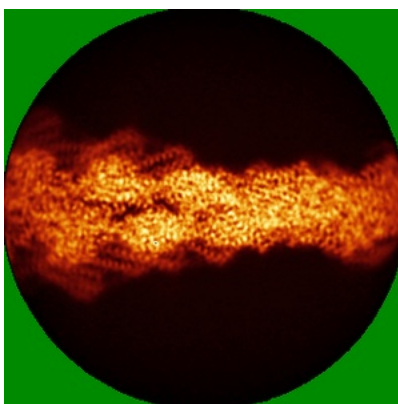
The images above show the largest variance slices of the map in three orthogonal directions.

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

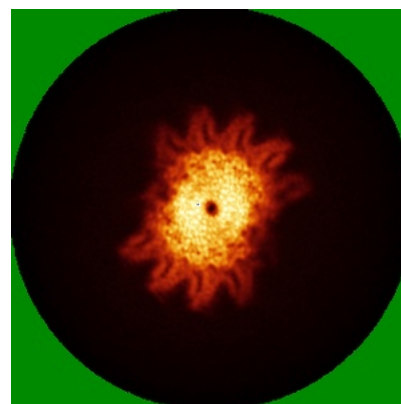
6.4.1 Primary map



X

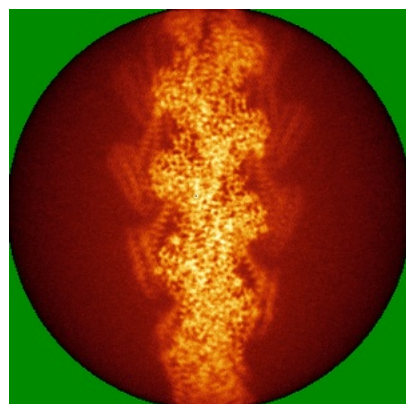


Y

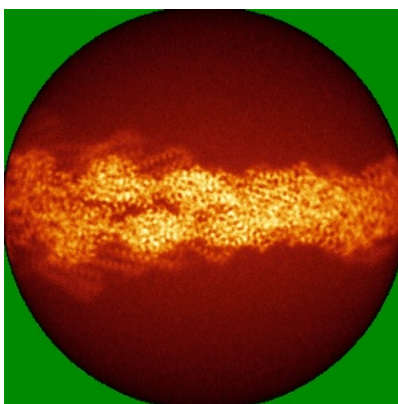


Z

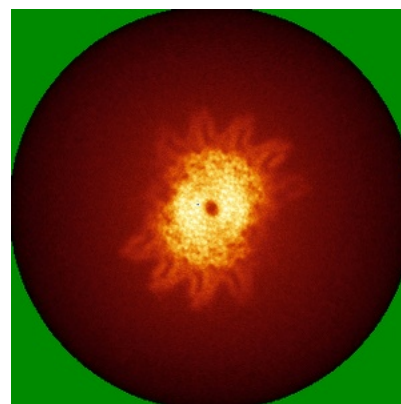
6.4.2 Raw map



X



Y

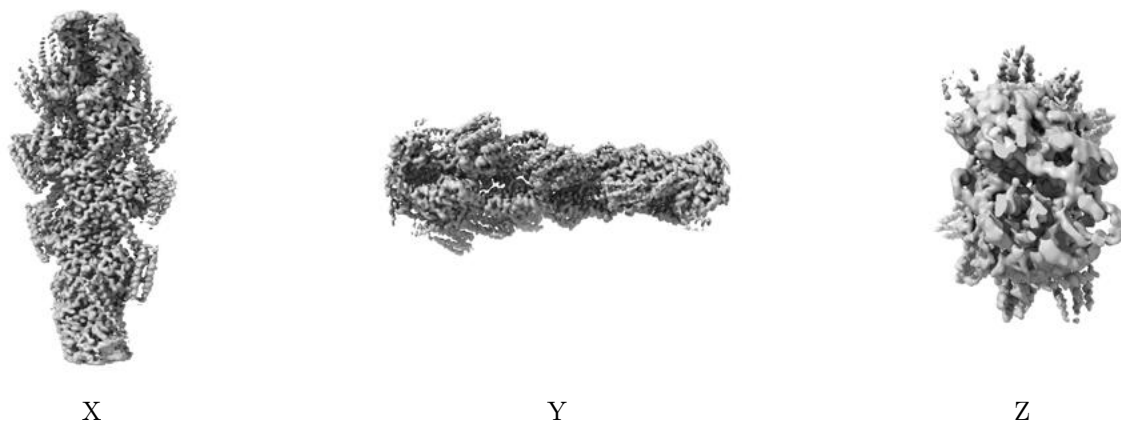


Z

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.

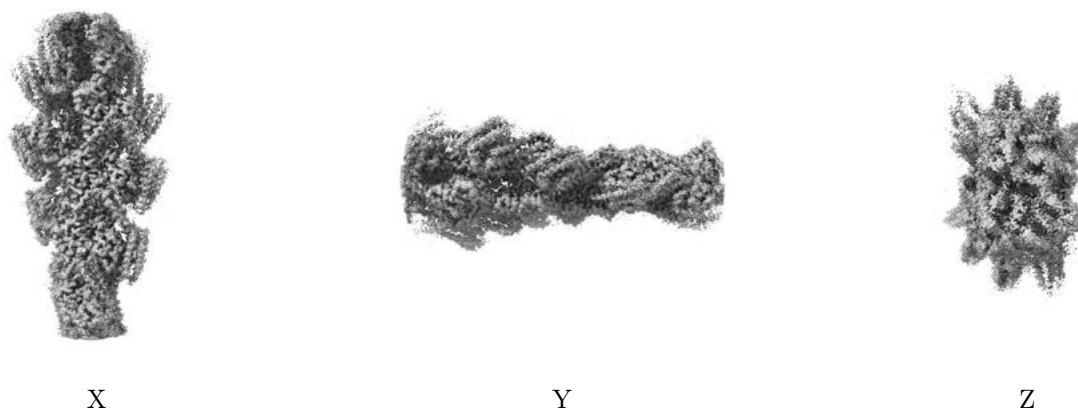
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

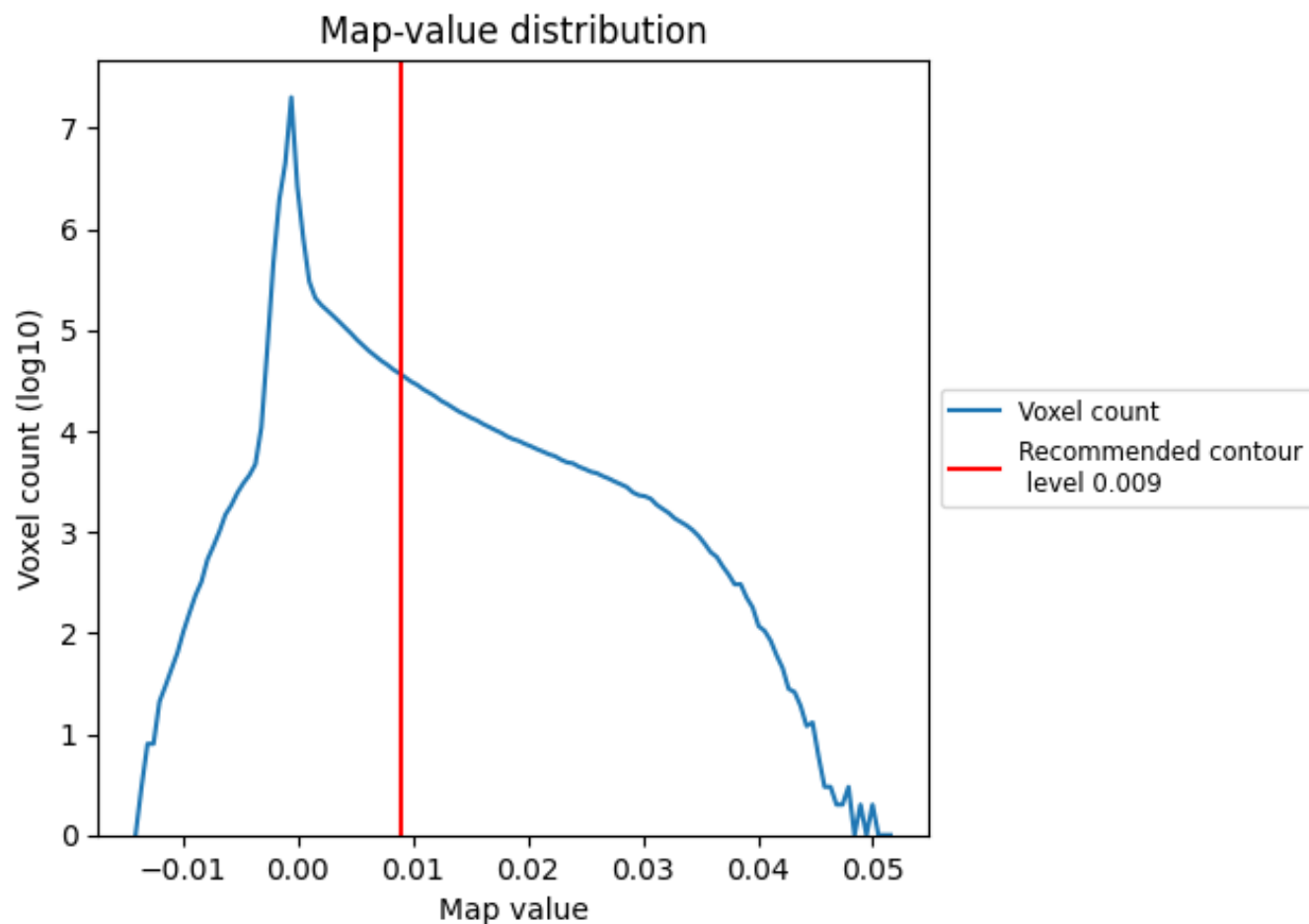
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

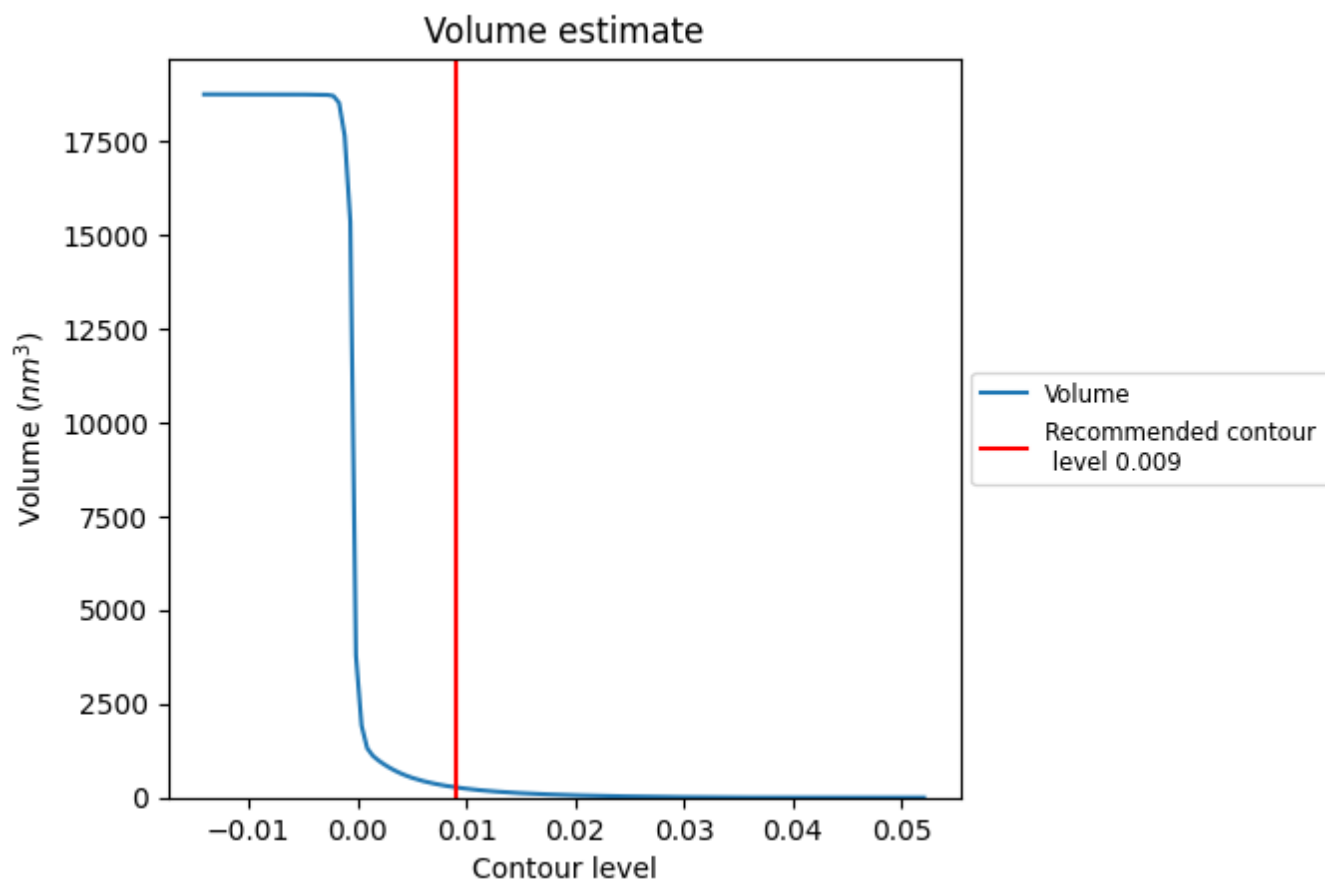
This section contains the results of statistical analysis of the map.

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.

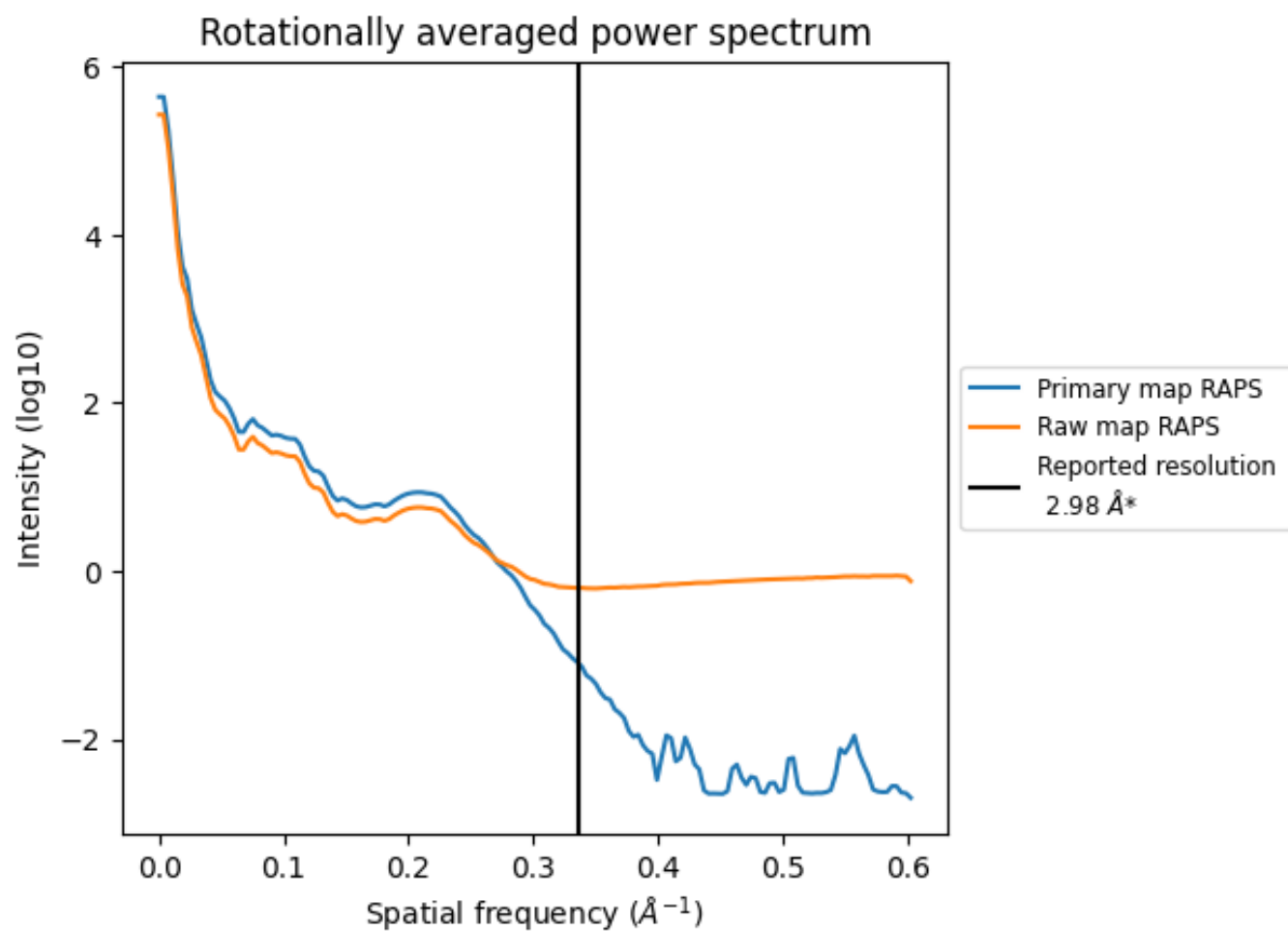
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 274 nm³; this corresponds to an approximate mass of 247 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 ⓘ

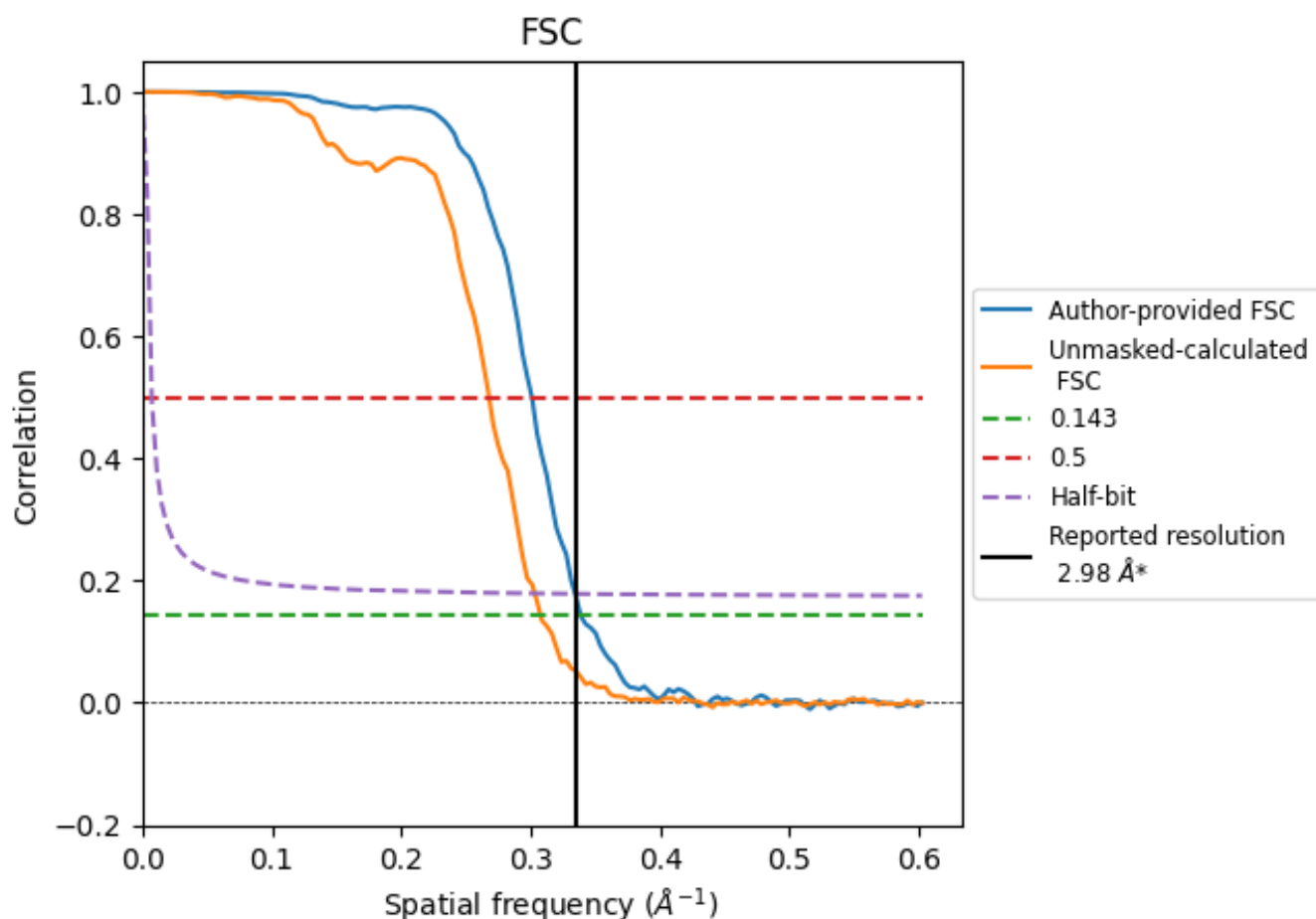


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8.2 Resolution estimates

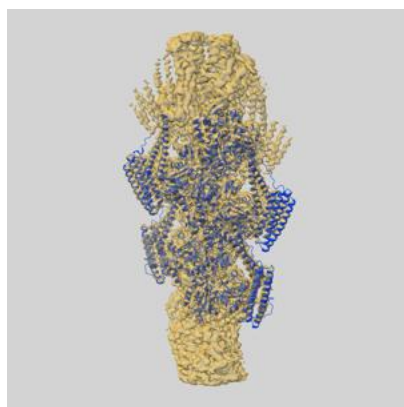
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.95	3.32	2.99
Unmasked-calculated*	3.25	3.73	3.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

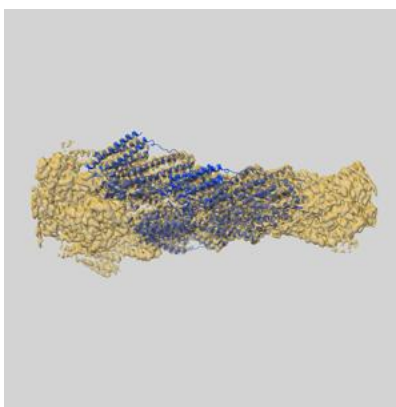
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44013 and PDB model 9AZ6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

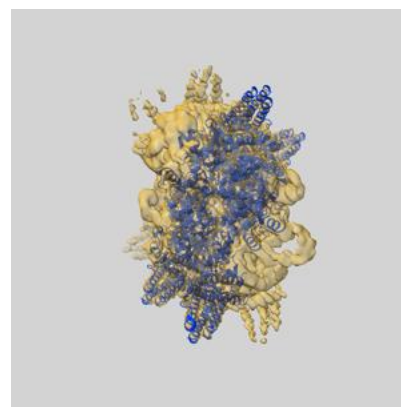
9.1 Map-model overlay [i](#)



X



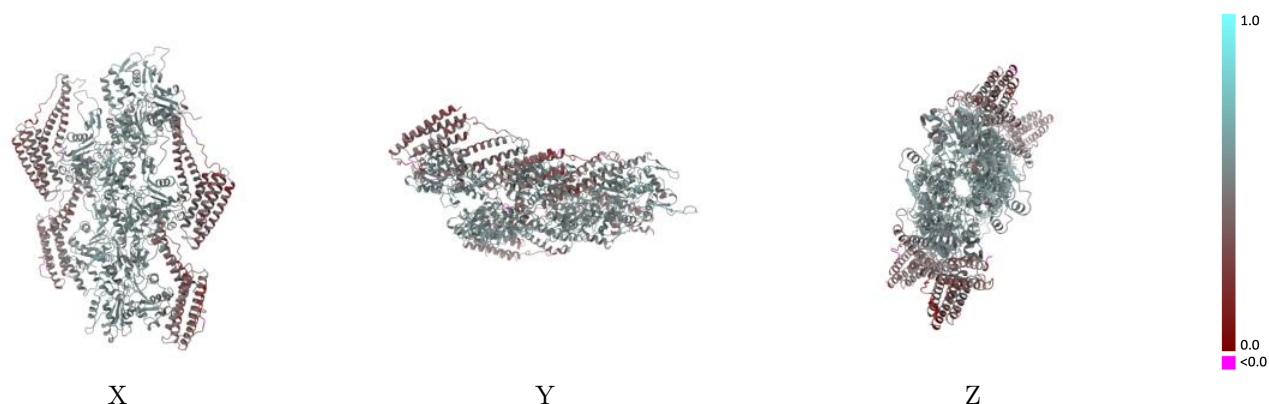
Y



Z

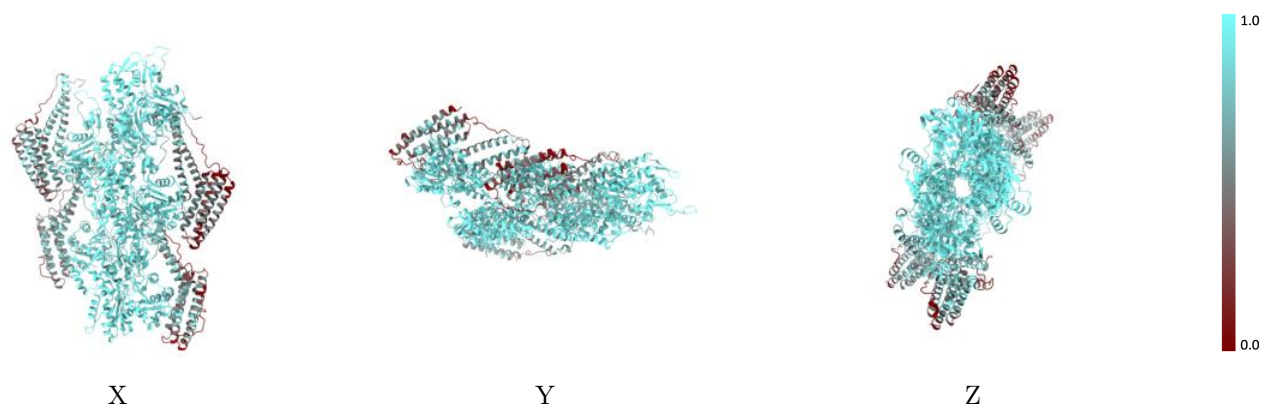
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



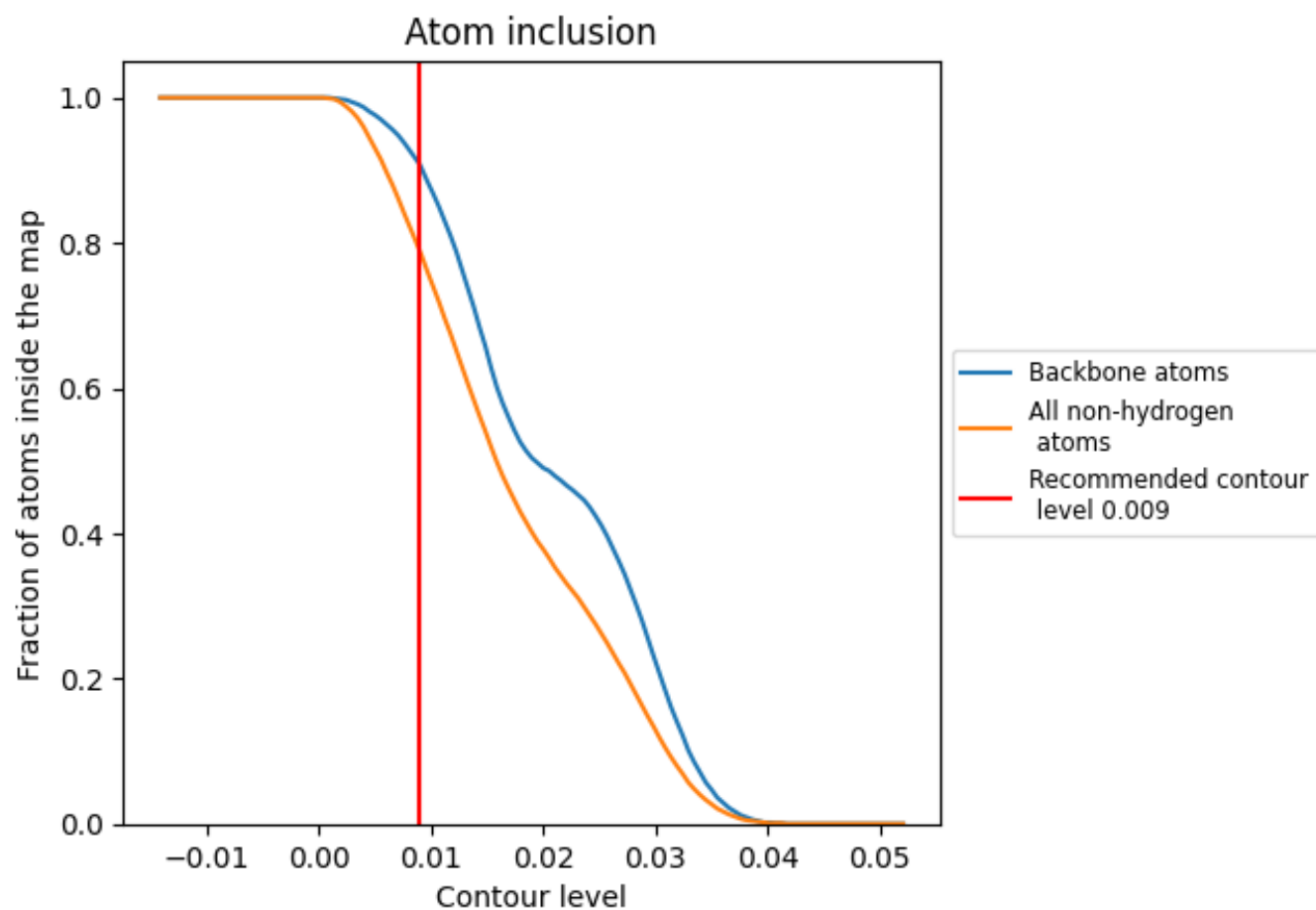
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 79% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.4850
A	0.9280	0.5390
B	0.9330	0.5460
C	0.9340	0.5500
D	0.9310	0.5460
E	0.9170	0.5410
F	0.5350	0.3560
G	0.6150	0.3750
H	0.3650	0.3540
I	0.4740	0.4050
J	0.5470	0.3610
K	0.7080	0.4030
L	0.4590	0.3480
M	0.5940	0.4020

