wwPDB EM Validation Summary Report (i)

Dec 1, 2021 – 05:13 am GMT

PDB ID	:	7P3X
EMDB ID	:	EMD-13187
Title	:	Homology model of the full-length AP-3 complex in a compact open conformation
Authors	:	Schubert, E.; Raunser, S.
Deposited on	:	2021-07-09
Resolution	:	9.10 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

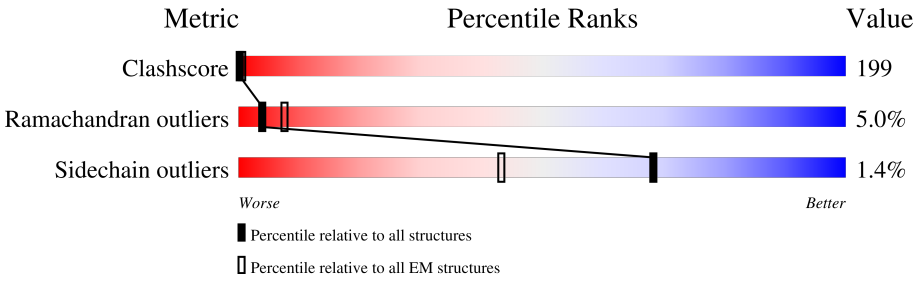
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	964	21% · 20% 30% 6% 40%
2	B	809	28% 5% 24% 42% 6% 23%
3	S	194	57% 8% 25% 44% 9% 13%
4	M	483	25% 6% 40% 30% 7% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14104 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 AP-3 complex subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	576	4625	2978	738	881	28	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	933	ARG	-	expression tag	UNP A0A7I9C4X2
A	934	THR	-	expression tag	UNP A0A7I9C4X2
A	935	LEU	-	expression tag	UNP A0A7I9C4X2
A	936	GLN	-	expression tag	UNP A0A7I9C4X2
A	937	VAL	-	expression tag	UNP A0A7I9C4X2
A	938	ASP	-	expression tag	UNP A0A7I9C4X2
A	939	GLY	-	expression tag	UNP A0A7I9C4X2
A	940	SER	-	expression tag	UNP A0A7I9C4X2
A	941	ASP	-	expression tag	UNP A0A7I9C4X2
A	942	TYR	-	expression tag	UNP A0A7I9C4X2
A	943	LYS	-	expression tag	UNP A0A7I9C4X2
A	944	ASP	-	expression tag	UNP A0A7I9C4X2
A	945	ASP	-	expression tag	UNP A0A7I9C4X2
A	946	ASP	-	expression tag	UNP A0A7I9C4X2
A	947	ASP	-	expression tag	UNP A0A7I9C4X2
A	948	LYS	-	expression tag	UNP A0A7I9C4X2
A	949	ASP	-	expression tag	UNP A0A7I9C4X2
A	950	TYR	-	expression tag	UNP A0A7I9C4X2
A	951	LYS	-	expression tag	UNP A0A7I9C4X2
A	952	ASP	-	expression tag	UNP A0A7I9C4X2
A	953	ASP	-	expression tag	UNP A0A7I9C4X2
A	954	ASP	-	expression tag	UNP A0A7I9C4X2
A	955	ASP	-	expression tag	UNP A0A7I9C4X2
A	956	LYS	-	expression tag	UNP A0A7I9C4X2
A	957	ASP	-	expression tag	UNP A0A7I9C4X2
A	958	TYR	-	expression tag	UNP A0A7I9C4X2
A	959	LYS	-	expression tag	UNP A0A7I9C4X2
A	960	ASP	-	expression tag	UNP A0A7I9C4X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ASP	-	expression tag	UNP A0A7I9C4X2
A	962	ASP	-	expression tag	UNP A0A7I9C4X2
A	963	ASP	-	expression tag	UNP A0A7I9C4X2
A	964	LYS	-	expression tag	UNP A0A7I9C4X2

- Molecule 2 is a protein called Y55_G0035830.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	621	Total	C	N	O	S	0	0
			4963	3168	830	937	28		

- Molecule 3 is a protein called AP complex subunit sigma.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	168	Total	C	N	O	S	0	0
			1358	867	215	272	4		

- Molecule 4 is a protein called AP-3 complex subunit mu.

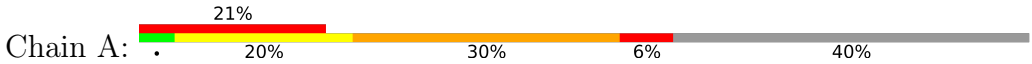
Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	397	Total	C	N	O	S	0	0
			3158	2018	516	612	12		

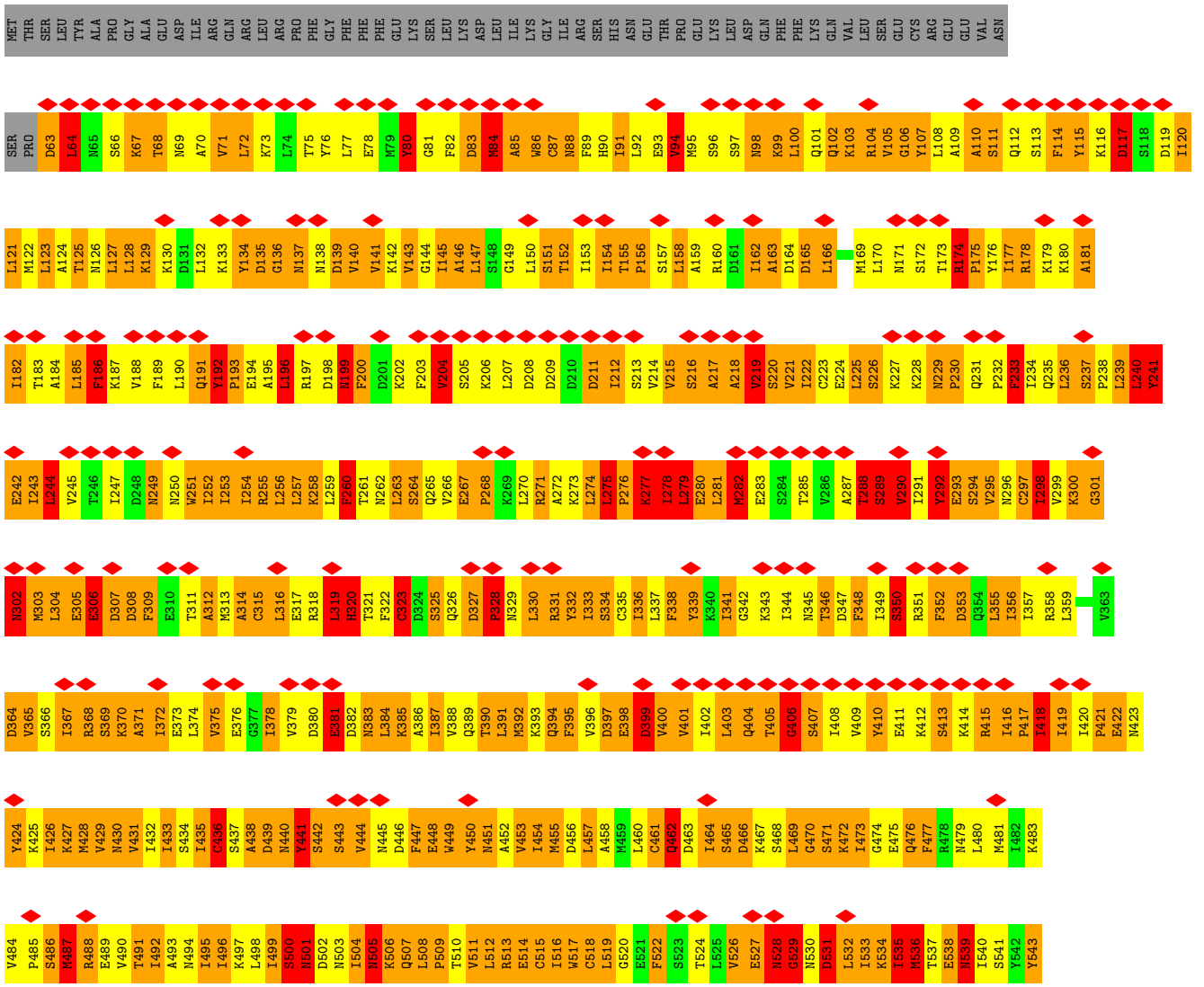
3 Residue-property plots (i)

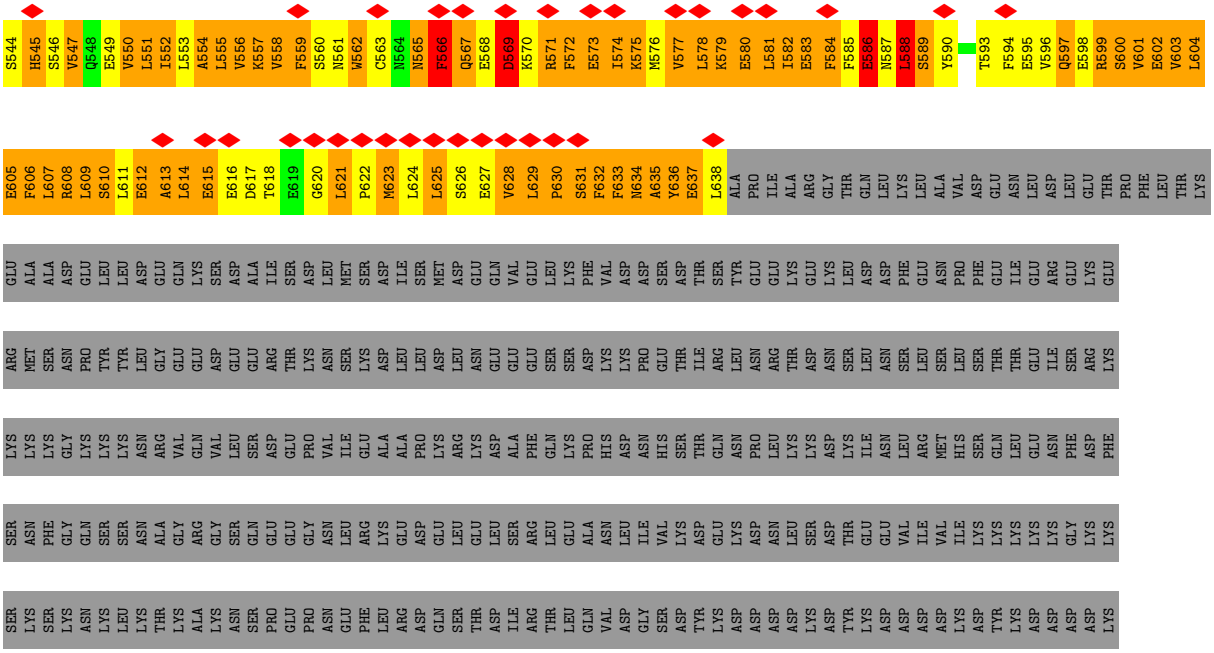
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: AP-3 complex subunit delta

Chain A:

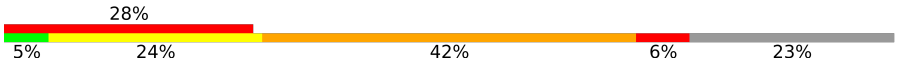


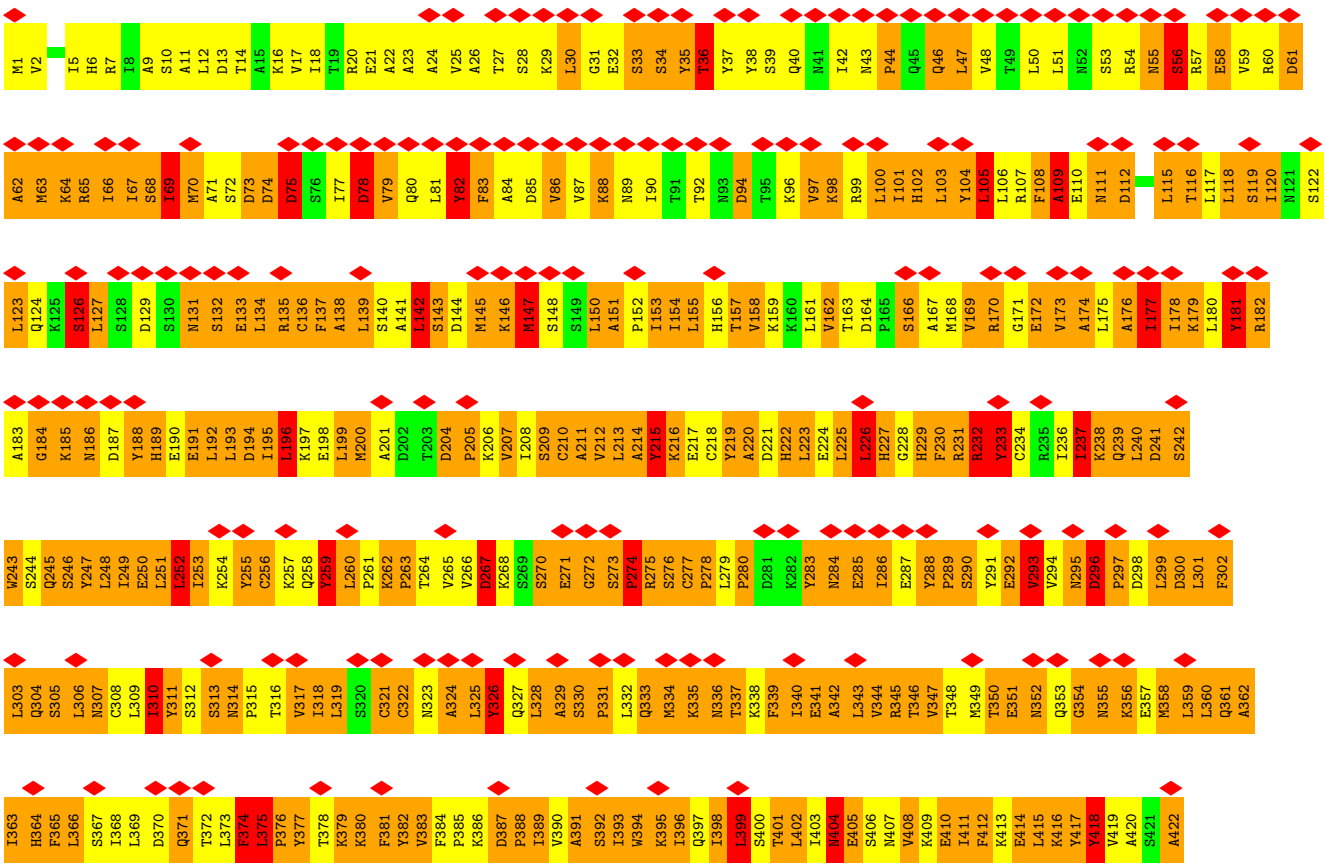


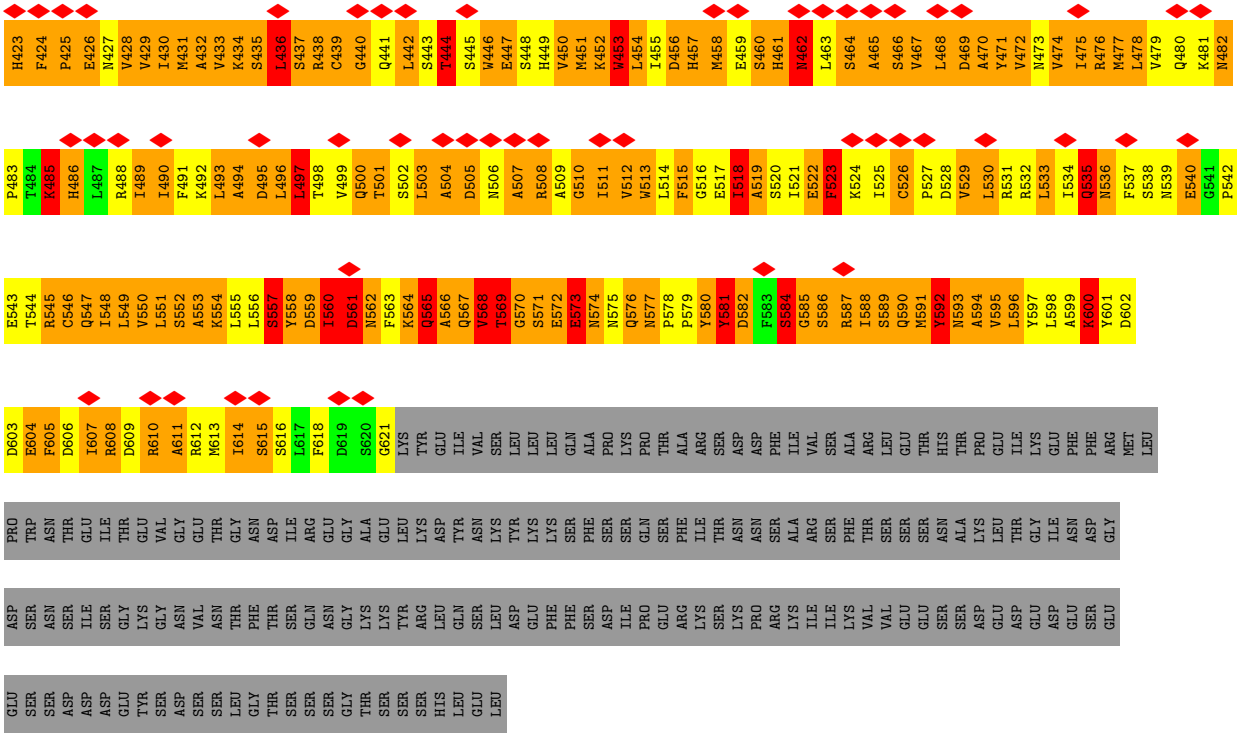


• Molecule 2: Y55_G0035830.mRNA.1.CDS.1

Chain B:

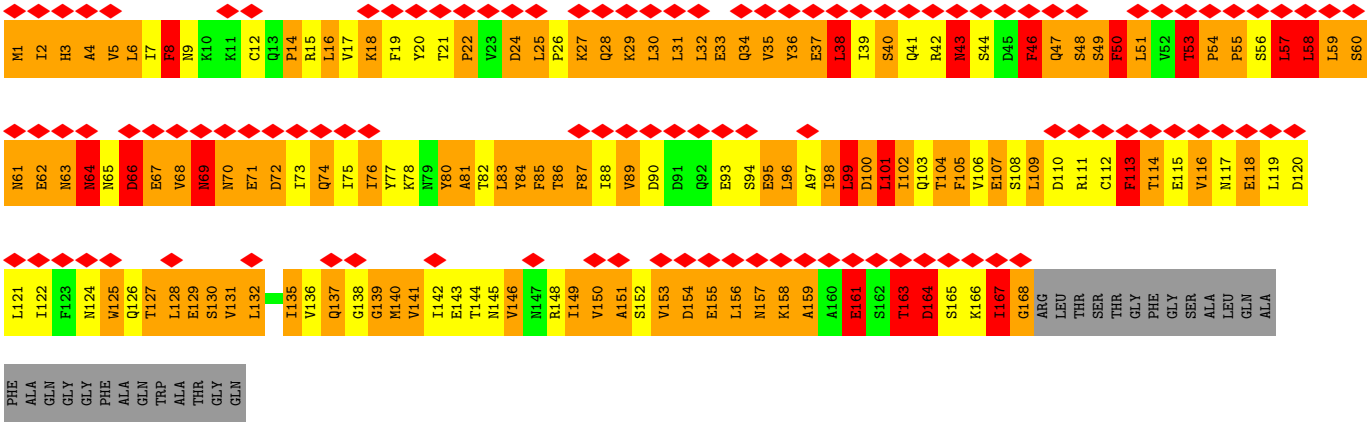






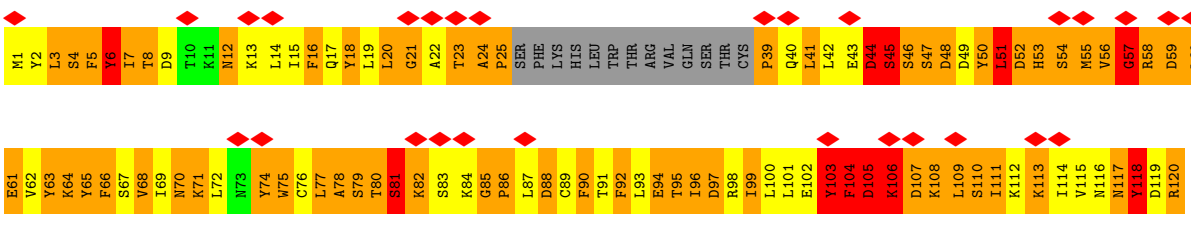
• Molecule 3: AP complex subunit sigma

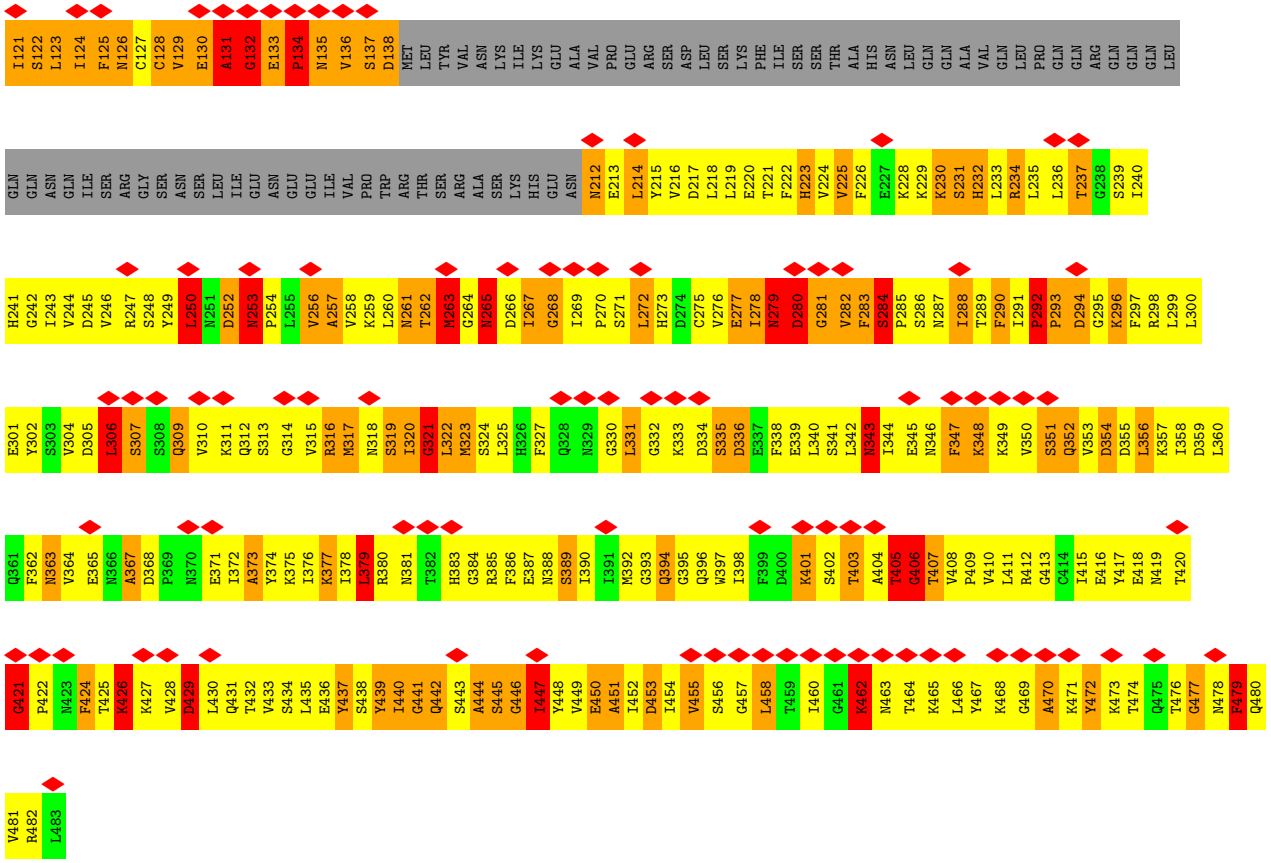
Chain S:



• Molecule 4: AP-3 complex subunit mu

Chain M:




I121 S122 L123 I124 F125 N126 C127 C128 V129 E130 A131 G132 E133 P134 N135 V136 S137 D138 MET LEU TYR VAL ASN LYS ILE LYS GLU ALA VAL PRO GLU ARG SER ASP LEU SER LYS PHE ILE SER SER THR ALA HIS ASN LEU GLN GLN ALA VAL GLN LEU PRO GLN GLN ARG GLN GLN GLN LEU
GLN GLN ASN GLN ILE SER ARG GLY SER ASN SER LEU ILE GLU ASN GLU GLU ILE VAL PRO TRP ARG THR SER ARG ALA SER LYS HIS GLU ASN N212 E213 L214 Y215 V216 D217 L218 L219 E220 T221 F222 H223 V224 V225 F226 E227 K228 K229 K230 S231 H232 L233 R234 L235 L236 T237 G238 S239 I240
H241 G242 I243 V244 D245 V246 R247 S248 Y249 L250 N251 D252 N253 P254 L255 V256 A257 V258 K259 L260 N261 T262 M263 G264 N265 D266 I267 G268 I269 P270 S271 L272 H273 D274 C275 V276 E277 I278 N279 D280 G281 V282 F283 S284 P285 S286 N287 I288 T289 F290 I291 P292 P293 D294 G295 K296 F297 R298 L299 L300
E301 Y302 S303 V304 D305 L306 S307 S308 Q309 V310 K311 Q312 S313 G314 V315 R316 M317 N318 S319 I320 G321 L322 M323 S324 L325 H326 F327 Q328 N329 G330 L331 G332 K333 D334 S335 D336 E337 F338 E339 L340 S341 L342 N343 I344 E345 N346 F347 K348 K349 V350 S351 Q352 V353 D354 D355 L356 K357 I358 D359 L360
Q361 F362 N363 V364 E365 N366 A367 D368 P369 N370 E371 I372 A373 Y374 K375 I376 K377 I378 L379 R380 N381 T382 H383 G384 R385 F386 E387 N388 S389 I390 I391 M392 G393 Q394 G395 Q396 W397 I398 F399 D400 K401 S402 T403 A404 T405 G406 T407 V408 P409 V410 L411 R412 G413 C414 I415 E416 Y417 E418 N419 T420
G421 P422 N423 F424 T425 K426 K427 V428 D429 L430 Q431 T432 V433 S434 L435 E436 Y437 S438 Y439 I440 G441 Q442 S443 A444 S445 G446 I447 Y448 V449 E450 A451 I452 D453 I454 V455 S456 G457 L458 T459 I460 G461 K462 N463 T464 K465 L466 Y467 K468 G469 A470 K471 Y472 K473 T474 Q475 T476 G477 N478 F479 Q480
V481 R482 L483

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23039	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	81	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	282.48, 282.48, 282.48	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	1.85	106/4699 (2.3%)	2.69	616/6358 (9.7%)
2	B	1.71	91/5057 (1.8%)	2.45	596/6855 (8.7%)
3	S	2.51	75/1379 (5.4%)	2.79	167/1874 (8.9%)
4	M	2.39	156/3217 (4.8%)	2.55	283/4346 (6.5%)
All	All	2.01	428/14352 (3.0%)	2.59	1662/19433 (8.6%)

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	0	54
2	B	0	31
3	S	1	18
4	M	1	24
All	All	2	127

The worst 5 of 428 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	104	PHE	N-CA	-22.48	1.01	1.46
4	M	64	LYS	N-CA	-18.25	1.09	1.46
4	M	135	ASN	C-N	-17.55	0.93	1.34
4	M	132	GLY	CA-C	-17.17	1.24	1.51
4	M	281	GLY	CA-C	16.88	1.78	1.51

The worst 5 of 1662 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	404	ALA	CB-CA-C	24.95	147.53	110.10
3	S	69	ASN	N-CA-C	23.29	173.89	111.00
1	A	242	GLU	C-N-CA	22.94	179.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	130	GLU	N-CA-C	-19.38	58.67	111.00
1	A	265	GLN	N-CA-C	-19.25	59.04	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	S	69	ASN	CA
4	M	22	ALA	CA

5 of 127 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ASP	Mainchain
1	A	64	LEU	Mainchain
1	A	80	TYR	Mainchain
1	A	84	MET	Mainchain
1	A	94	VAL	Mainchain

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	4625	0	4703	1294	0
2	B	4963	0	4983	2778	0
3	S	1358	0	1335	469	0
4	M	3158	0	3098	1734	0
All	All	14104	0	14119	5611	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 199.

The worst 5 of 5611 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:B:17:VAL:HG21	2:B:35:TYR:CD2	1.29	1.68
2:B:243:TRP:CH2	4:M:98:ARG:HD3	1.17	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LEU:CD1	2:B:144:ASP:HB3	1.23	1.62
1:A:606:PHE:CZ	1:A:633:PHE:HB2	1.23	1.62
2:B:578:PRO:HD2	2:B:581:TYR:CE2	1.21	1.61

There are no symmetry-related clashes.

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	A	574/964 (60%)	529 (92%)	32 (6%)	13 (2%)	6 34
2	B	619/809 (76%)	500 (81%)	72 (12%)	47 (8%)	1 13
3	S	166/194 (86%)	160 (96%)	4 (2%)	2 (1%)	13 50
4	M	391/483 (81%)	315 (81%)	51 (13%)	25 (6%)	1 16
All	All	1750/2450 (71%)	1504 (86%)	159 (9%)	87 (5%)	4 20

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	TRP
1	A	267	GLU
1	A	278	ILE
1	A	305	GLU
1	A	306	GLU

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	536/898 (60%)	530 (99%)	6 (1%)	73 84
2	B	566/738 (77%)	561 (99%)	5 (1%)	78 87
3	S	159/175 (91%)	156 (98%)	3 (2%)	57 75
4	M	360/441 (82%)	351 (98%)	9 (2%)	47 68
All	All	1621/2252 (72%)	1598 (99%)	23 (1%)	68 80

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	6	TYR
4	M	250	LEU
4	M	214	LEU
4	M	343	ASN
2	B	233	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	441	GLN
2	B	574	ASN
4	M	346	ASN
2	B	486	HIS
3	S	64	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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
4	M	33
3	S	11
1	A	9
2	B	6

The worst 5 of 59 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	68:VAL	C	69:ASN	N	1.67
1	A	244:LEU	C	245:VAL	N	1.20
1	A	277:LYS	C	278:ILE	N	1.20
1	A	464:ILE	C	465:SER	N	1.20
1	B	259:TYR	C	260:LEU	N	1.20

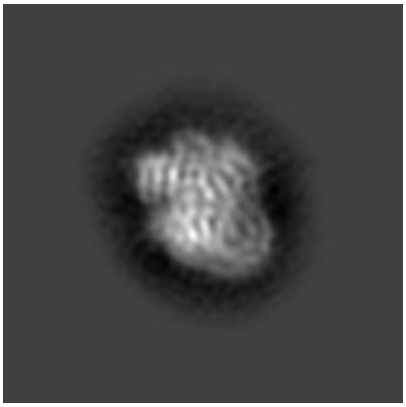
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13187. These allow visual inspection of the internal detail of the map and identification of artifacts.

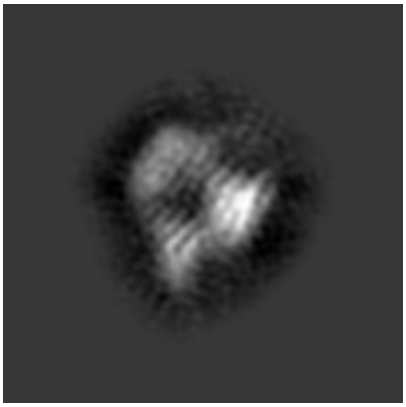
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

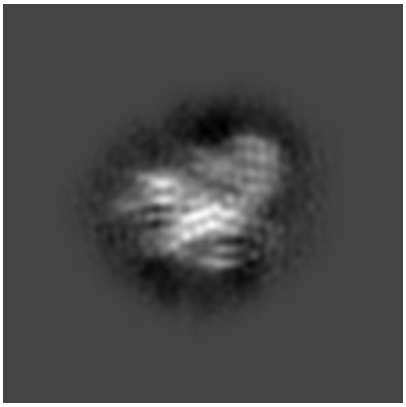
6.1.1 Primary map



X



Y

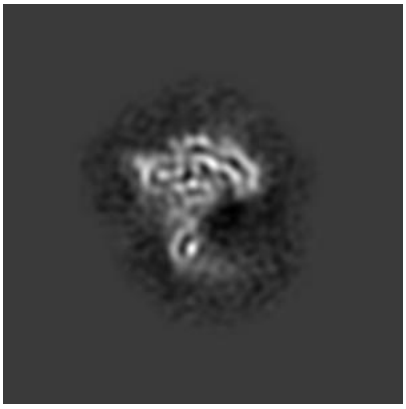


Z

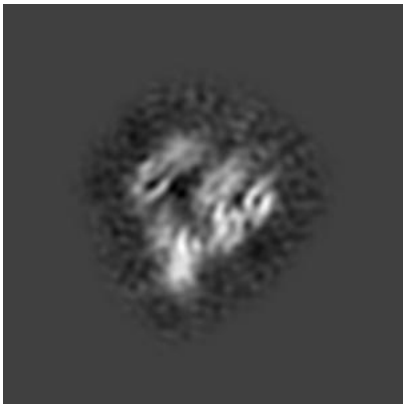
The images above show the map projected in three orthogonal directions.

6.2 Central slices

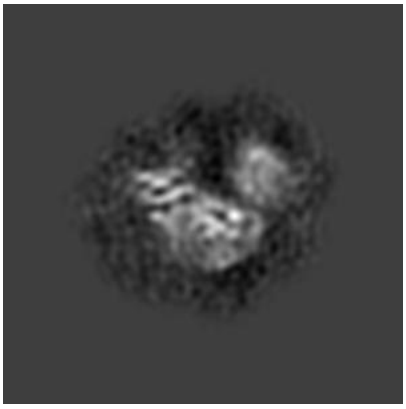
6.2.1 Primary map



X Index: 132



Y Index: 132

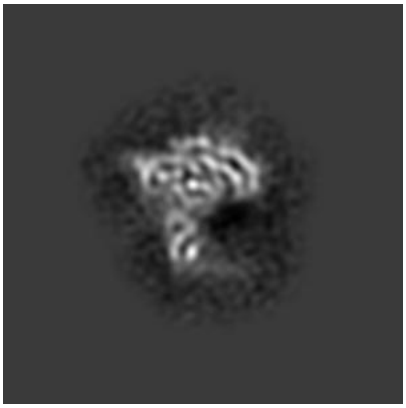


Z Index: 132

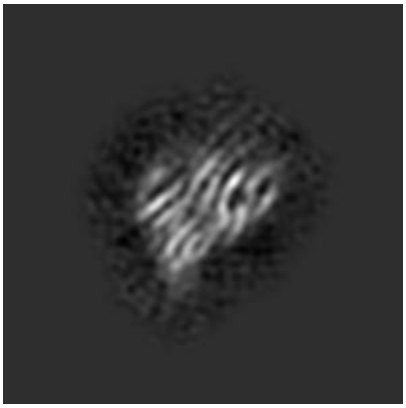
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

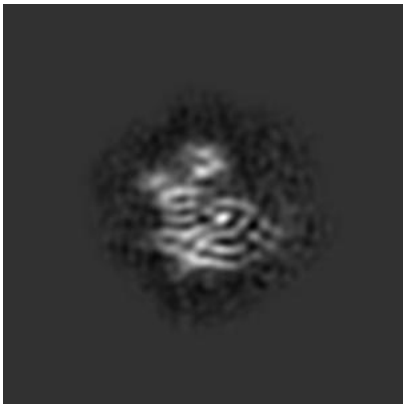
6.3.1 Primary map



X Index: 130



Y Index: 123

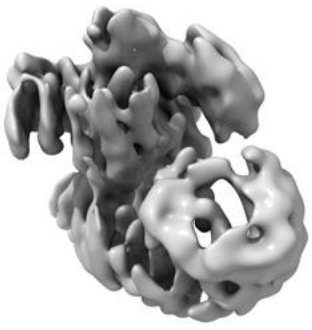


Z Index: 150

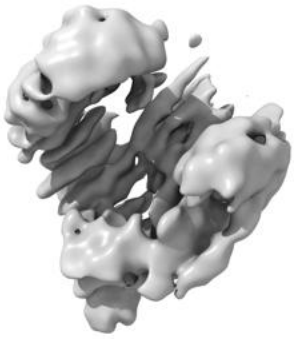
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

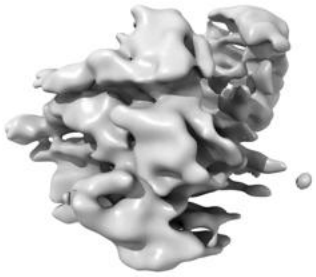
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

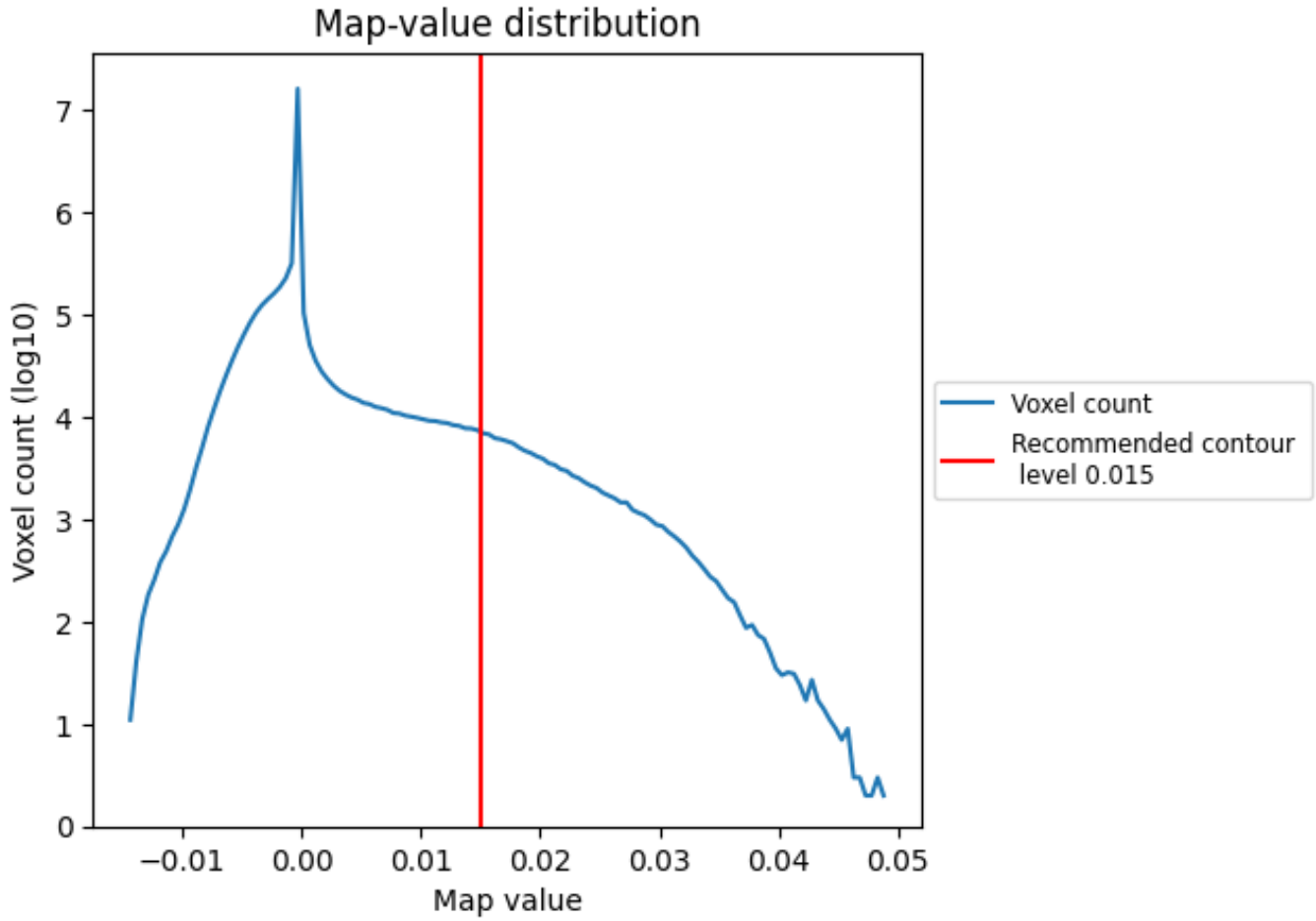
6.5 Mask visualisation (i)

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

7 Map analysis

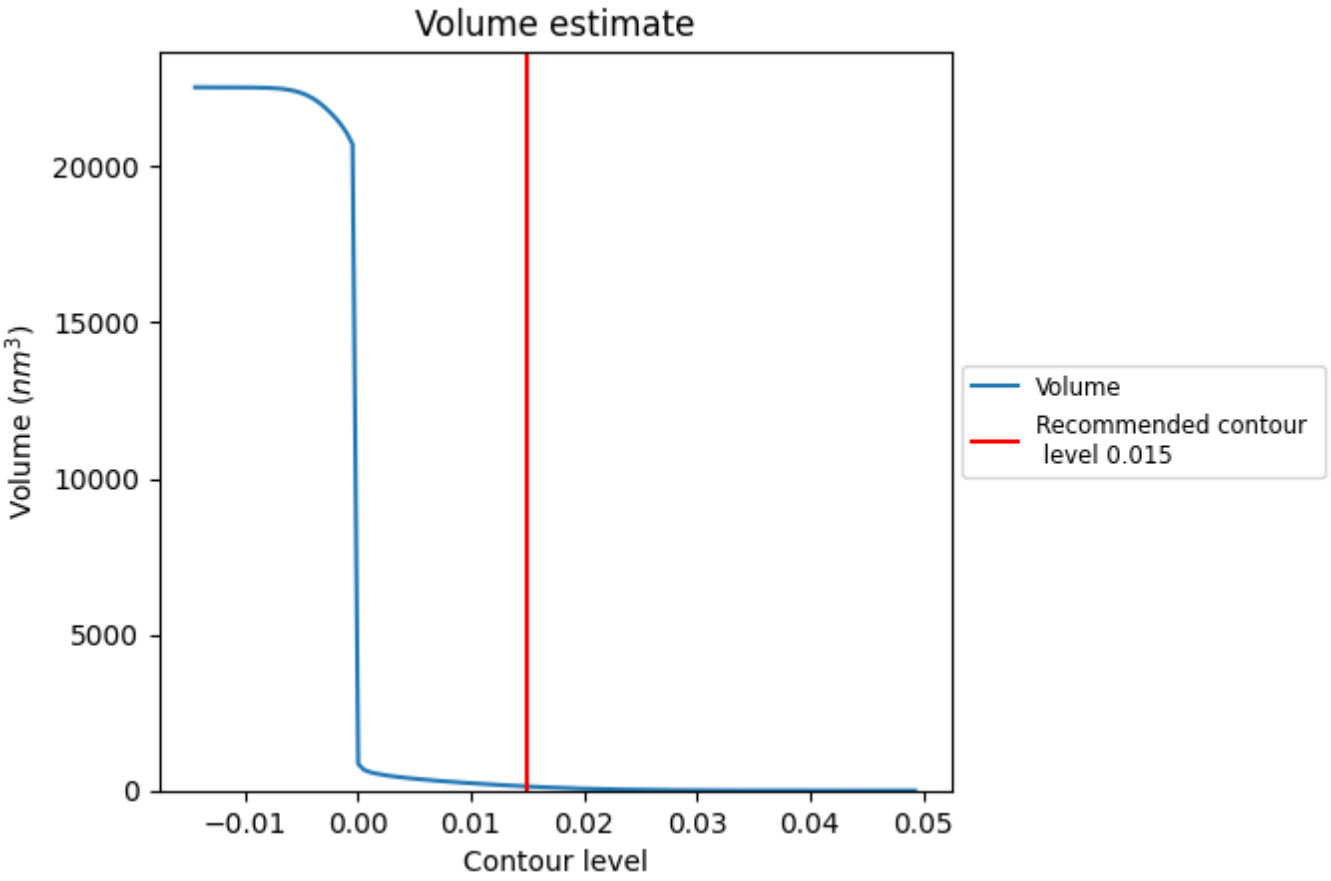
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

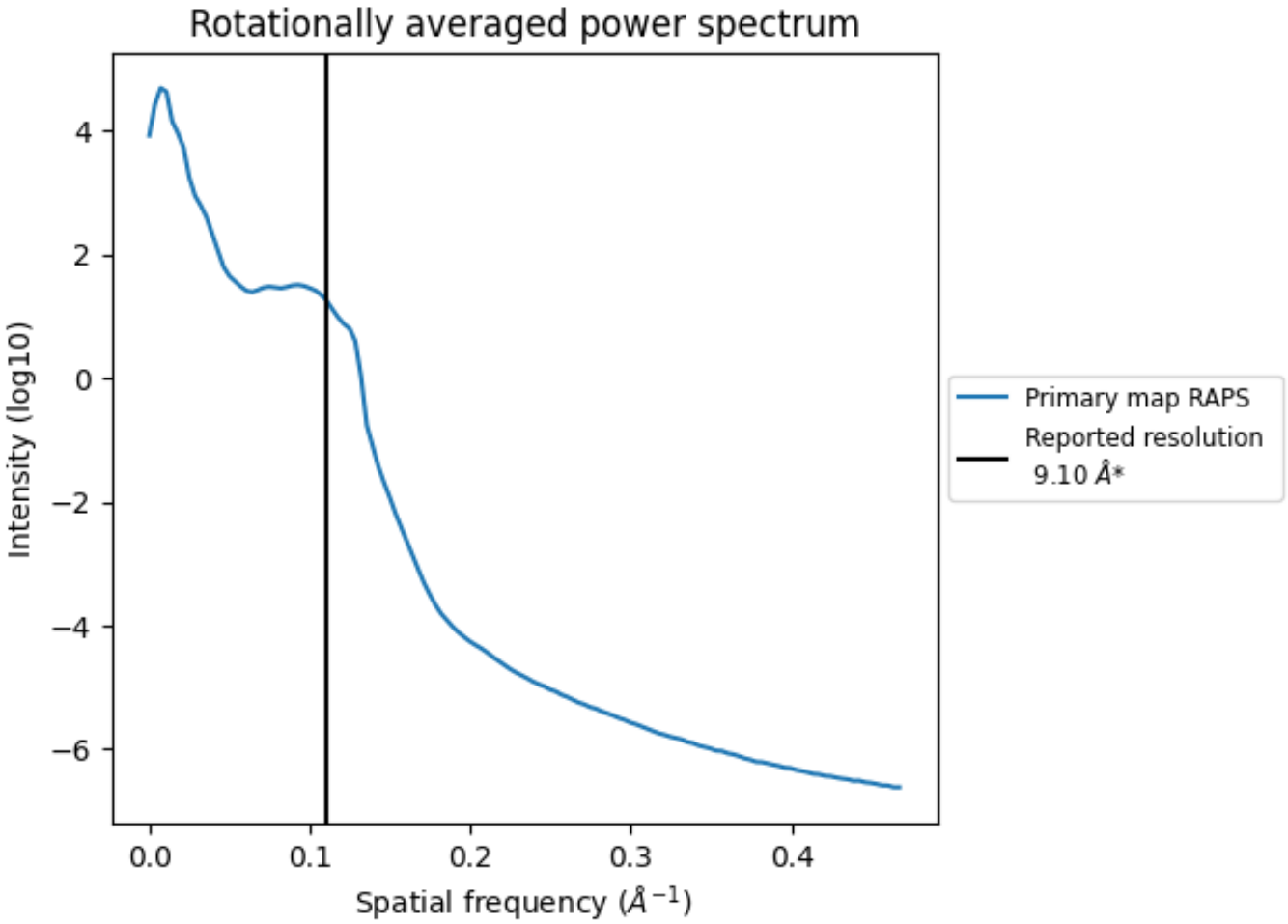
7.2 Volume estimate (i)



The volume at the recommended contour level is 131 nm^3; this corresponds to an approximate mass of 119 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 0.110 Å^{-1}

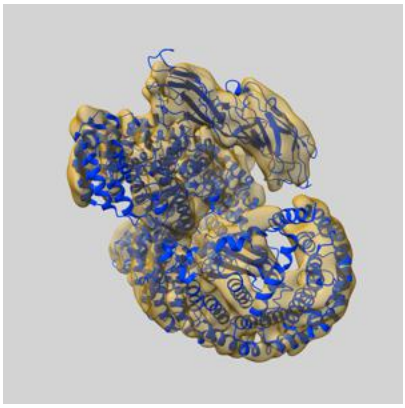
8 Fourier-Shell correlation

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

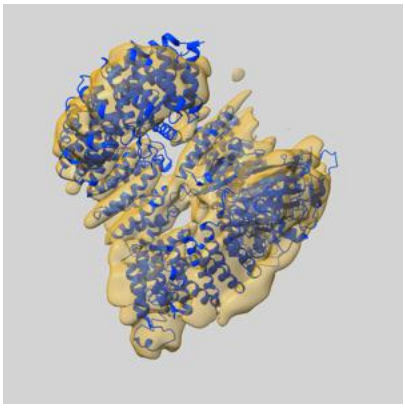
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13187 and PDB model 7P3X. Per-residue inclusion information can be found in section 3 on page 5.

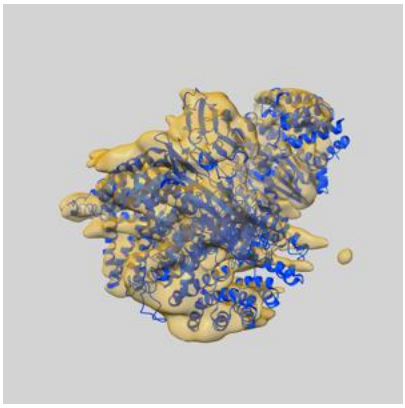
9.1 Map-model overlay



X



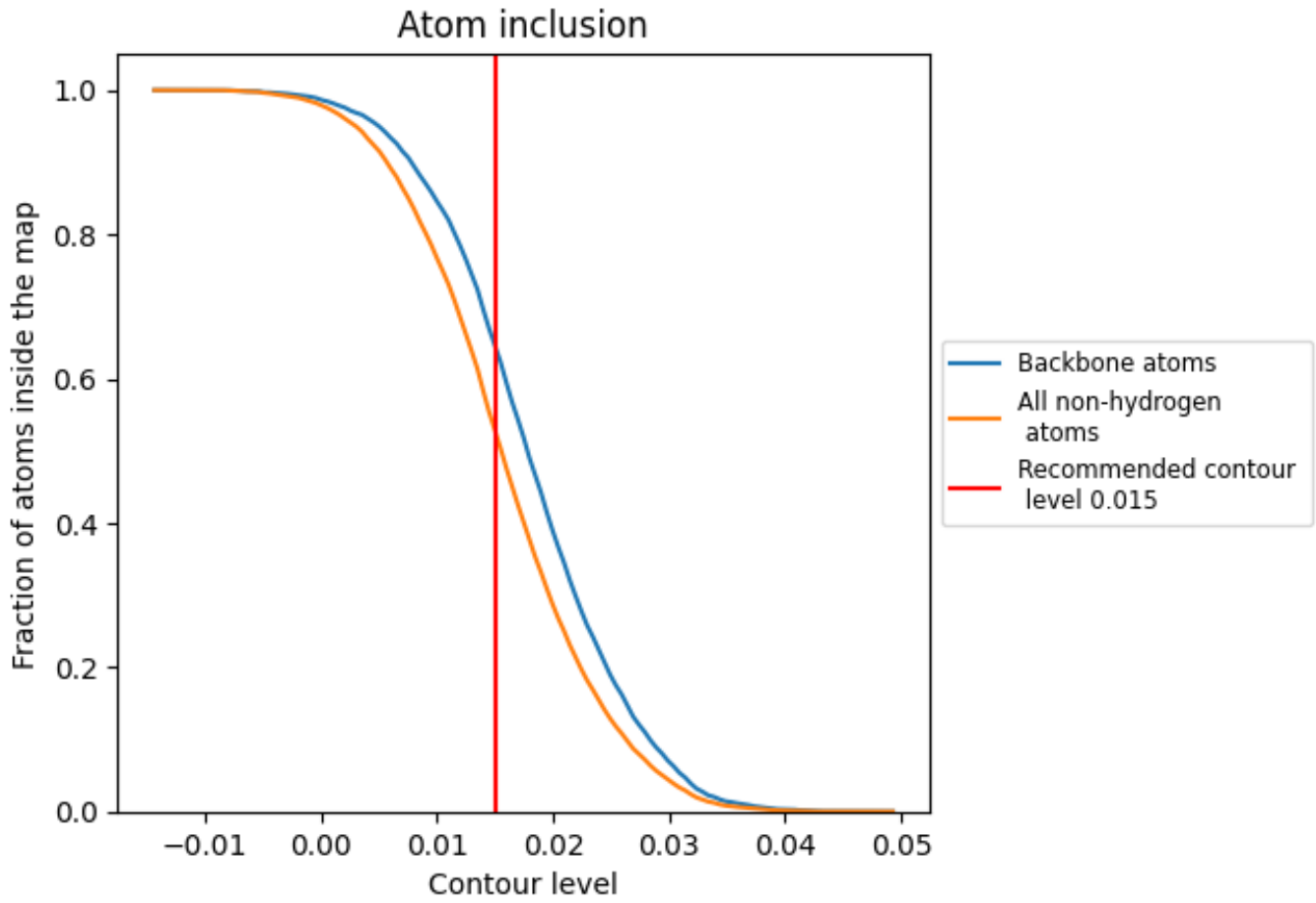
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.