wwPDB EM Validation Summary Report ⓘ

May 2, 2026 – 03:21 PM EDT

PDB ID	:	9EGL / pdb_00009egl
EMDB ID	:	EMD-47990
Title	:	Cryo-EM structure of COP9 signalosome precatalytic state with neddylated cullin-3
Authors	:	Shi, H.; Zheng, N.
Deposited on	:	2024-11-21
Resolution	:	3.93 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:

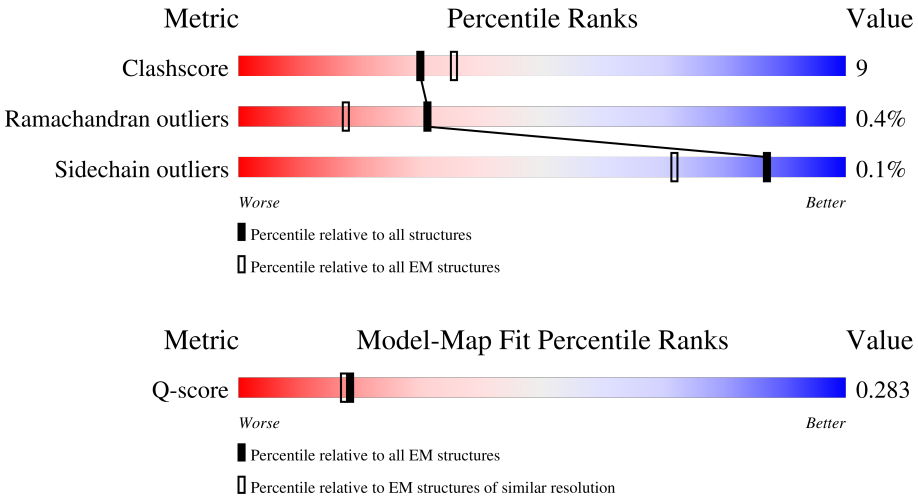
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 3.93 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	7811 (3.43 - 4.43)

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	491	68% 16% 17%
2	B	443	73% 19% 8%
3	C	423	78% 18%
4	D	406	73% 26%

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Mol	Chain	Length	Quality of chain
5	E	334	64% 23% 13%
6	F	327	66% 18% 16%
7	G	264	66% 15% 19%
8	H	209	66% 16% 18%
9	I	81	54% 38% 6%
10	J	768	8% 42% 14% 44%
11	K	108	53% 23% 24%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 25393 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 COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	409	3271	2066	573	610	22	0	0

- Molecule 2 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	408	3342	2126	574	627	15	0	0

- Molecule 3 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	405	3222	2051	541	604	26	0	0

- Molecule 4 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	405	3241	2042	564	619	16	0	0

- Molecule 5 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	291	2309	1476	386	433	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	76	ALA	GLU	engineered mutation	UNP Q92905
E	151	ASN	ASP	engineered mutation	UNP Q92905

- Molecule 6 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	275	Total	C	N	O	S	0	0
			2201	1407	366	415	13		

- Molecule 7 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	213	Total	C	N	O	S	0	0
			1687	1070	287	324	6		

- Molecule 8 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	172	Total	C	N	O	S	0	0
			1374	880	239	251	4		

- Molecule 9 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	76	Total	C	N	O	S	0	0
			599	378	104	115	2		

- Molecule 10 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	427	Total	C	N	O	S	0	0
			3451	2176	608	648	19		

- Molecule 11 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	82	Total	C	N	O	S	0	0
			693	443	127	114	9		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	K	3	Total	Zn	0
			3	3	

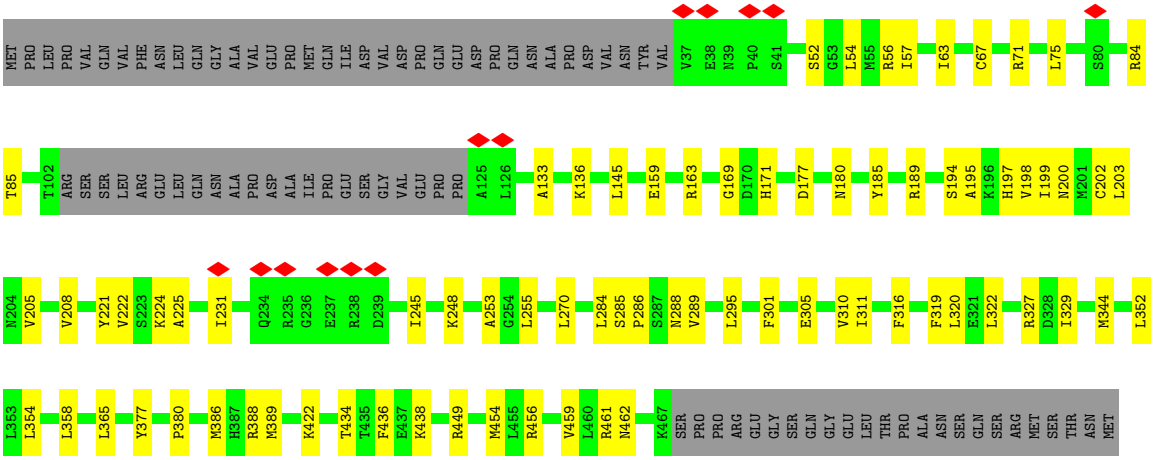
3 Residue-property plots (i)

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: COP9 signalosome complex subunit 1

Chain A:

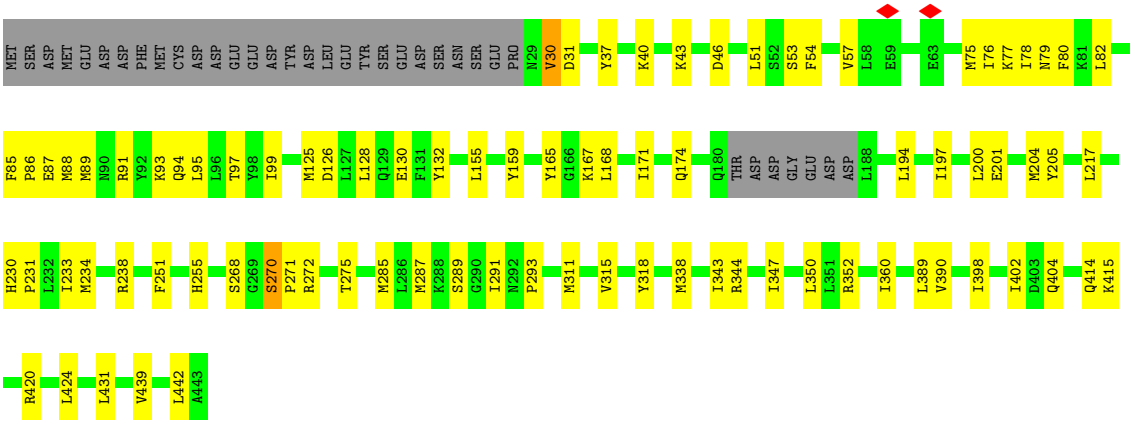




- Molecule 2: COP9 signalosome complex subunit 2

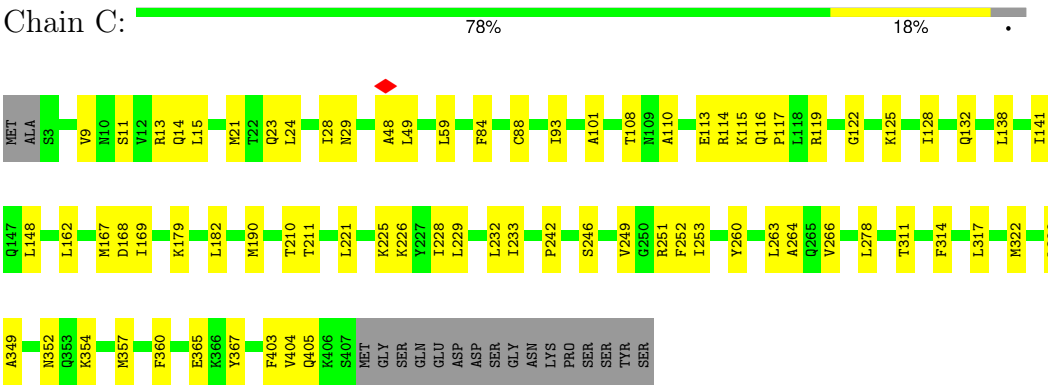
Chain B:





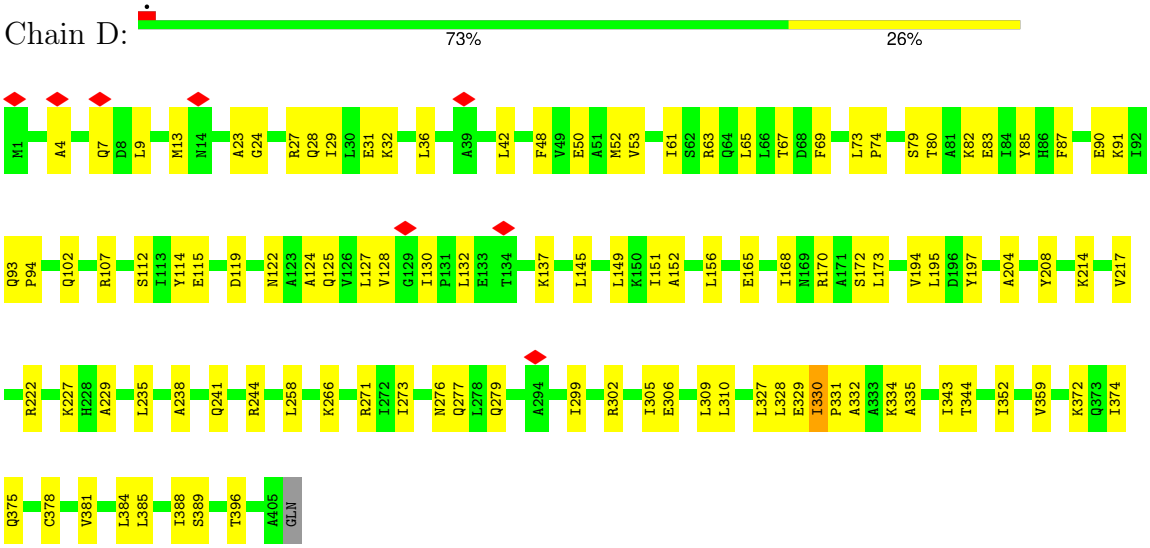
- Molecule 3: COP9 signalosome complex subunit 3

Chain C:



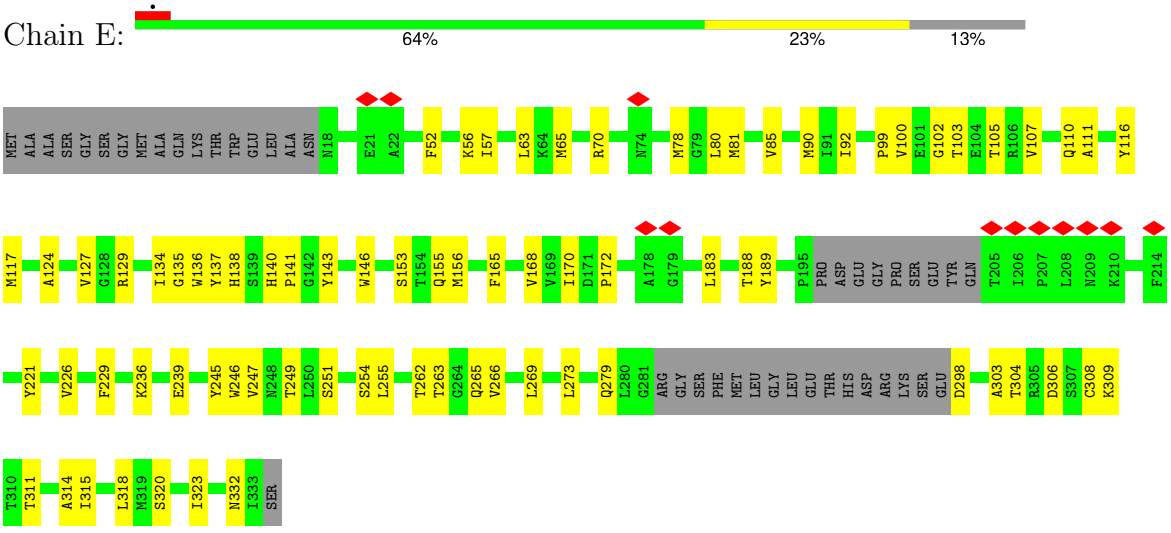
• Molecule 4: COP9 signalosome complex subunit 4

Chain D:



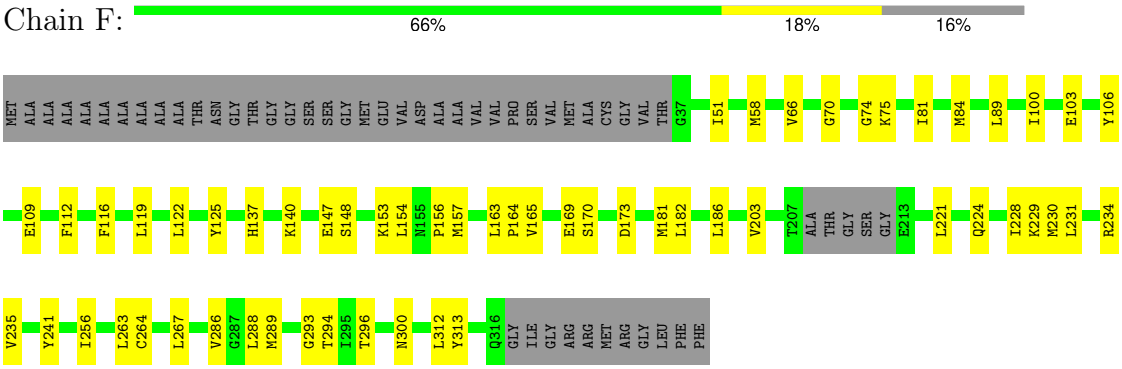
• Molecule 5: COP9 signalosome complex subunit 5

Chain E:



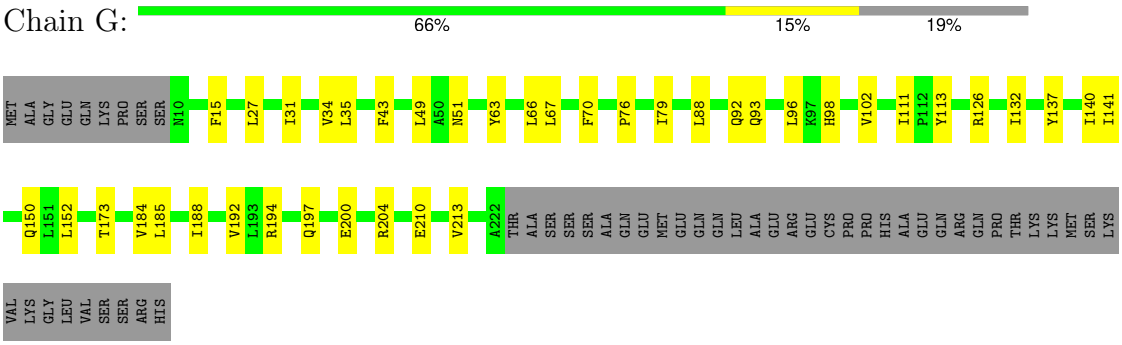
• Molecule 6: COP9 signalosome complex subunit 6

Chain F:



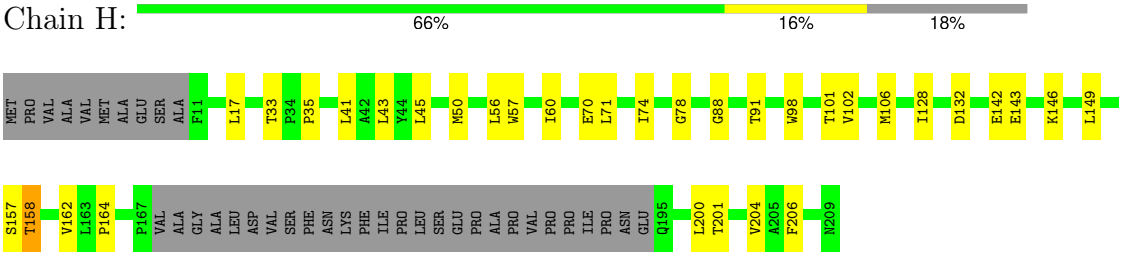
• Molecule 7: COP9 signalosome complex subunit 7b

Chain G:



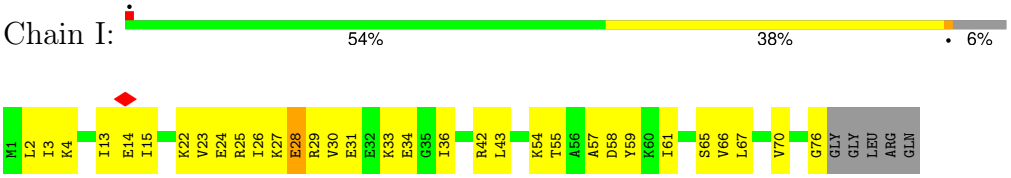
• Molecule 8: COP9 signalosome complex subunit 8

Chain H:



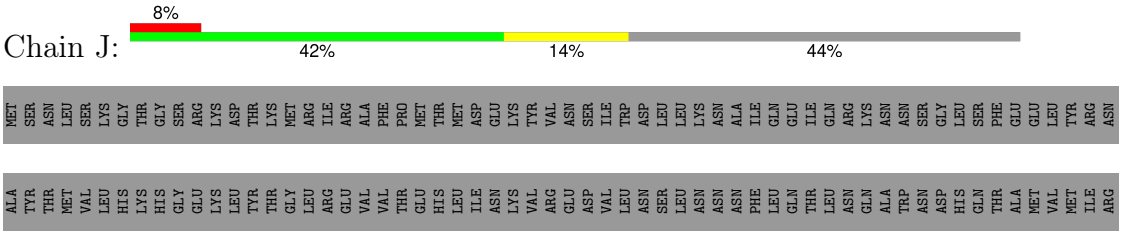
• Molecule 9: NEDD8

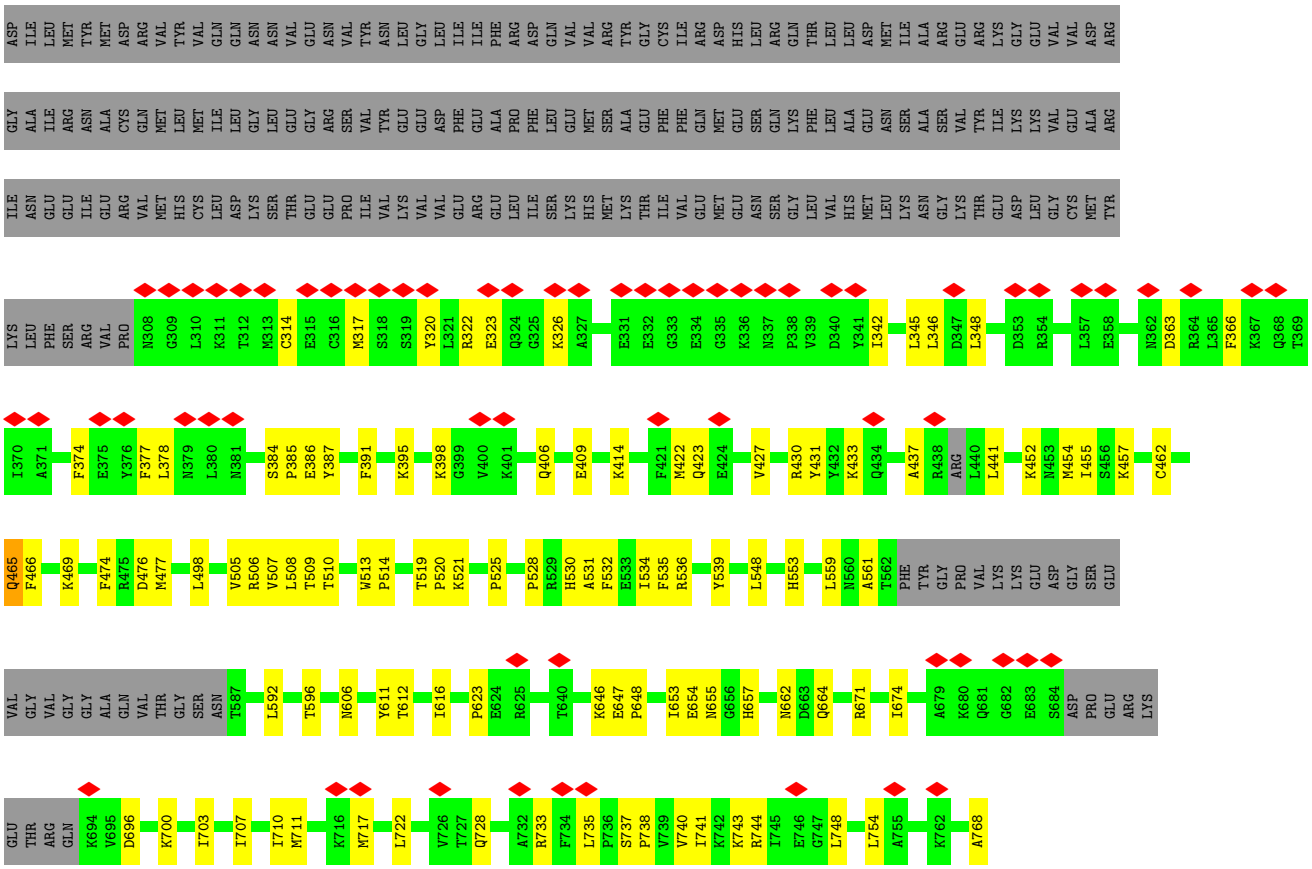
Chain I:



• Molecule 10: Cullin-3

Chain J:

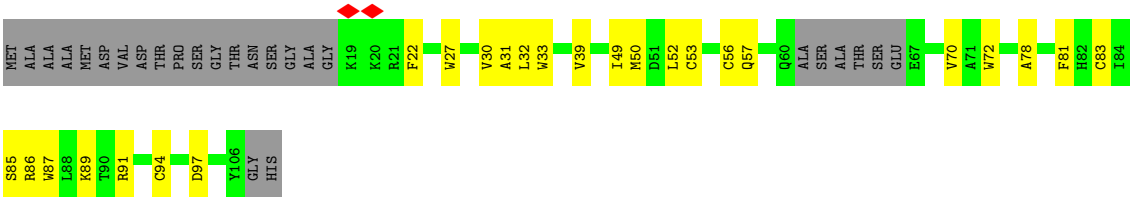




• Molecule 11: E3 ubiquitin-protein ligase RBX1

Chain K:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	308367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.371	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	354.0, 354.0, 354.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.885, 0.885, 0.885	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.11	0/3324	0.31	0/4478
2	B	0.12	0/3399	0.37	0/4571
3	C	0.11	0/3281	0.33	0/4431
4	D	0.11	0/3293	0.33	0/4448
5	E	0.12	0/2356	0.34	0/3181
6	F	0.12	0/2247	0.31	0/3044
7	G	0.10	0/1707	0.25	0/2309
8	H	0.14	0/1407	0.37	0/1912
9	I	0.19	0/604	0.49	0/808
10	J	0.13	0/3506	0.37	0/4706
11	K	0.14	0/713	0.41	0/965
All	All	0.12	0/25837	0.34	0/34853

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

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	3271	0	3309	49	0
2	B	3342	0	3397	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3222	0	3243	49	0
4	D	3241	0	3245	68	0
5	E	2309	0	2300	66	0
6	F	2201	0	2182	47	0
7	G	1687	0	1730	29	0
8	H	1374	0	1360	22	0
9	I	599	0	638	25	0
10	J	3451	0	3483	77	0
11	K	693	0	655	24	0
12	K	3	0	0	0	0
All	All	25393	0	25542	461	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 9.

The worst 5 of 461 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)
11:K:94:CYS:HB3	11:K:97:ASP:OD1	1.70	0.91
11:K:52:LEU:O	11:K:53:CYS:SG	2.39	0.81
9:I:61:ILE:HG23	9:I:65:SER:HB3	1.62	0.80
3:C:352:ASN:HB3	3:C:357:MET:HB2	1.64	0.78
11:K:52:LEU:HB3	11:K:56:CYS:HB2	1.66	0.76

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	405/491 (82%)	387 (96%)	17 (4%)	1 (0%)	43 75
2	B	404/443 (91%)	366 (91%)	34 (8%)	4 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	403/423 (95%)	381 (94%)	20 (5%)	2 (0%)	24	60
4	D	403/406 (99%)	378 (94%)	22 (6%)	3 (1%)	18	53
5	E	285/334 (85%)	262 (92%)	23 (8%)	0	100	100
6	F	271/327 (83%)	256 (94%)	15 (6%)	0	100	100
7	G	211/264 (80%)	206 (98%)	5 (2%)	0	100	100
8	H	168/209 (80%)	166 (99%)	1 (1%)	1 (1%)	21	56
9	I	74/81 (91%)	68 (92%)	6 (8%)	0	100	100
10	J	419/768 (55%)	376 (90%)	40 (10%)	3 (1%)	18	53
11	K	78/108 (72%)	72 (92%)	6 (8%)	0	100	100
All	All	3121/3854 (81%)	2918 (94%)	189 (6%)	14 (0%)	31	65

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	30	VAL
2	B	270	SER
3	C	404	VAL
4	D	332	ALA
2	B	442	LEU

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	356/429 (83%)	356 (100%)	0	100	100
2	B	371/405 (92%)	371 (100%)	0	100	100
3	C	362/377 (96%)	362 (100%)	0	100	100
4	D	346/347 (100%)	346 (100%)	0	100	100
5	E	248/282 (88%)	248 (100%)	0	100	100
6	F	246/276 (89%)	246 (100%)	0	100	100
7	G	185/229 (81%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	143/173 (83%)	143 (100%)	0	100 100
9	I	66/69 (96%)	64 (97%)	2 (3%)	36 57
10	J	383/693 (55%)	383 (100%)	0	100 100
11	K	74/90 (82%)	74 (100%)	0	100 100
All	All	2780/3370 (82%)	2778 (100%)	2 (0%)	87 90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	2	LEU
9	I	28	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	53	GLN
8	H	51	ASN
8	H	39	GLN
10	J	423	GLN
2	B	406	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.

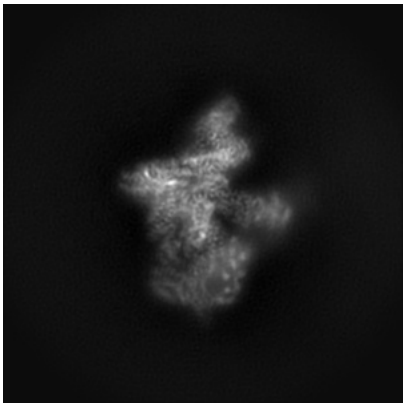
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47990. These allow visual inspection of the internal detail of the map and identification of artifacts.

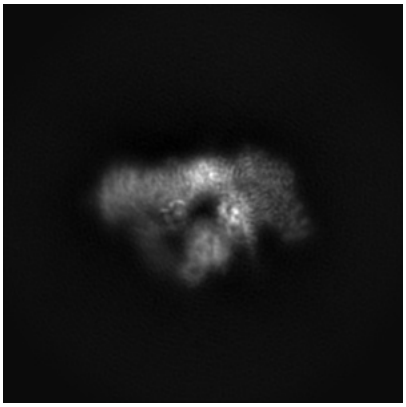
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

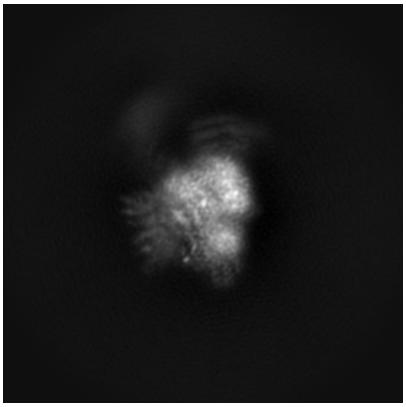
6.1.1 Primary map



X



Y

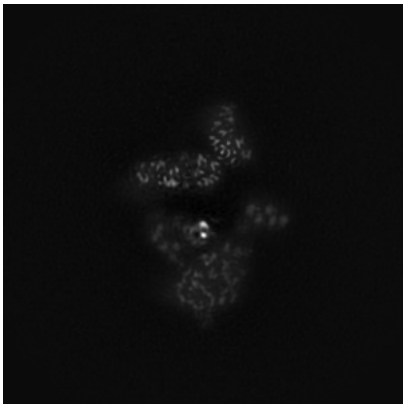


Z

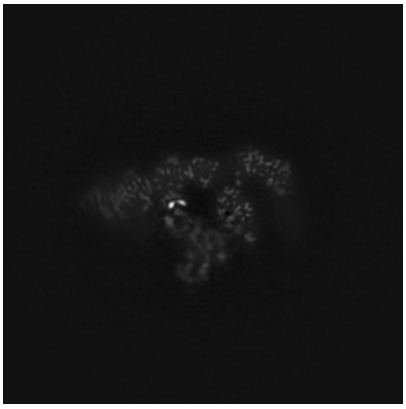
The images above show the map projected in three orthogonal directions.

6.2 Central slices

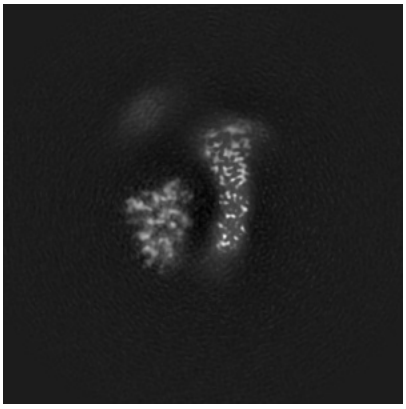
6.2.1 Primary map



X Index: 200



Y Index: 200

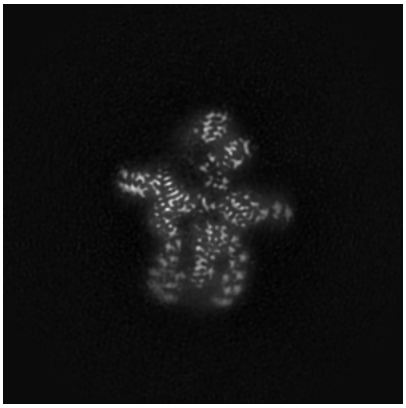


Z Index: 200

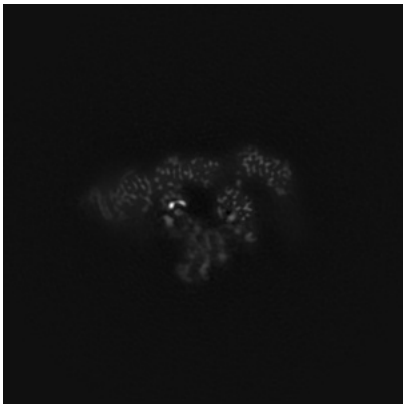
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

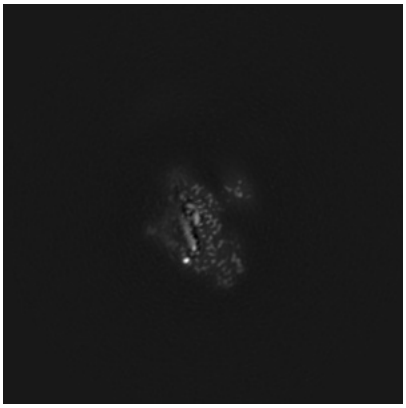
6.3.1 Primary map



X Index: 222



Y Index: 199

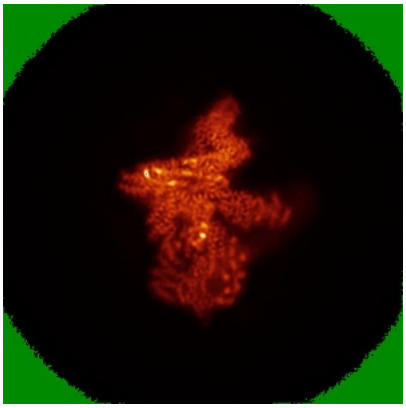


Z Index: 230

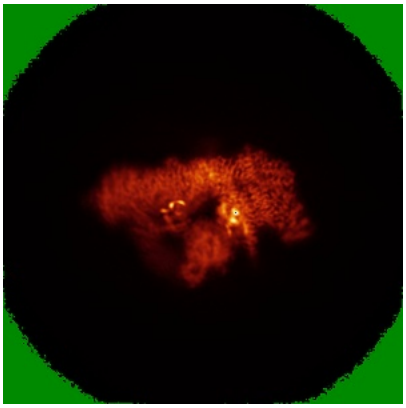
The images above show the largest variance slices of the map in three orthogonal directions.

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

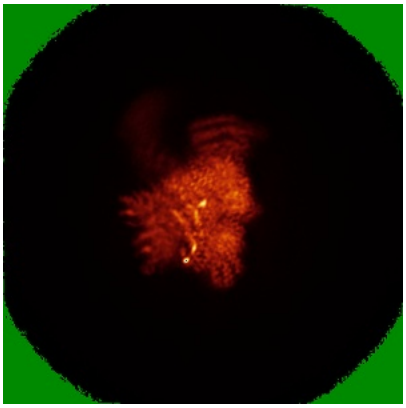
6.4.1 Primary map



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

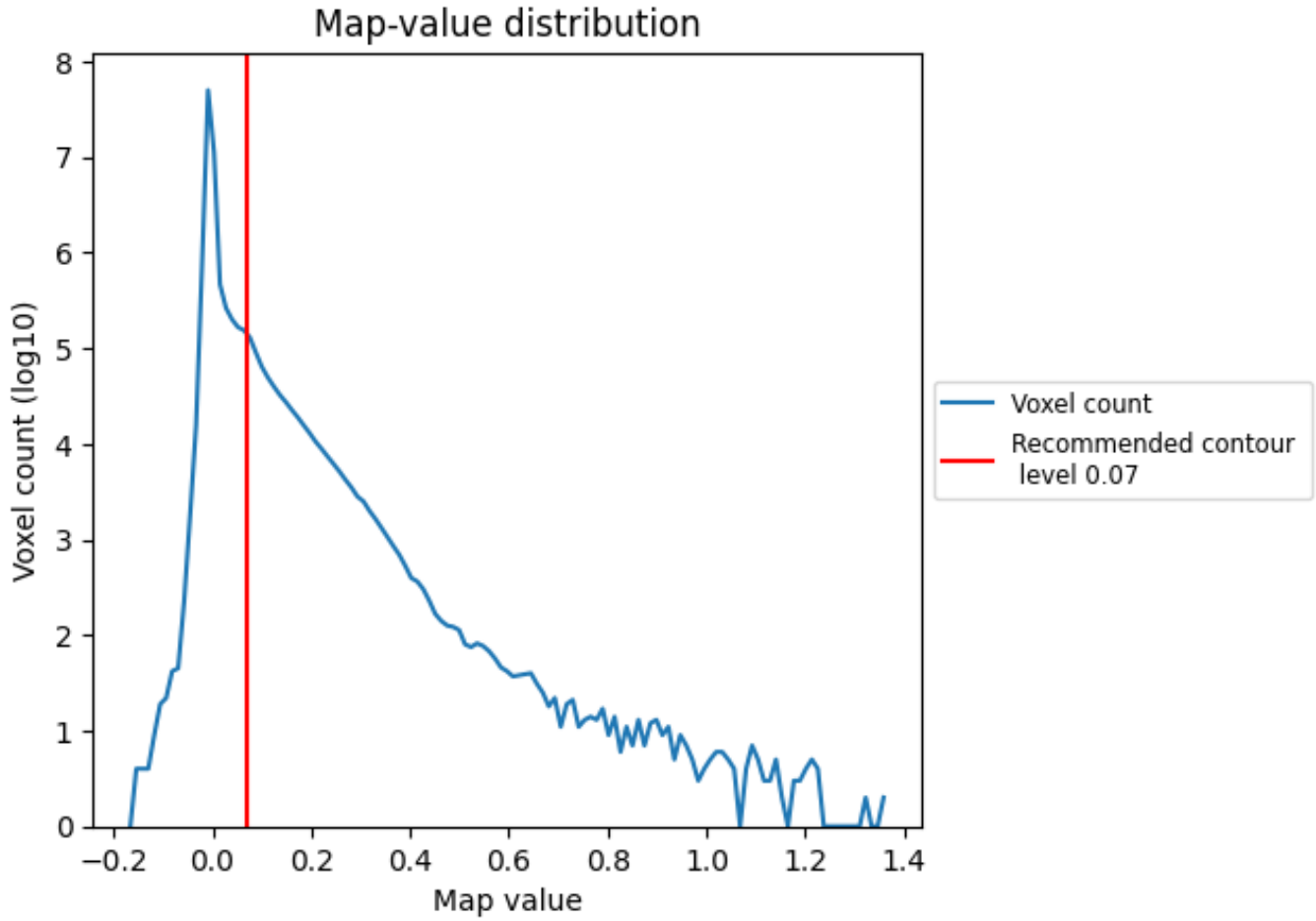
6.6 Mask visualisation (i)

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

7 Map analysis

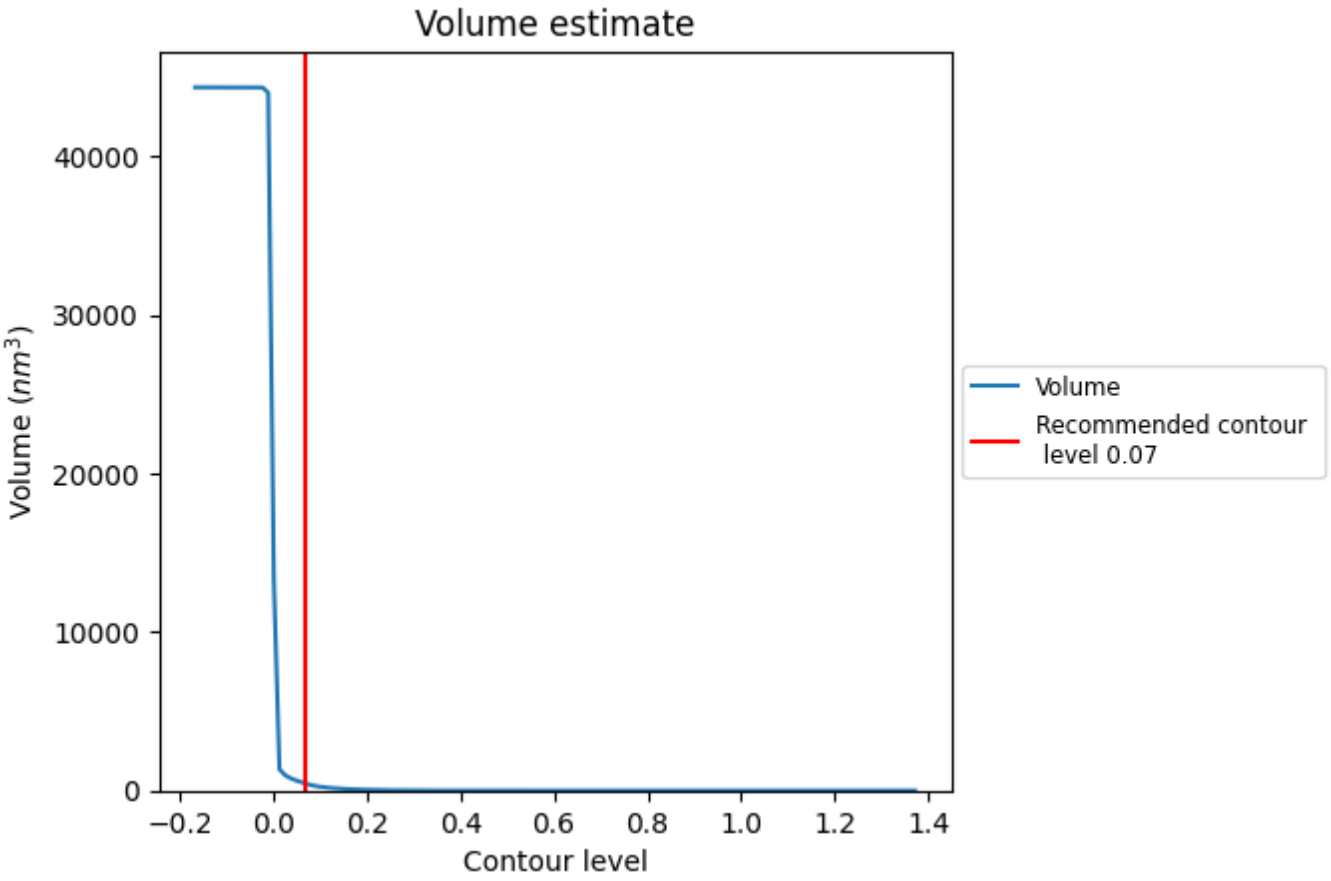
This section contains the results of statistical analysis of the map.

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.

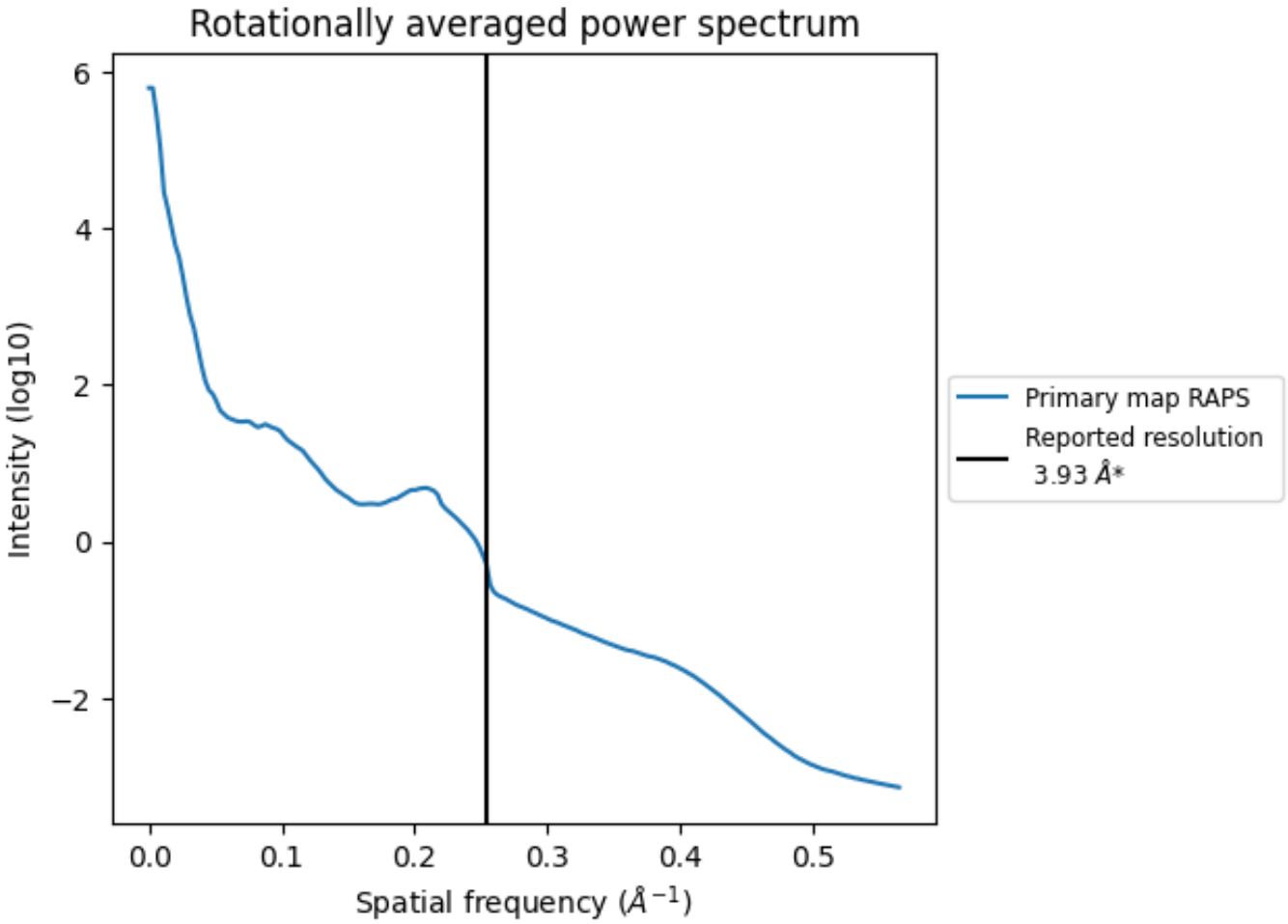
7.2 Volume estimate (i)



The volume at the recommended contour level is 443 nm^3; this corresponds to an approximate mass of 400 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 0.254 Å^{-1}

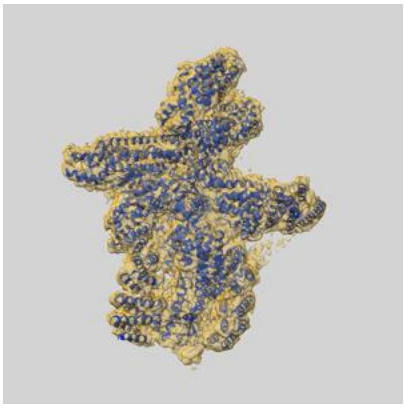
8 Fourier-Shell correlation (i)

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

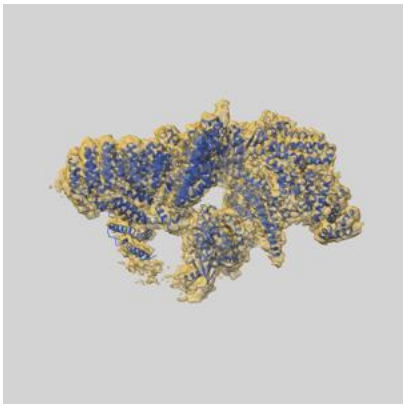
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47990 and PDB model 9EGL. Per-residue inclusion information can be found in section 3 on page 6.

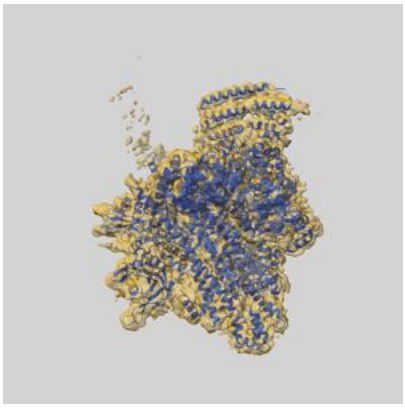
9.1 Map-model overlay



X



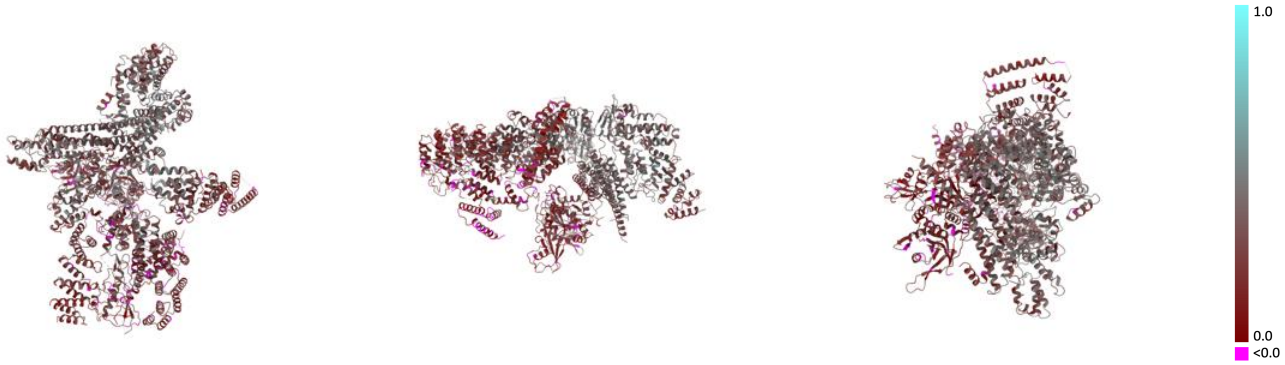
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

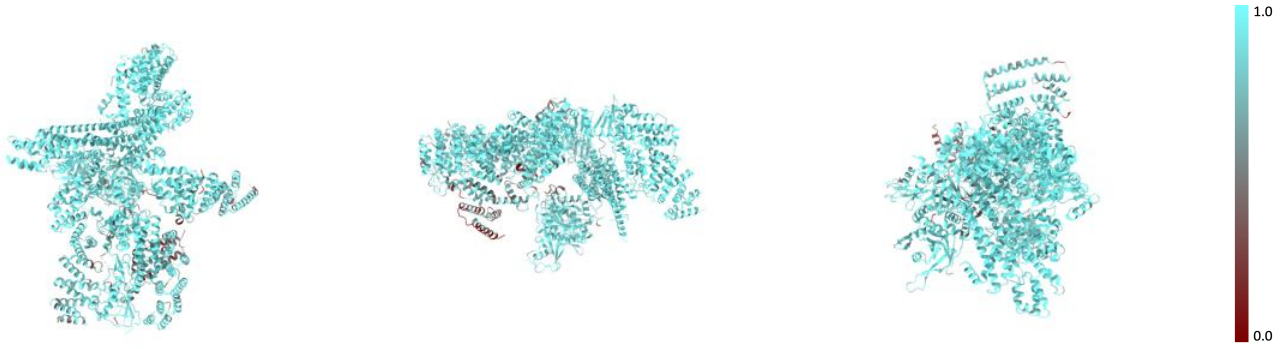
9.2 Q-score mapped to coordinate model



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.

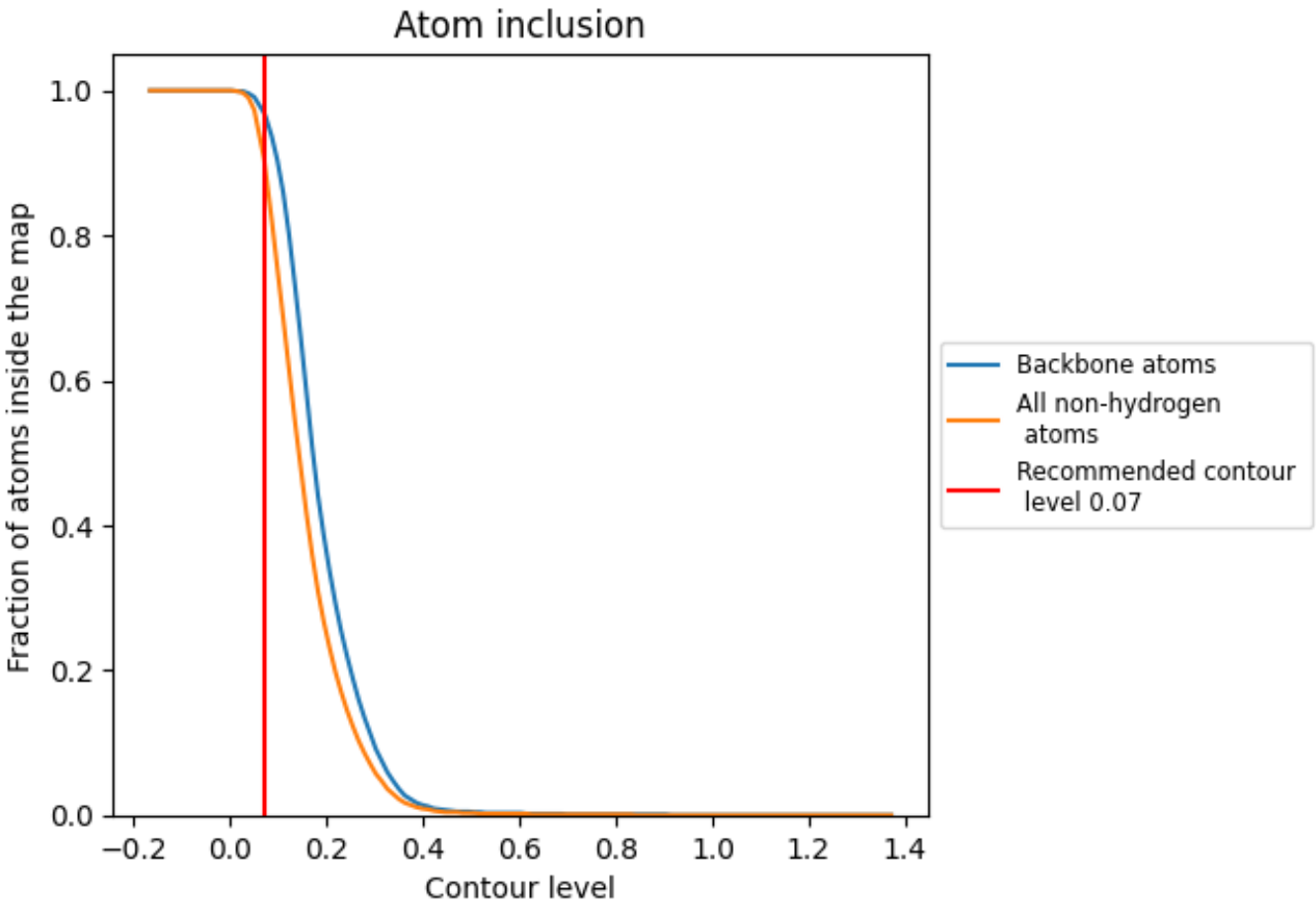
9.3 Atom inclusion mapped to coordinate model



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.2830
A	0.8900	0.2990
B	0.9410	0.3000
C	0.9580	0.3870
D	0.9120	0.2810
E	0.9010	0.2000
F	0.9540	0.2520
G	0.9580	0.3670
H	0.9550	0.3770
I	0.8900	0.1800
J	0.7560	0.1730
K	0.9250	0.2530

