Full wwPDB EM Validation Report

May 18, 2024 – 10:30 am BST

PDB ID	:	6YLF
EMDB ID	:	EMD-10837
Title	:	Rix1-Rea1 pre-60S particle - Rea1, body 3 (rigid body refinement, composite structure of Rea1 ring and tail)
Authors	:	Kater, L.; Beckmann, R.
Deposited on	:	2020-04-07
Resolution	:	4.20 Å(reported)
Based on initial models	:	6OR5, 6HYP, 6HYD, 6QTA

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 (i) 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 (i)) were used in the production of this report:

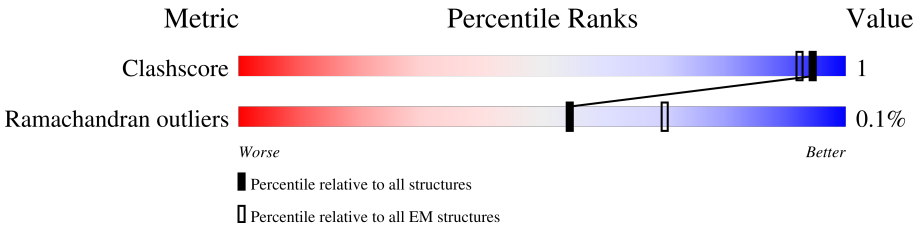
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.20 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

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	AP1	4910	10% 73% · 26%
2	xP1	515	7% 14% 86%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18362 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 Midasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	AP1	3629	18010	10752	3629	3629	0	0

- Molecule 2 is a protein called Ribosome assembly protein 4.

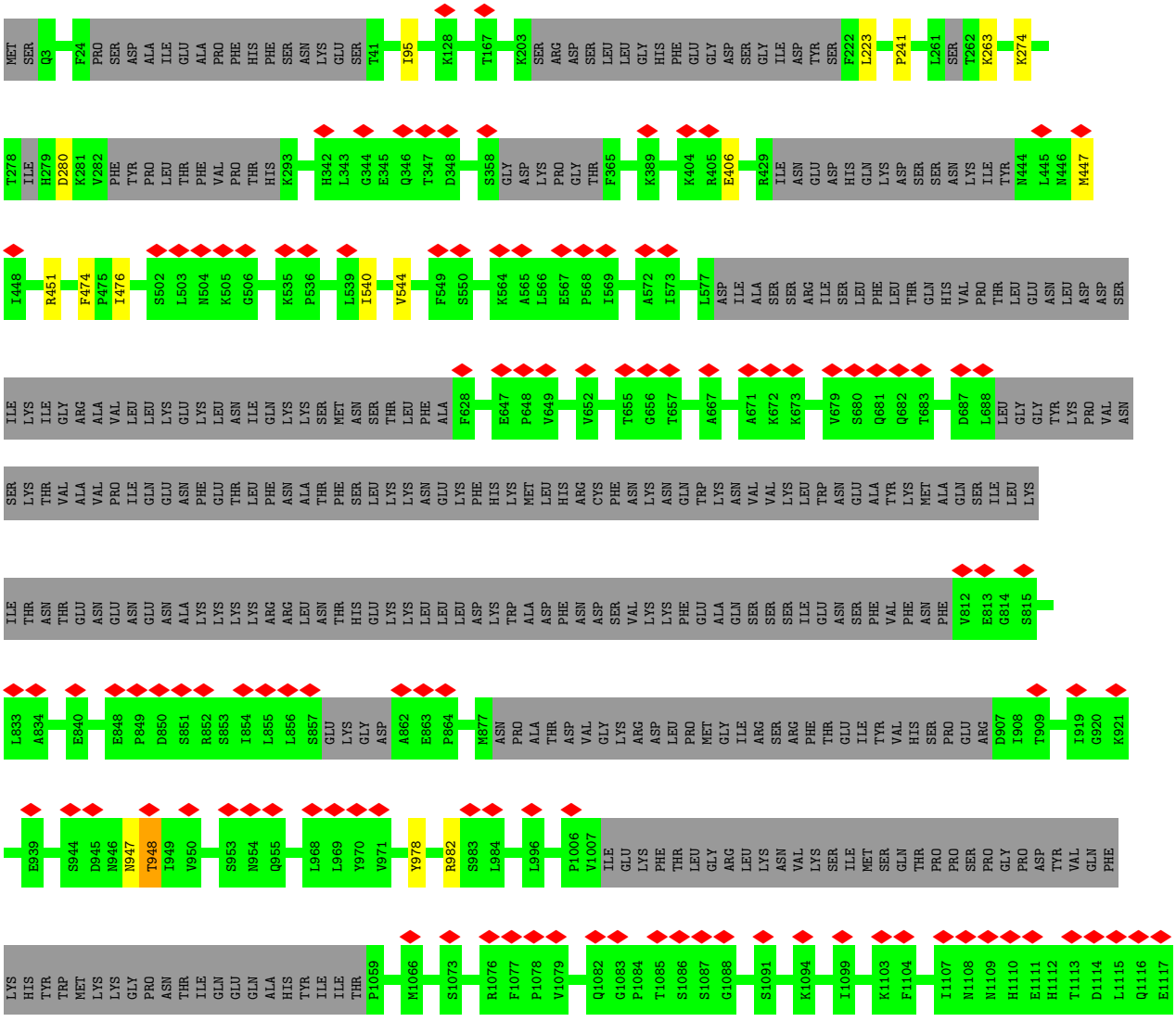
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	xP1	71	352	210	71	71	0	0

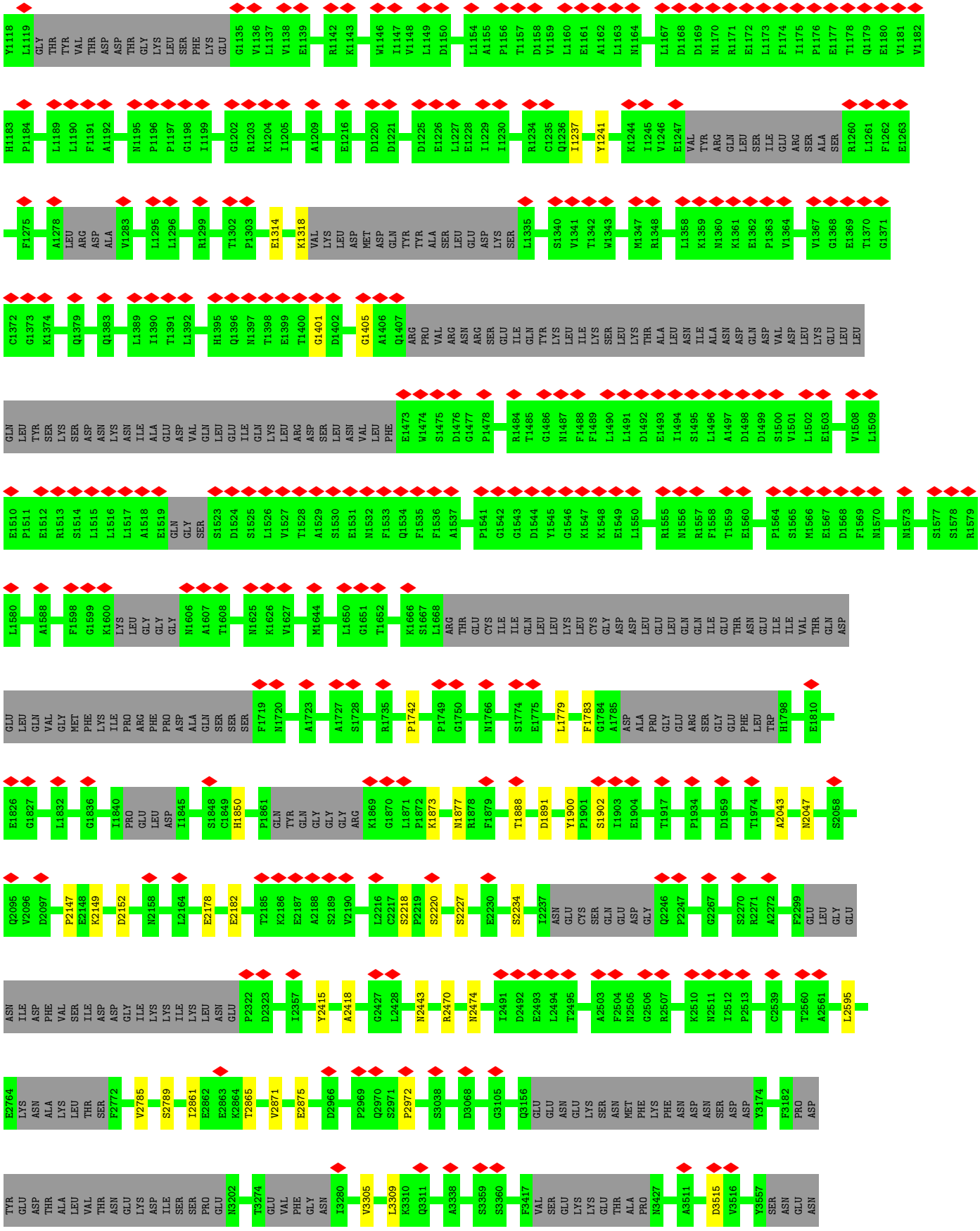
3 Residue-property plots (i)

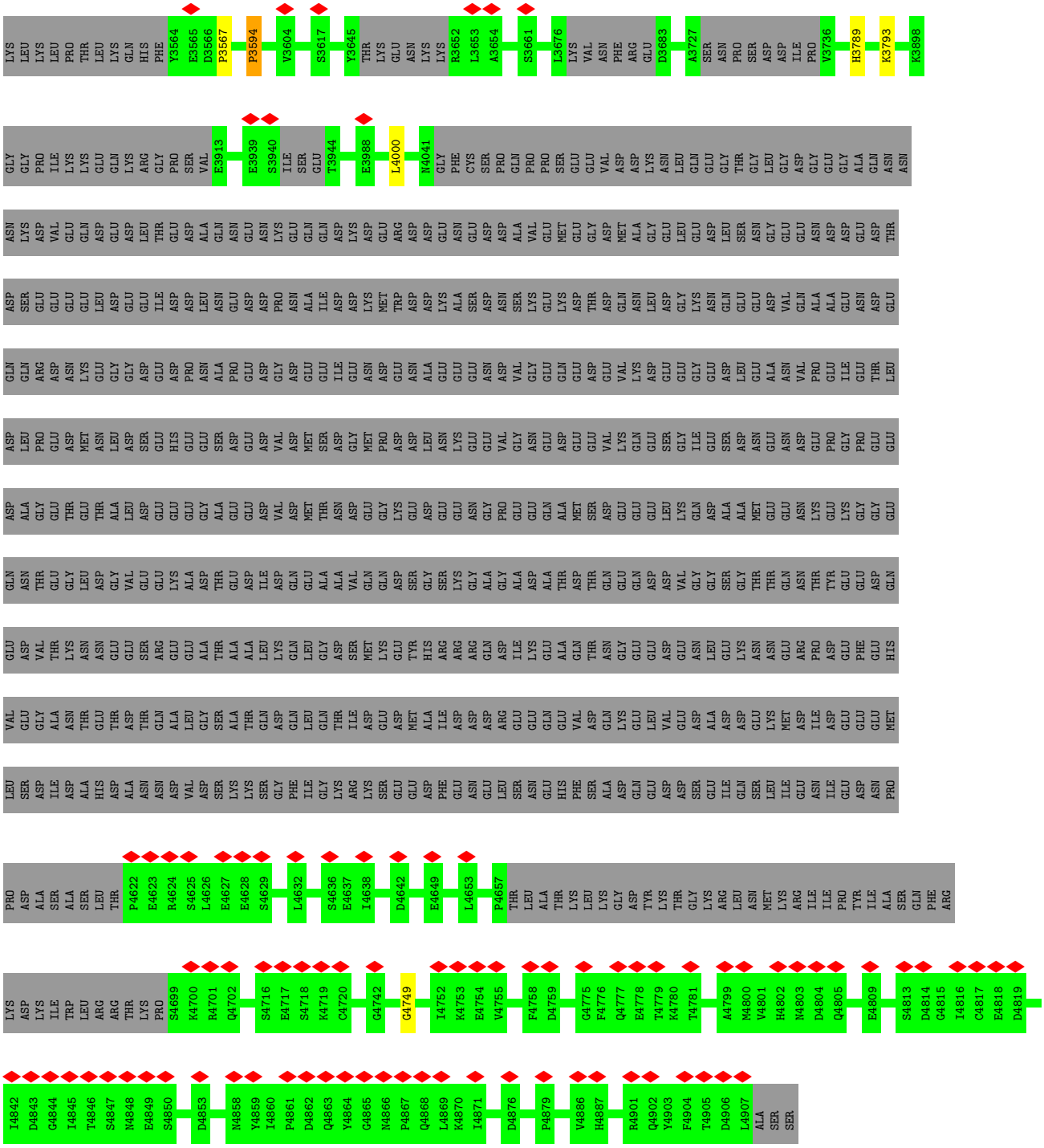
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain AP1:

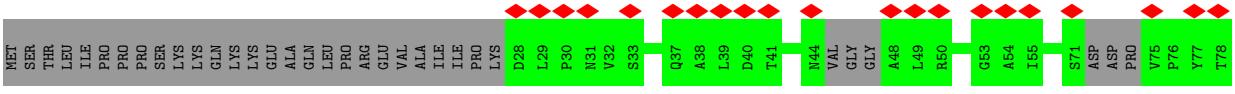


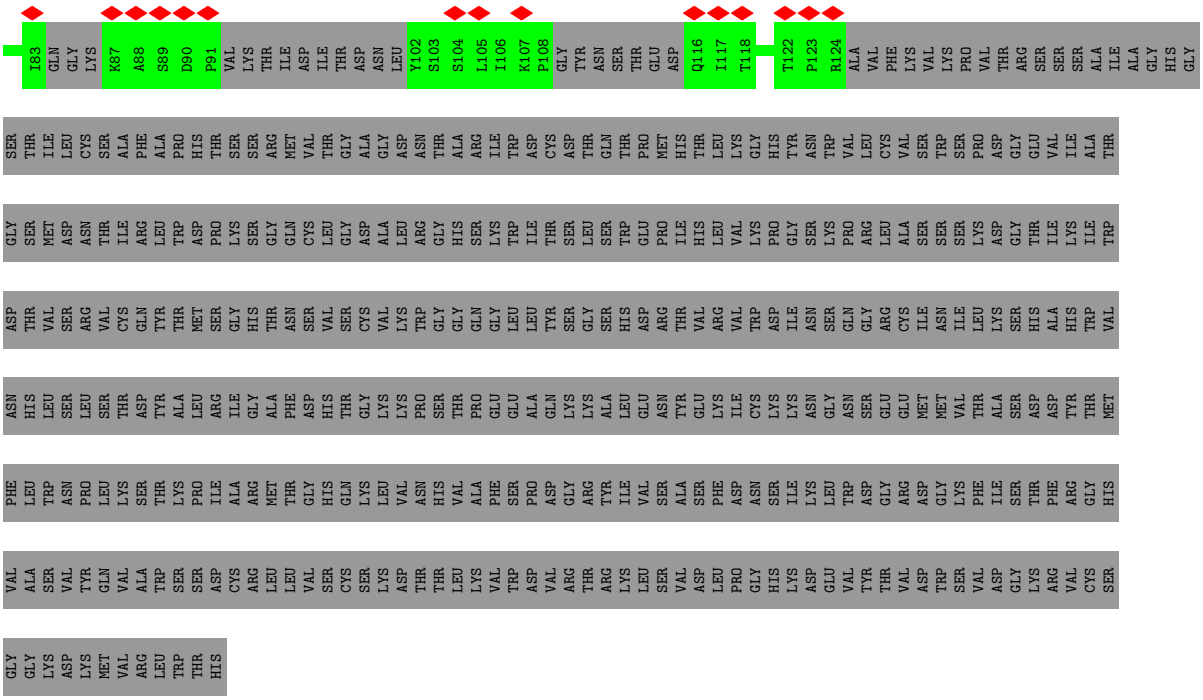




• Molecule 2: Ribosome assembly protein 4

Chain xP1:




I83 GLN GLY LYS K87 A88 S89 D90 P91 VAL LYS THR ILE ASP ILE THR ASP ASN LEU Y102 S103 S104 L105 I106 K107 P108 GLY TYR ASN SER THR GLU ASP Q116 I117 T118 T122 P123 R124 ALA VAL PHE LYS VAL LYS PRO VAL THR ARG SER SER SER ALA ILE ALA GLY HIS GLY
SER THR ILE LEU CYS SER ALA PHE ALA PRO HIS THR SER SER ARG MET VAL THR GLY ALA GLY ASP ASN THR ALA ARG ILE TRP ASP CYS ASP THR GLN THR PRO MET HIS THR LEU LYS GLY HIS TYR ASN TRP VAL LEU CYS VAL SER TRP SER PRO ASP GLY GLU VAL ILE ALA THR
GLY SER MET ASP ASN THR ILE ARG LEU TRP ASP PRO LYS SER GLY GLN CYS LEU GLY ASP ALA LEU ARG GLY HIS SER LYS TRP ILE THR SER LEU SER TRP GLU PRO ILE HIS LEU VAL LYS PRO GLY SER LYS PRO ARG LEU ALA SER SER SER LYS ASP GLY THR ILE LYS ILE TRP
ASP THR VAL SER ARG VAL CYS GLN TYR THR MET SER GLY HIS THR ASN SER VAL SER CYS VAL LYS TRP GLY GLY GLN GLY LEU LEU TYR SER GLY SER HIS ASP ARG THR VAL ARG VAL TRP ASP ILE ASN SER GLN GLY ARG CYS ILE ASN ILE LEU LYS SER HIS ALA HIS TRP VAL
ASN HIS LEU SER LEU SER THR ASP TYR ALA LEU ARG ILE GLY ALA PHE ASP HIS THR GLY LYS LYS PRO SER THR PRO GLU GLU ALA GLN LYS LYS ALA LEU GLU GLU ASN TYR GLU LYS ILE CYS LYS LYS ASN GLY ASN SER GLU GLU MET MET VAL THR ALA SER ASP ASP TYR THR MET
PHE LEU TRP ASN PRO LEU LYS SER THR LYS PRO ILE ALA ARG MET THR GLY HIS GLN LYS LEU VAL ASN HIS VAL ALA PHE SER PRO ASP GLY ARG TYR ILE VAL SER ALA SER PHE ASP ASN SER ILE LYS LEU TRP ASP GLY ARG ASP GLY LYS PHE ILE SER THR PHE ARG GLY HIS
VAL ALA SER VAL TYR GLN VAL ALA TRP SER SER ASP CYS ARG LEU LEU VAL SER CYS SER LYS ASP THR THR LEU LYS VAL TRP ASP VAL ARG THR ARG LYS LEU SER VAL ASP LEU PRO GLY HIS LYS ASP GLU VAL TYR THR VAL ASP TRP SER VAL ASP GLY LYS ARG VAL CYS SER
GLY GLY LYS ASP LYS MET VAL ARG LEU TRP THR HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55397	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	370.65, 370.65, 370.65	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	AP1	0.27	0/17970	0.50	2/25013 (0.0%)
2	xP1	0.24	0/346	0.51	0/473
All	All	0.27	0/18316	0.50	2/25486 (0.0%)

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	AP1	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AP1	3567	PRO	N-CA-CB	6.53	111.14	103.30
1	AP1	3594	PRO	N-CA-CB	6.18	110.72	103.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AP1	1742	PRO	Peptide
1	AP1	1850	HIS	Peptide
1	AP1	2147	PRO	Peptide
1	AP1	223	LEU	Peptide
1	AP1	2443	ASN	Peptide
1	AP1	2595	LEU	Peptide
1	AP1	2972	PRO	Peptide
1	AP1	3515	ASP	Peptide
1	AP1	4000	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	AP1	406	GLU	Peptide
1	AP1	4749	GLY	Peptide
1	AP1	947	ASN	Peptide
1	AP1	948	THR	Peptide
1	AP1	95	ILE	Peptide

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	AP1	18010	0	7839	27	0
2	xP1	352	0	145	0	0
All	All	18362	0	7984	27	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 1.

All (27) 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:AP1:263:LYS:HA	1:AP1:274:LYS:O	1.74	0.87
1:AP1:263:LYS:CA	1:AP1:274:LYS:O	2.40	0.69
1:AP1:263:LYS:CB	1:AP1:274:LYS:O	2.45	0.65
1:AP1:1779:LEU:O	1:AP1:1783:PHE:N	2.30	0.64
1:AP1:2178:GLU:O	1:AP1:2182:GLU:N	2.37	0.57
1:AP1:1237:ILE:O	1:AP1:1241:TYR:N	2.36	0.57
1:AP1:447:MET:O	1:AP1:451:ARG:N	2.39	0.56
1:AP1:1401:GLY:O	1:AP1:1405:GLY:N	2.39	0.55
1:AP1:2043:ALA:O	1:AP1:2047:ASN:N	2.41	0.54
1:AP1:3789:HIS:O	1:AP1:3793:LYS:N	2.40	0.53
1:AP1:1900:TYR:O	1:AP1:1902:SER:N	2.43	0.52
1:AP1:540:ILE:O	1:AP1:544:VAL:N	2.42	0.49
1:AP1:2871:VAL:O	1:AP1:2875:GLU:N	2.42	0.49
1:AP1:2227:SER:O	1:AP1:2234:SER:N	2.45	0.47
1:AP1:2861:ILE:O	1:AP1:2865:THR:N	2.47	0.47
1:AP1:2470:ARG:O	1:AP1:2474:ASN:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:1888:THR:O	1:AP1:1891:ASP:N	2.48	0.46
1:AP1:1314:GLU:O	1:AP1:1318:LYS:N	2.48	0.46
1:AP1:2218:SER:O	1:AP1:2220:SER:N	2.49	0.46
1:AP1:978:TYR:O	1:AP1:982:ARG:N	2.48	0.45
1:AP1:474:PHE:O	1:AP1:476:ILE:N	2.49	0.44
1:AP1:2785:VAL:O	1:AP1:2789:SER:N	2.48	0.43
1:AP1:1873:LYS:O	1:AP1:1877:ASN:N	2.50	0.43
1:AP1:2149:LYS:O	1:AP1:2152:ASP:N	2.53	0.42
1:AP1:263:LYS:O	1:AP1:274:LYS:N	2.53	0.42
1:AP1:2415:TYR:O	1:AP1:2418:ALA:N	2.53	0.41
1:AP1:3305:VAL:O	1:AP1:3309:LEU:N	2.53	0.41

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	AP1	3549/4910 (72%)	3232 (91%)	313 (9%)	4 (0%)	51 85
2	xP1	59/515 (12%)	53 (90%)	6 (10%)	0	100 100
All	All	3608/5425 (66%)	3285 (91%)	319 (9%)	4 (0%)	54 85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AP1	241	PRO
1	AP1	3594	PRO
1	AP1	280	ASP
1	AP1	948	THR

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AP1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AP1	3595:LEU	C	3599:ARG	N	4.97
1	AP1	3575:LEU	C	3579:VAL	N	3.43
1	AP1	3587:MET	C	3591:ARG	N	3.23

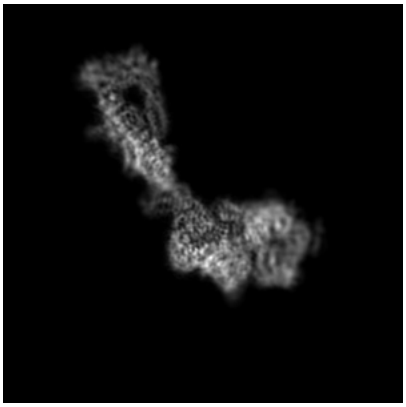
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10837. These allow visual inspection of the internal detail of the map and identification of artifacts.

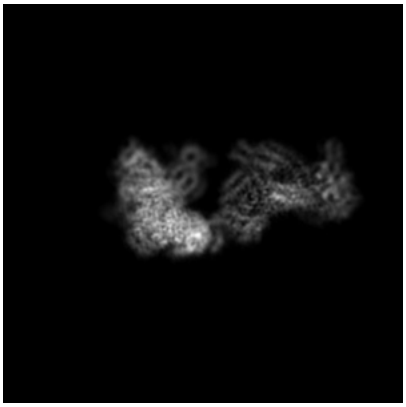
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

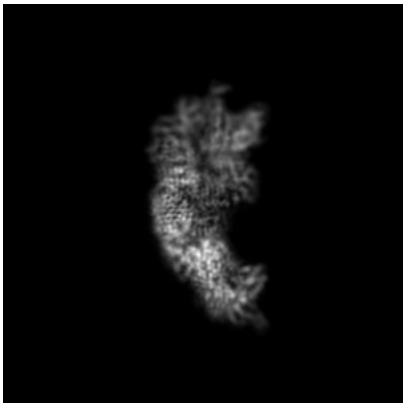
6.1.1 Primary map



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: 175

Y Index: 175

Z Index: 175

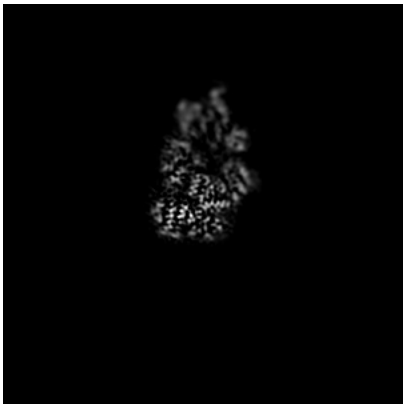
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 188

Y Index: 132

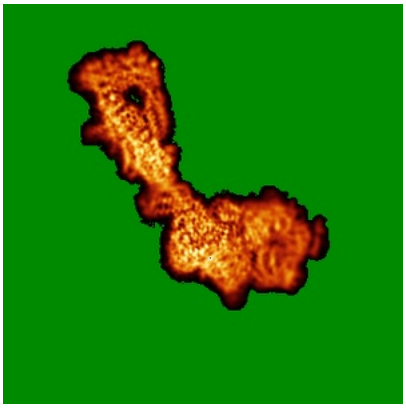


Z Index: 133

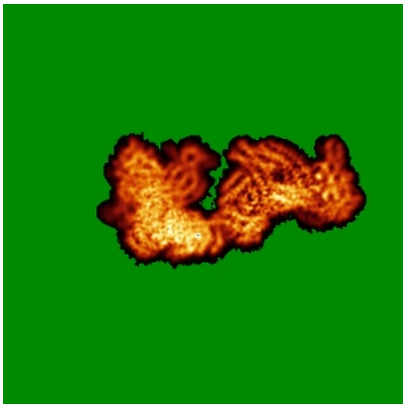
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

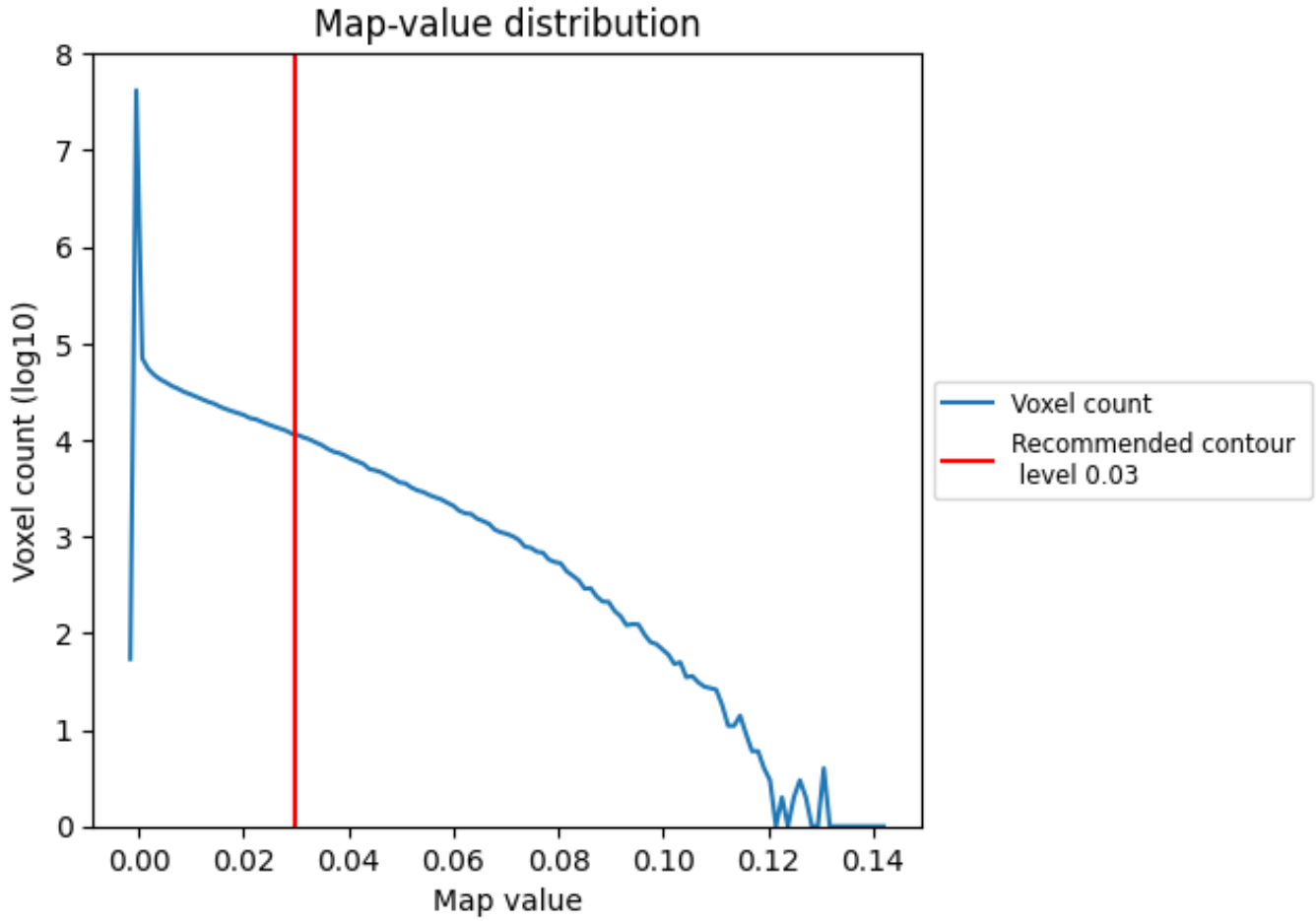
6.6 Mask visualisation (i)

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

7 Map analysis

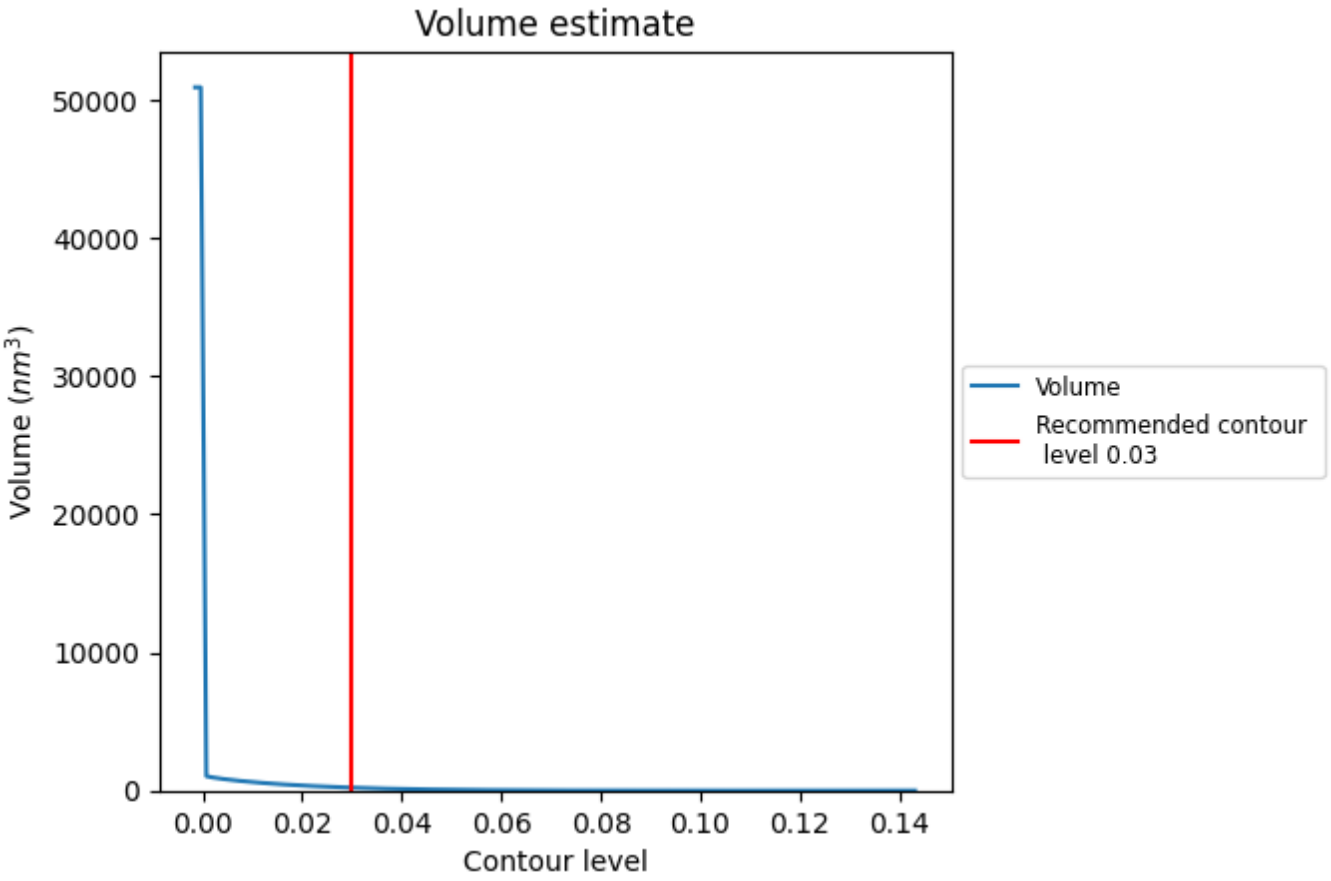
This section contains the results of statistical analysis of the map.

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.

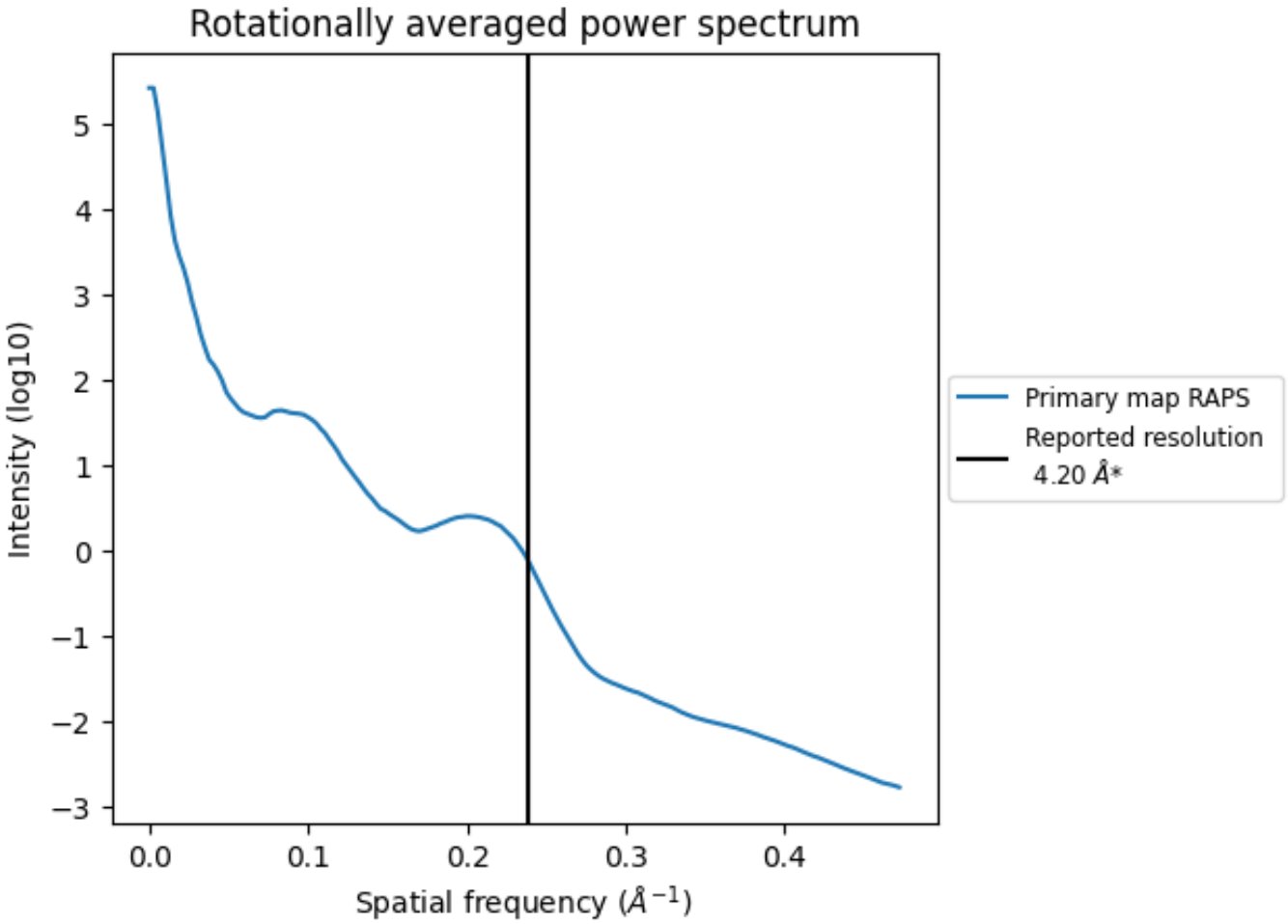
7.2 Volume estimate



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 189 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 0.238 Å^{-1}

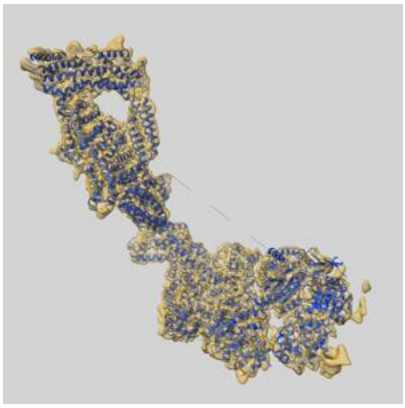
8 Fourier-Shell correlation

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

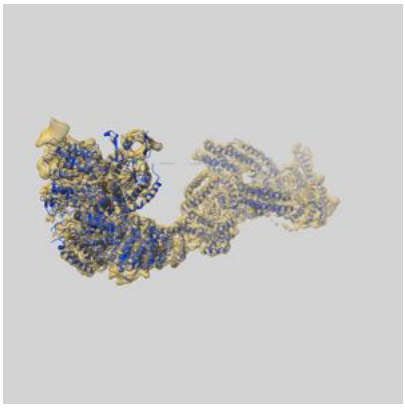
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10837 and PDB model 6YLF. Per-residue inclusion information can be found in section 3 on page 4.

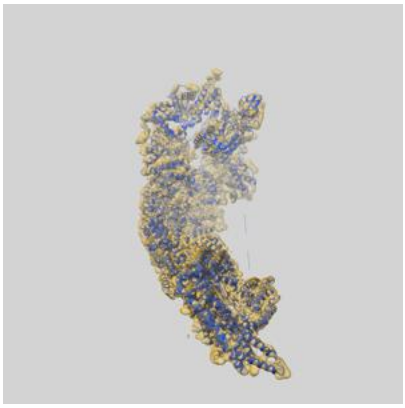
9.1 Map-model overlay



X



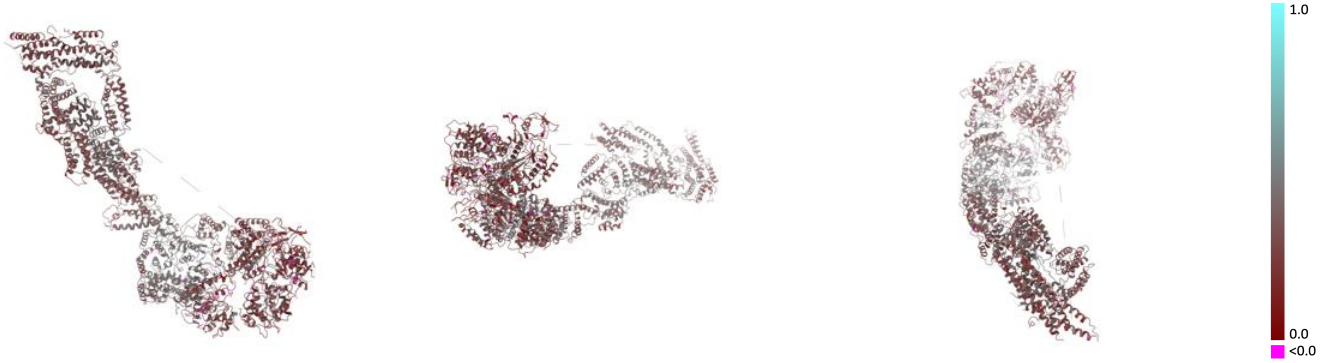
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

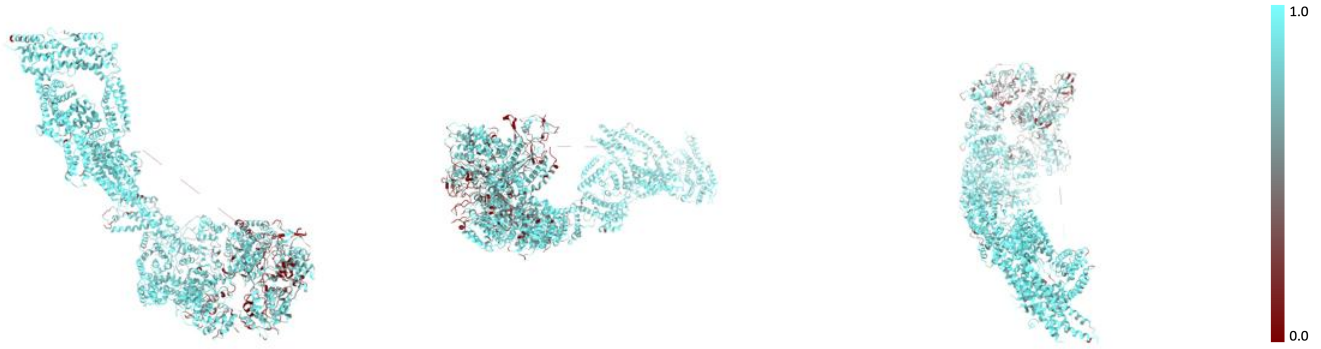
9.2 Q-score mapped to coordinate model (i)



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.

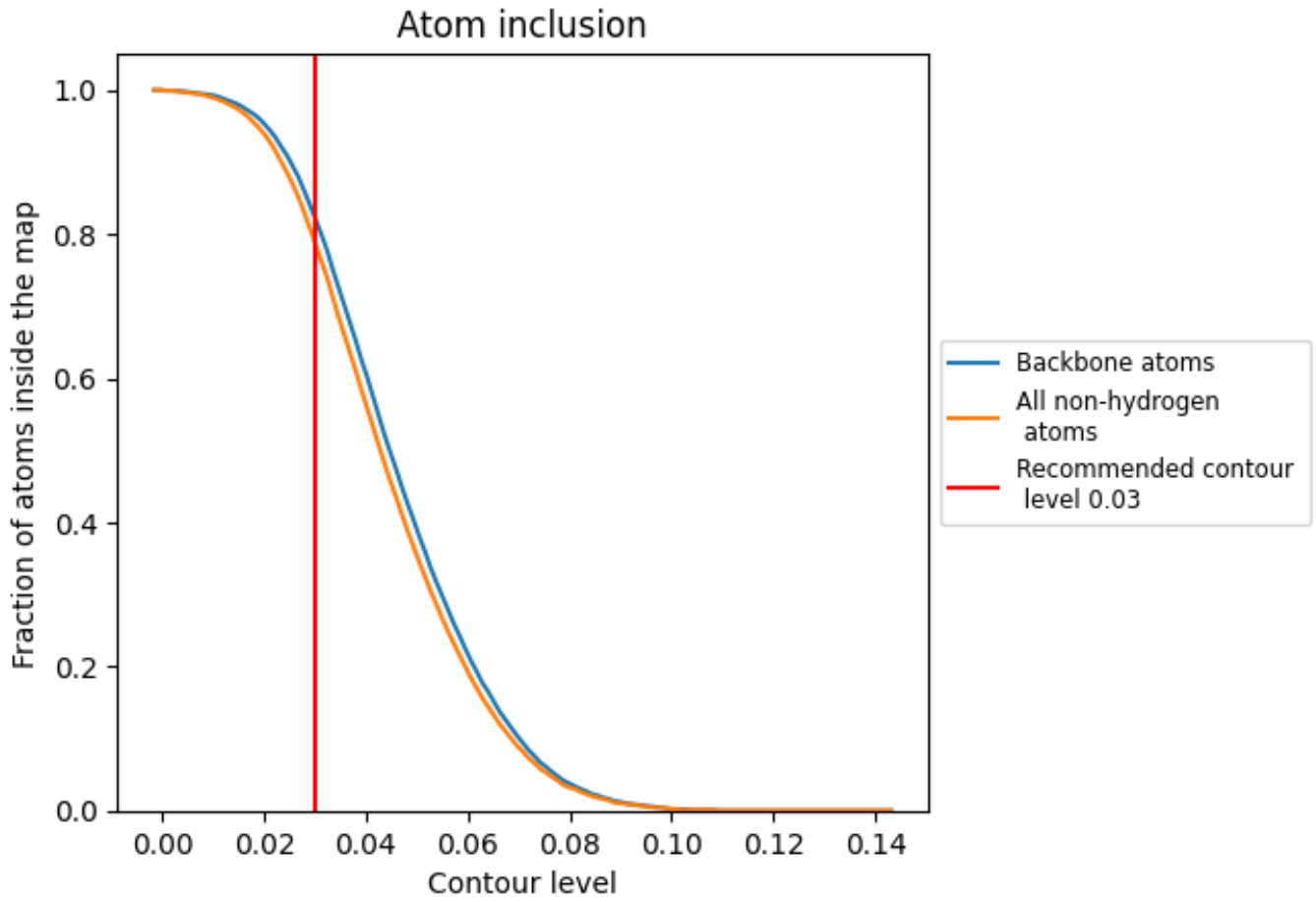
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 82% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.3360
AP1	0.7950	0.3380
xP1	0.4800	0.2400