



wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 11:55 pm GMT

PDB ID : 6R7F
EMDB ID : EMD-4739
Title : Structural basis of Cullin-2 RING E3 ligase regulation by the COP9 signalosome
Authors : Faull, S.V.; Lau, A.M.C.; Martens, C.; Ahdash, Z.; Yebenes, H.; Schmidt, C.; Beuron, F.; Cronin, N.B.; Morris, E.P.; Politis, A.
Deposited on : 2019-03-28
Resolution : 8.20 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

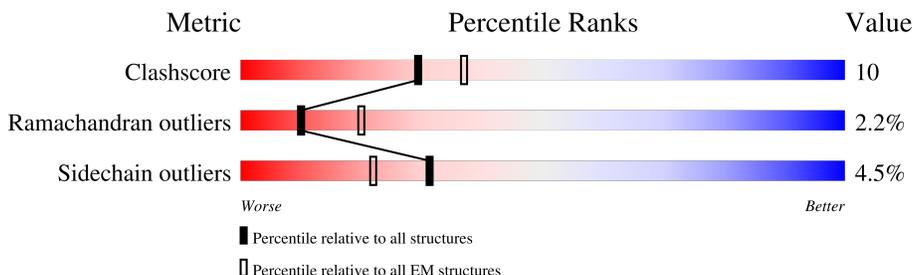
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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.



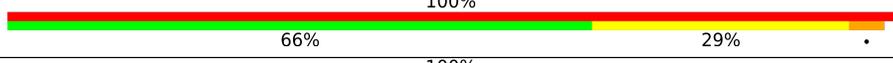
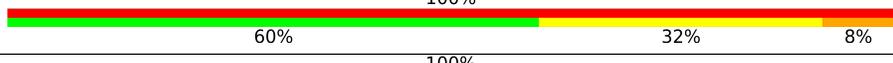
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	433	
2	B	443	
3	C	403	
4	D	406	
5	E	311	
6	F	288	
7	H	209	
8	G	208	

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Mol	Chain	Length	Quality of chain
9	V	160	
10	P	118	
11	Q	112	
12	O	745	
13	R	90	
14	N	76	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 31558 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	433	3450	2174	605	649	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	414	3386	2149	579	643	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	403	3205	2040	537	601	27	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	406	3251	2047	566	622	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	311	2472	1575	412	471	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	288	2280	1452	379	434	15	0	0

- Molecule 7 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	168	1340	859	232	245	4	0	0

- Molecule 8 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	208	1645	1039	279	321	6	0	0

- Molecule 9 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	V	160	1308	824	245	235	4	0	0

- Molecule 10 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	118	921	575	156	185	5	0	0

- Molecule 11 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	112	873	553	139	173	8	0	0

- Molecule 12 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	744	6090	3869	1029	1146	46	0	0

- Molecule 13 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	R	90	746	472	137	128	9	0	0

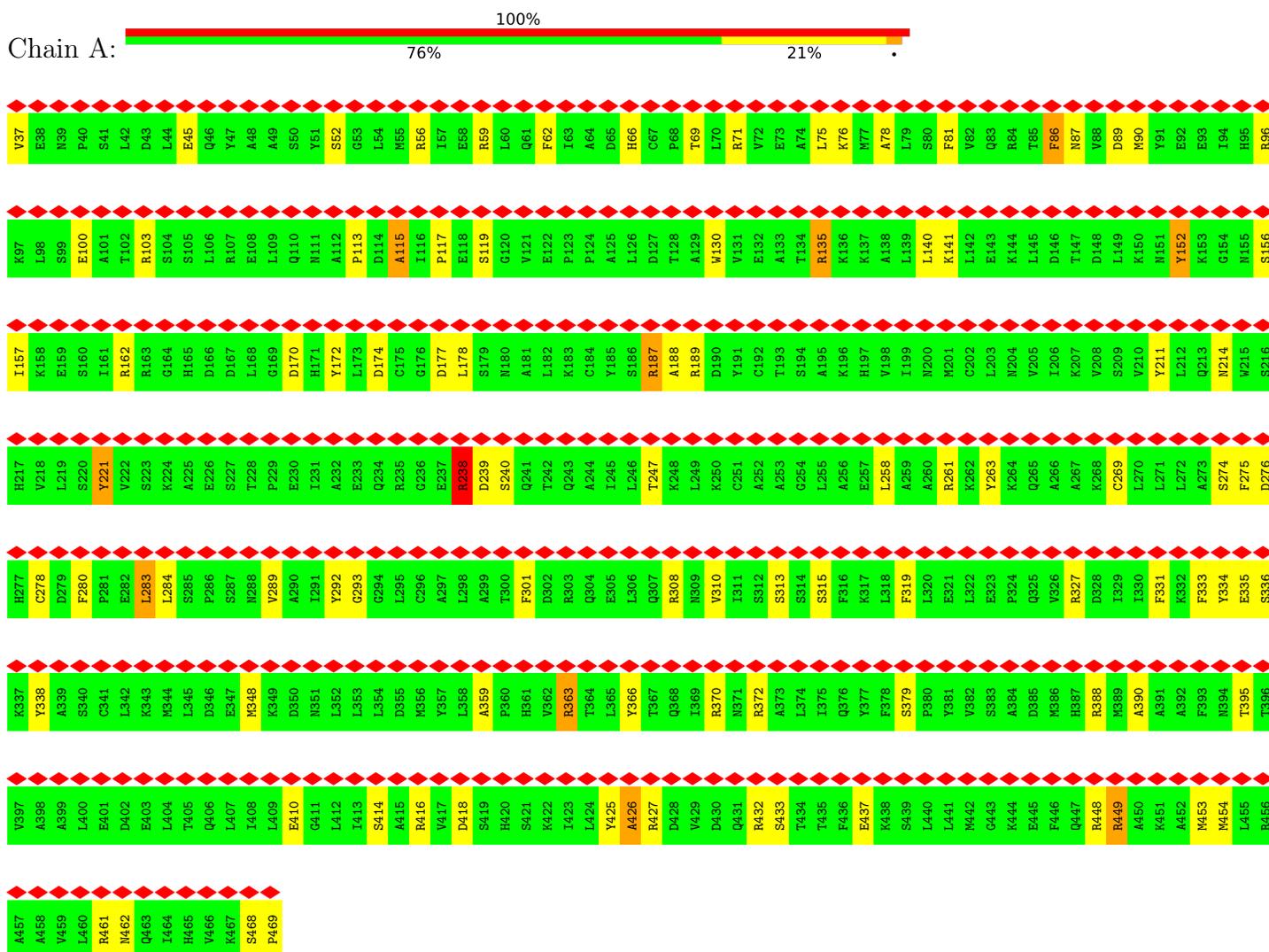
- Molecule 14 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	76	591	372	102	115	2	0	0

3 Residue-property plots

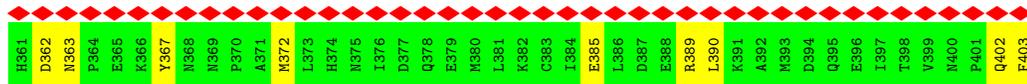
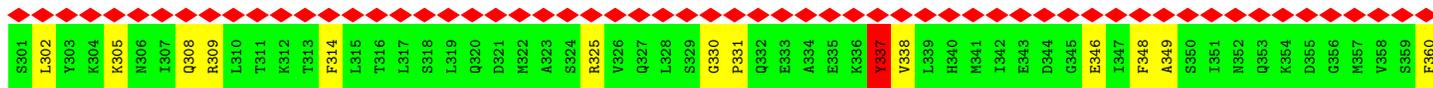
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: COP9 signalosome complex subunit 1

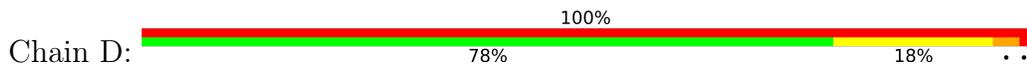


- Molecule 2: COP9 signalosome complex subunit 2





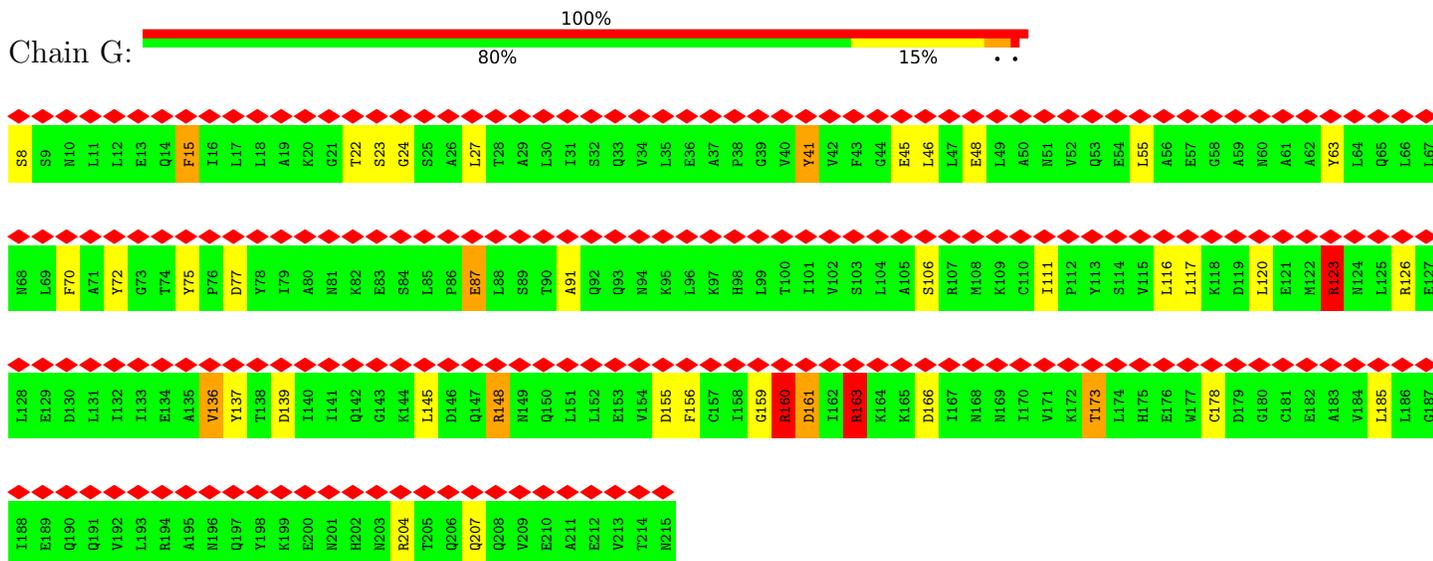
• Molecule 4: COP9 signalosome complex subunit 4



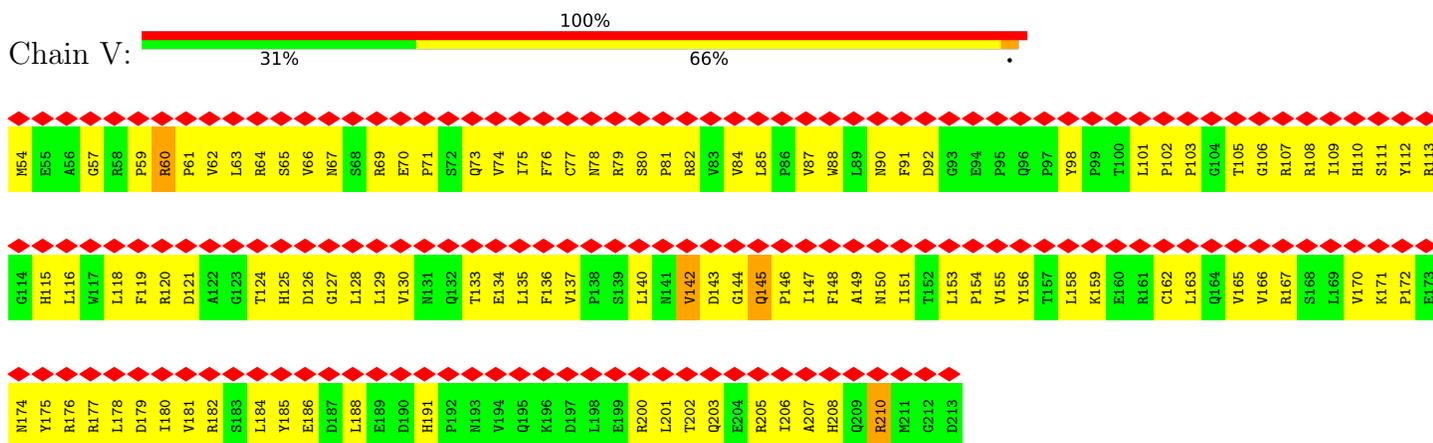
• Molecule 5: COP9 signalosome complex subunit 5



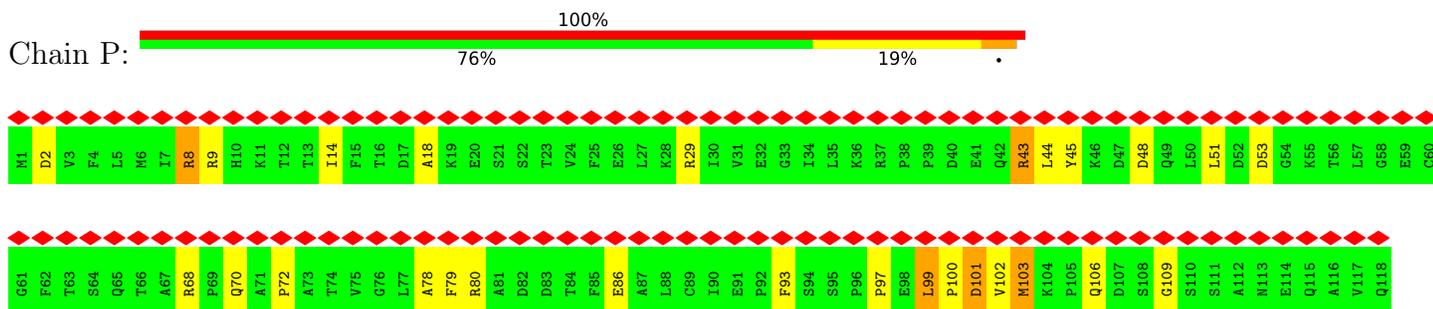
- Molecule 8: COP9 signalosome complex subunit 7b



- Molecule 9: von Hippel-Lindau disease tumor suppressor



- Molecule 10: Elongin-B

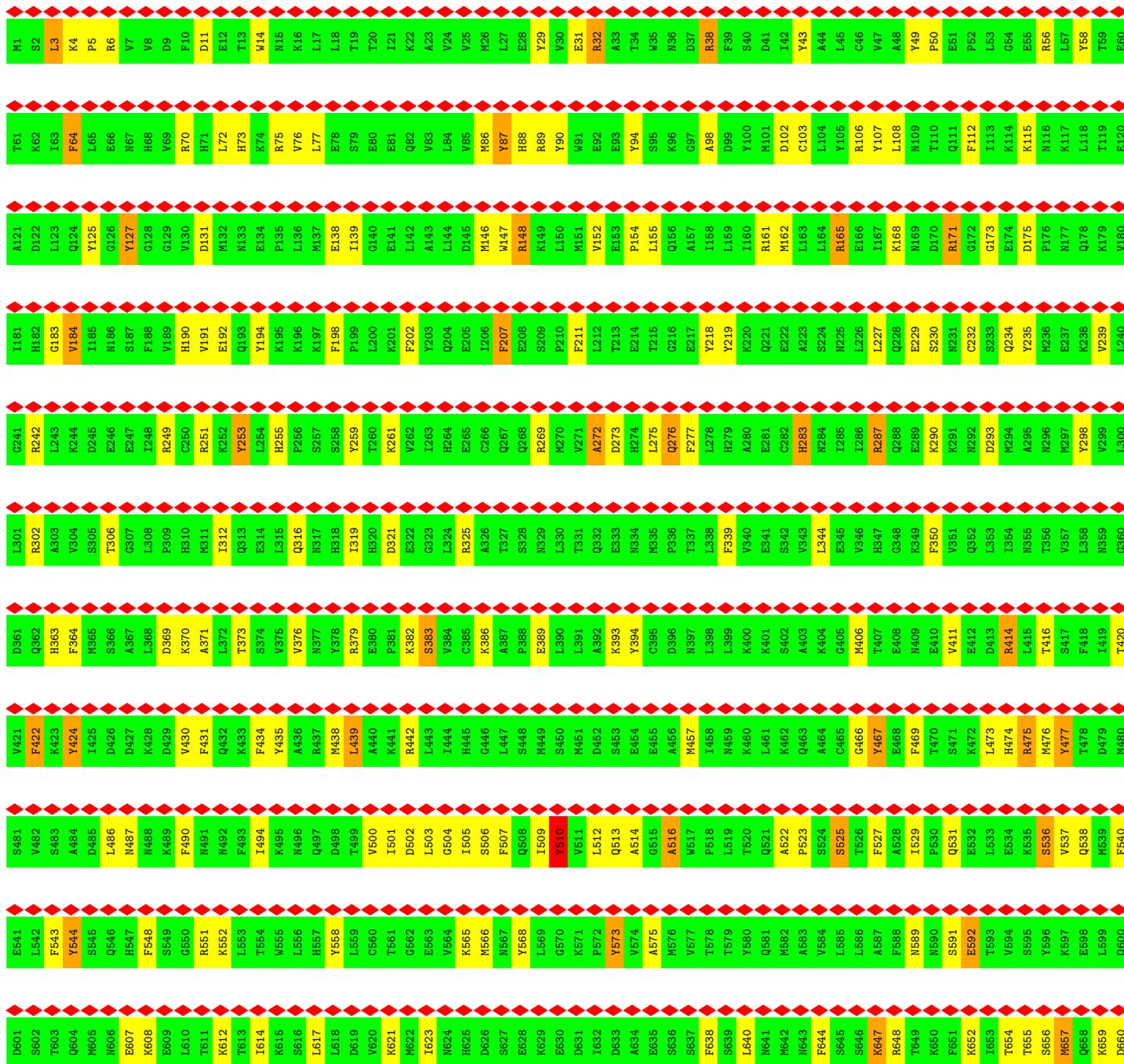


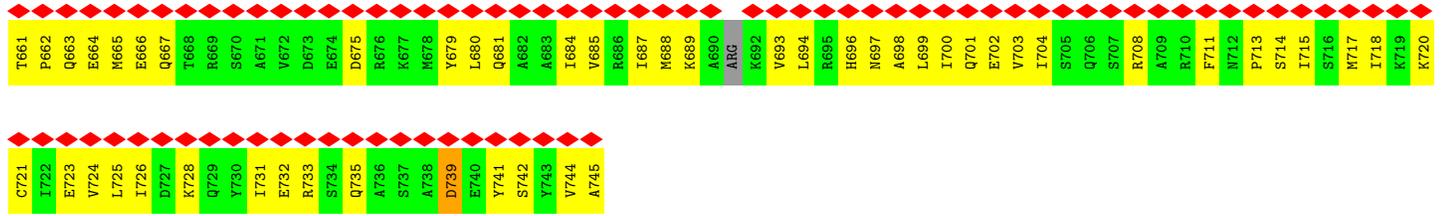
- Molecule 11: Elongin-C



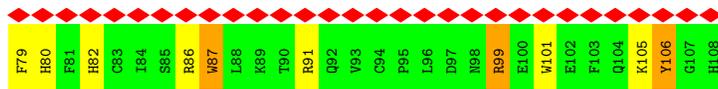
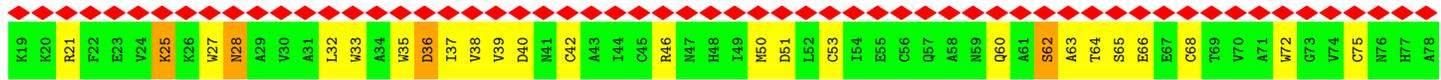


● Molecule 12: Cullin-2

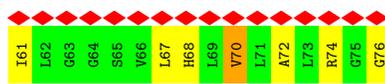
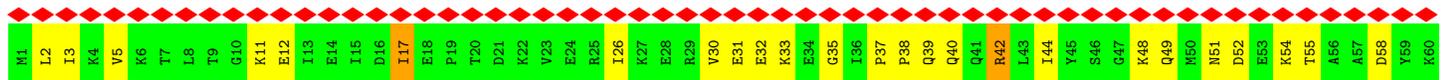




• Molecule 13: E3 ubiquitin-protein ligase RBX1



• Molecule 14: NEDD8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20055	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	17.442	Depositor
Minimum map value	-4.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (\AA)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

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	1.70	38/3509 (1.1%)	1.85	69/4733 (1.5%)
2	B	2.07	30/3444 (0.9%)	1.94	86/4634 (1.9%)
3	C	1.63	20/3264 (0.6%)	1.85	65/4407 (1.5%)
4	D	1.69	31/3303 (0.9%)	1.87	71/4460 (1.6%)
5	E	2.67	31/2526 (1.2%)	1.94	64/3411 (1.9%)
6	F	1.68	15/2327 (0.6%)	1.99	56/3153 (1.8%)
7	H	1.71	14/1372 (1.0%)	1.91	29/1865 (1.6%)
8	G	1.60	7/1665 (0.4%)	1.90	30/2253 (1.3%)
9	V	1.05	0/1341	1.07	0/1824
10	P	1.75	8/938 (0.9%)	1.93	21/1267 (1.7%)
11	Q	1.72	8/892 (0.9%)	1.82	19/1204 (1.6%)
12	O	1.60	37/6207 (0.6%)	1.84	131/8358 (1.6%)
13	R	2.63	12/768 (1.6%)	1.93	20/1040 (1.9%)
14	N	0.36	0/596	0.56	0/800
All	All	1.80	251/32152 (0.8%)	1.84	661/43409 (1.5%)

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	12
2	B	0	15
3	C	0	6
4	D	0	10
5	E	0	10
6	F	0	7
7	H	0	7
8	G	0	9
10	P	0	2
11	Q	0	5
12	O	0	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	R	0	2
All	All	0	102

The worst 5 of 251 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	309	LYS	CA-CB	85.10	3.41	1.53
2	B	294	PHE	CA-C	70.42	3.36	1.52
5	E	203	TYR	CE1-CZ	26.85	1.73	1.38
5	E	203	TYR	CG-CD2	26.55	1.73	1.39
13	R	106	TYR	CG-CD2	26.45	1.73	1.39

The worst 5 of 661 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	98	TYR	CB-CG-CD2	-18.83	109.70	121.00
6	F	205	ARG	NE-CZ-NH1	-16.75	111.93	120.30
4	D	6	ARG	NE-CZ-NH2	-16.17	112.22	120.30
6	F	45	PRO	N-CA-C	15.86	153.33	112.10
12	O	87	TYR	CB-CG-CD2	-15.76	111.55	121.00

There are no chirality outliers.

5 of 102 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ARG	Sidechain
1	A	152	TYR	Sidechain
1	A	187	ARG	Sidechain
1	A	221	TYR	Sidechain
1	A	66	HIS	Sidechain

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	3450	0	3482	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3386	0	3424	37	0
3	C	3205	0	3225	15	0
4	D	3251	0	3253	13	0
5	E	2472	0	2444	74	0
6	F	2280	0	2263	35	0
7	H	1340	0	1324	2	0
8	G	1645	0	1667	3	0
9	V	1308	0	1299	327	0
10	P	921	0	908	92	0
11	Q	873	0	845	90	0
12	O	6090	0	6071	181	0
13	R	746	0	705	29	0
14	N	591	0	616	45	0
All	All	31558	0	31526	644	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 644 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)
9:V:178:LEU:CD2	10:P:103:MET:HG3	1.06	1.53
9:V:171:LYS:NZ	10:P:106:GLN:CB	1.70	1.52
9:V:178:LEU:CD2	10:P:103:MET:CG	1.75	1.50
9:V:178:LEU:HD21	10:P:103:MET:CG	1.27	1.50
9:V:178:LEU:HD13	10:P:103:MET:CE	1.32	1.50

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	431/433 (100%)	399 (93%)	26 (6%)	6 (1%)	11	46
2	B	412/443 (93%)	364 (88%)	33 (8%)	15 (4%)	3	25
3	C	401/403 (100%)	361 (90%)	26 (6%)	14 (4%)	3	25
4	D	404/406 (100%)	387 (96%)	8 (2%)	9 (2%)	6	35
5	E	309/311 (99%)	290 (94%)	15 (5%)	4 (1%)	12	48
6	F	286/288 (99%)	272 (95%)	8 (3%)	6 (2%)	7	36
7	H	164/209 (78%)	158 (96%)	5 (3%)	1 (1%)	25	66
8	G	206/208 (99%)	189 (92%)	13 (6%)	4 (2%)	8	38
9	V	158/160 (99%)	154 (98%)	1 (1%)	3 (2%)	8	38
10	P	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
11	Q	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
12	O	738/745 (99%)	691 (94%)	29 (4%)	18 (2%)	6	33
13	R	88/90 (98%)	70 (80%)	13 (15%)	5 (6%)	1	18
14	N	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
All	All	3897/4002 (97%)	3617 (93%)	195 (5%)	85 (2%)	10	35

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ALA
1	A	426	ALA
2	B	61	GLU
2	B	141	ASP
2	B	186	ASP

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	377/377 (100%)	363 (96%)	14 (4%)	34	58
2	B	376/405 (93%)	356 (95%)	20 (5%)	22	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	359/359 (100%)	348 (97%)	11 (3%)	40	62
4	D	347/347 (100%)	342 (99%)	5 (1%)	67	80
5	E	267/267 (100%)	250 (94%)	17 (6%)	17	42
6	F	255/255 (100%)	237 (93%)	18 (7%)	14	39
7	H	139/173 (80%)	133 (96%)	6 (4%)	29	53
8	G	181/181 (100%)	171 (94%)	10 (6%)	21	47
9	V	147/147 (100%)	145 (99%)	2 (1%)	67	80
10	P	103/103 (100%)	99 (96%)	4 (4%)	32	56
11	Q	96/96 (100%)	95 (99%)	1 (1%)	76	86
12	O	680/681 (100%)	644 (95%)	36 (5%)	22	47
13	R	79/79 (100%)	70 (89%)	9 (11%)	5	21
14	N	64/66 (97%)	60 (94%)	4 (6%)	18	43
All	All	3470/3536 (98%)	3313 (96%)	157 (4%)	31	52

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	O	131	ASP
12	O	657	MET
12	O	175	ASP
12	O	420	THR
13	R	82	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
11	Q	108	ASN
12	O	310	HIS
14	N	41	GLN
12	O	73	HIS
12	O	190	HIS

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
12	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	654:THR	C	655:THR	N	4.12

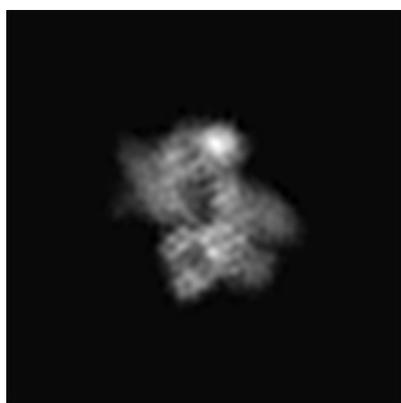
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4739. These allow visual inspection of the internal detail of the map and identification of artifacts.

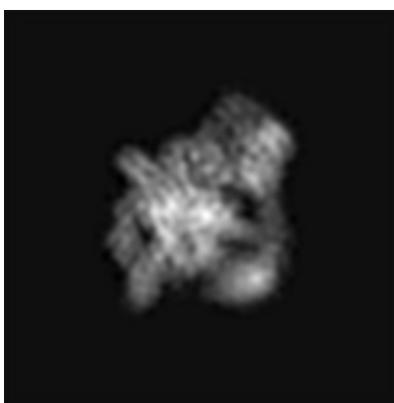
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

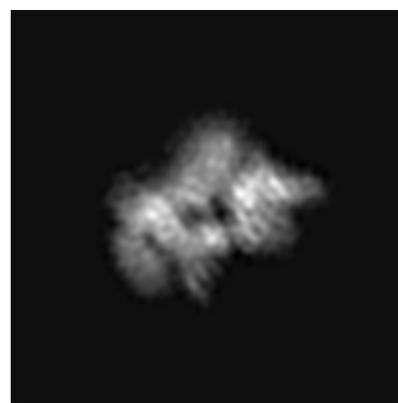
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

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

6.3 Largest variance slices [i](#)

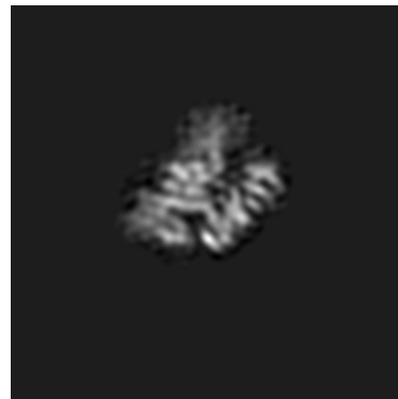
6.3.1 Primary map



X Index: 145



Y Index: 160

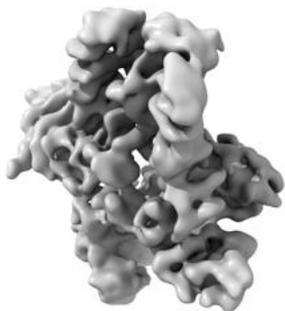


Z Index: 126

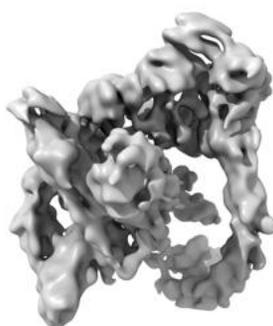
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

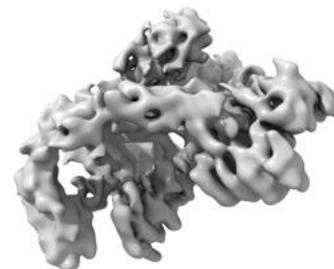
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

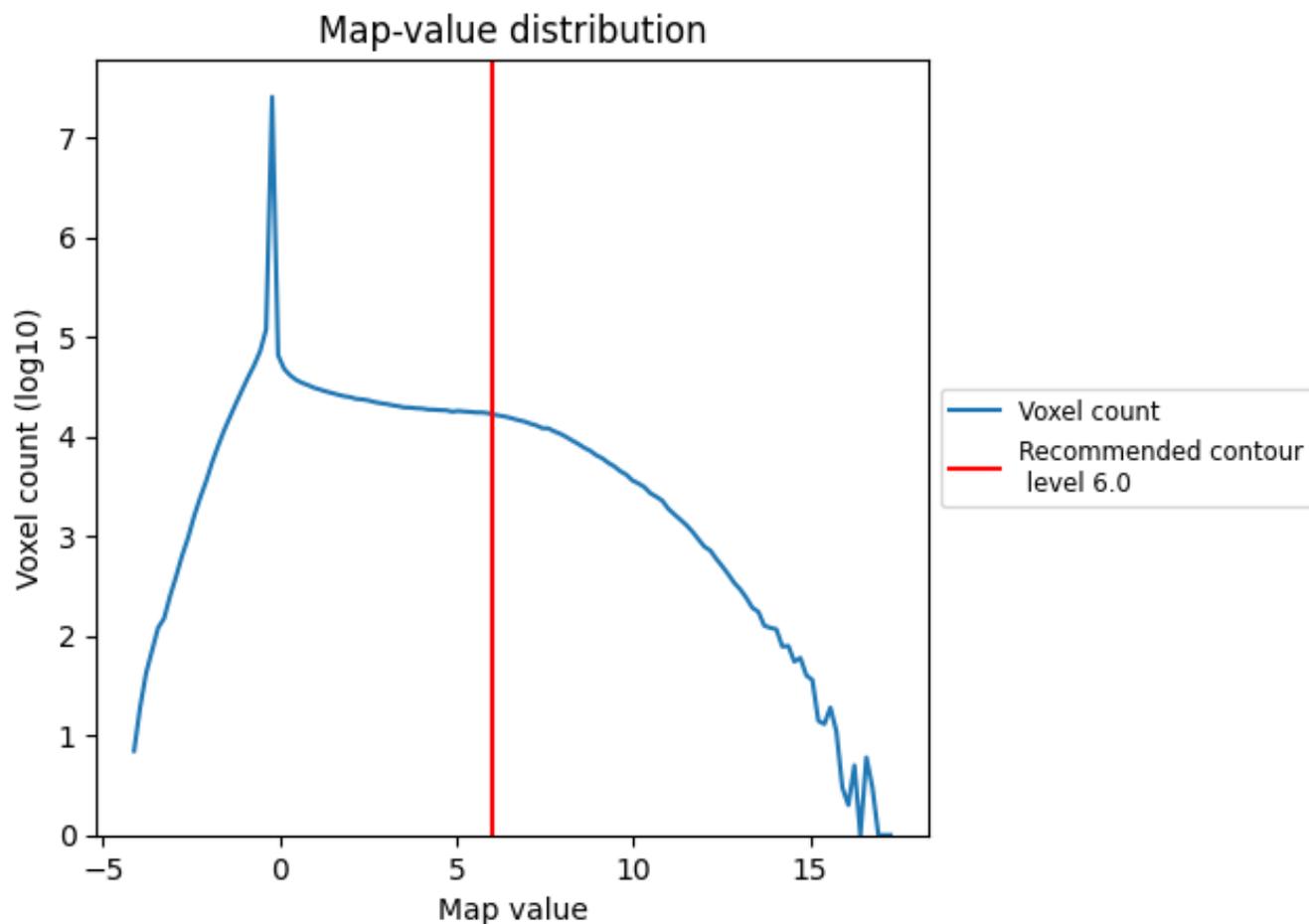
6.5 Mask visualisation

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

7 Map analysis [i](#)

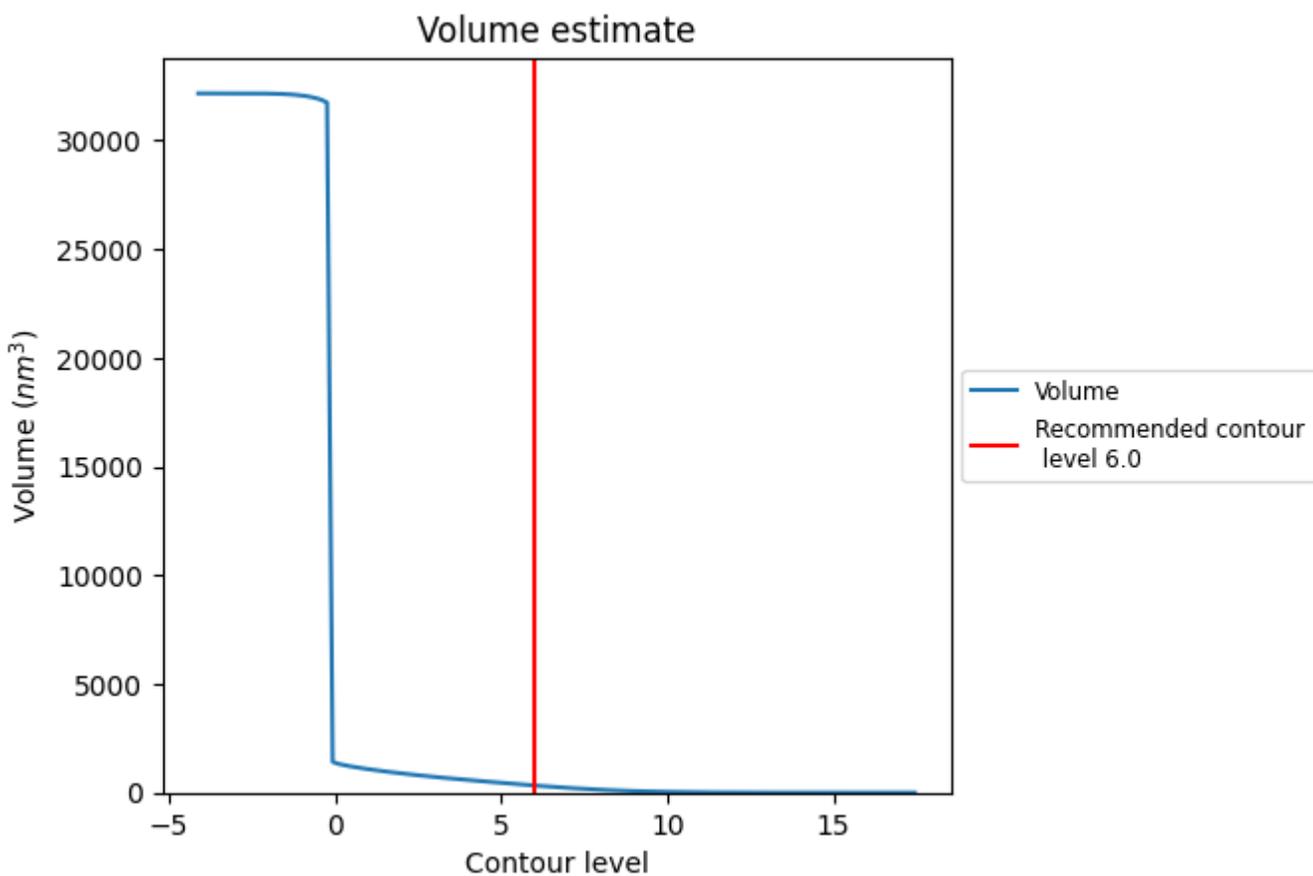
This section contains the results of statistical analysis of the map.

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.

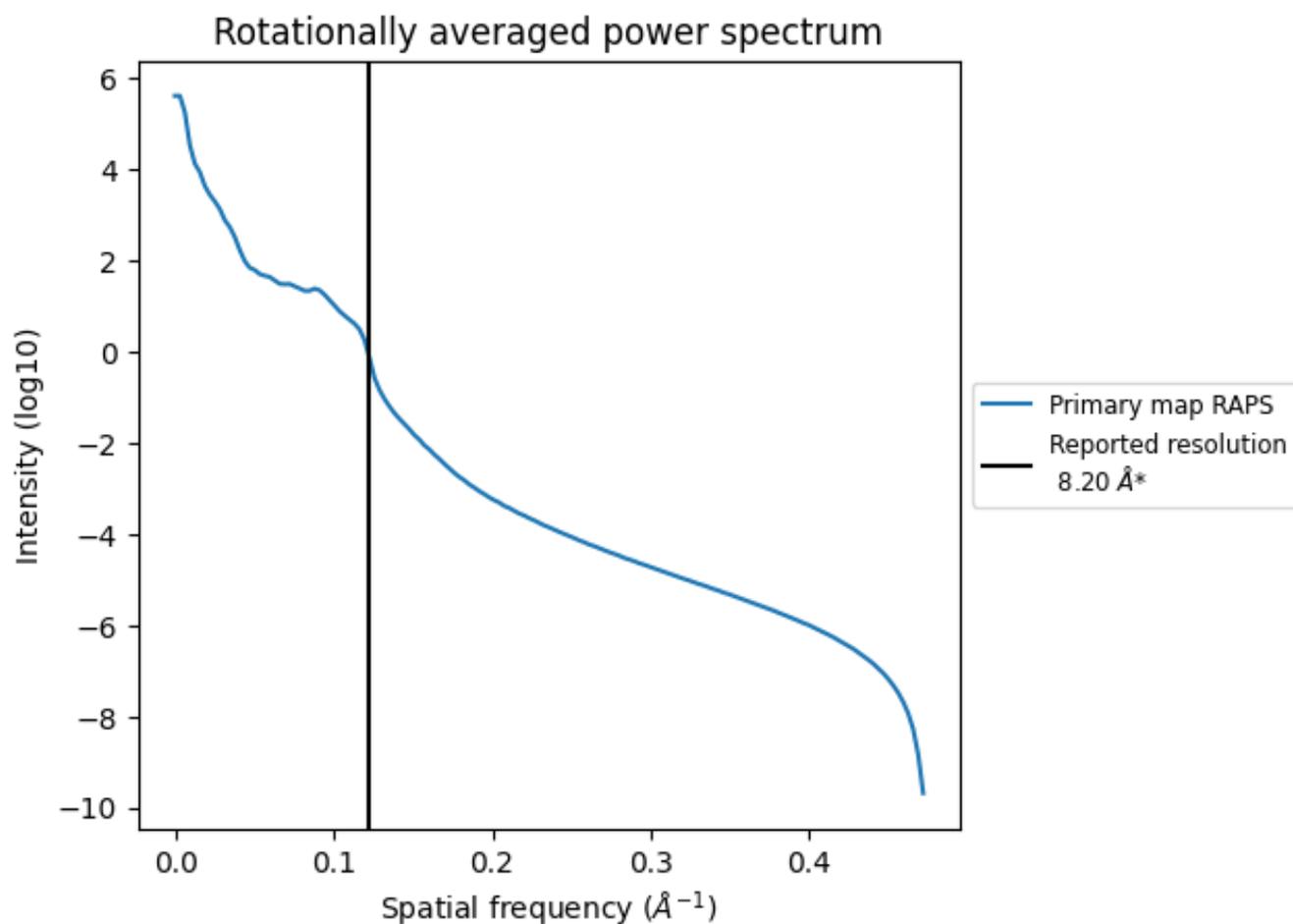
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm³; this corresponds to an approximate mass of 296 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 0.122 Å⁻¹

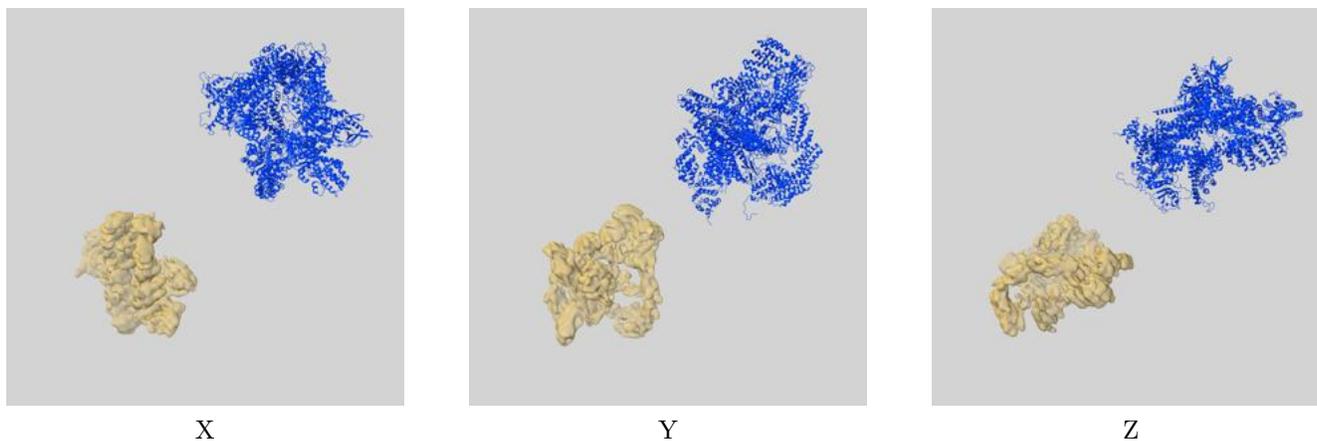
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

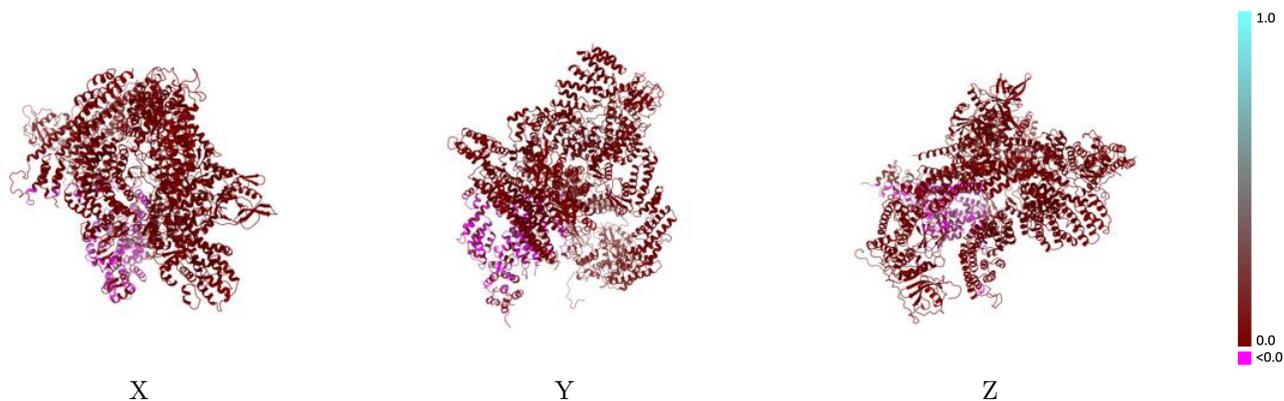
This section contains information regarding the fit between EMDB map EMD-4739 and PDB model 6R7F. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



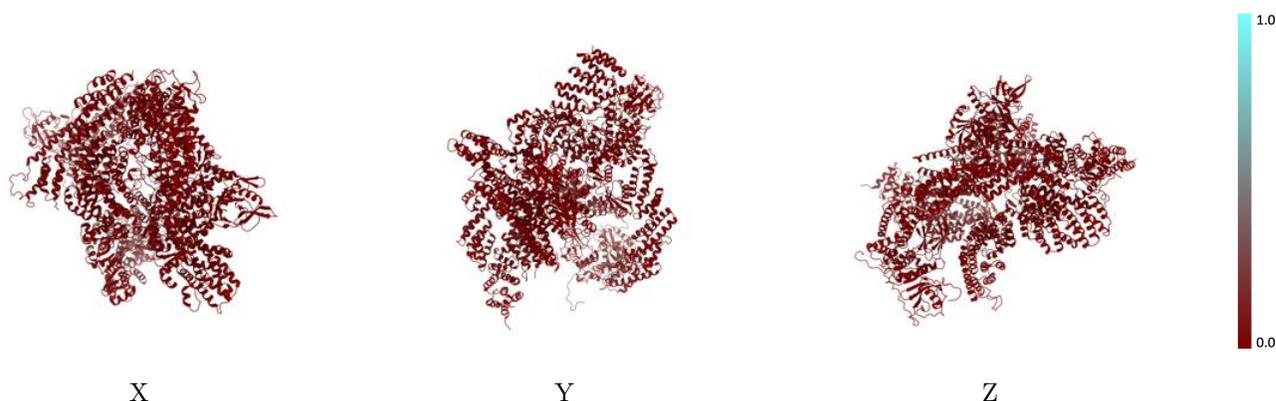
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



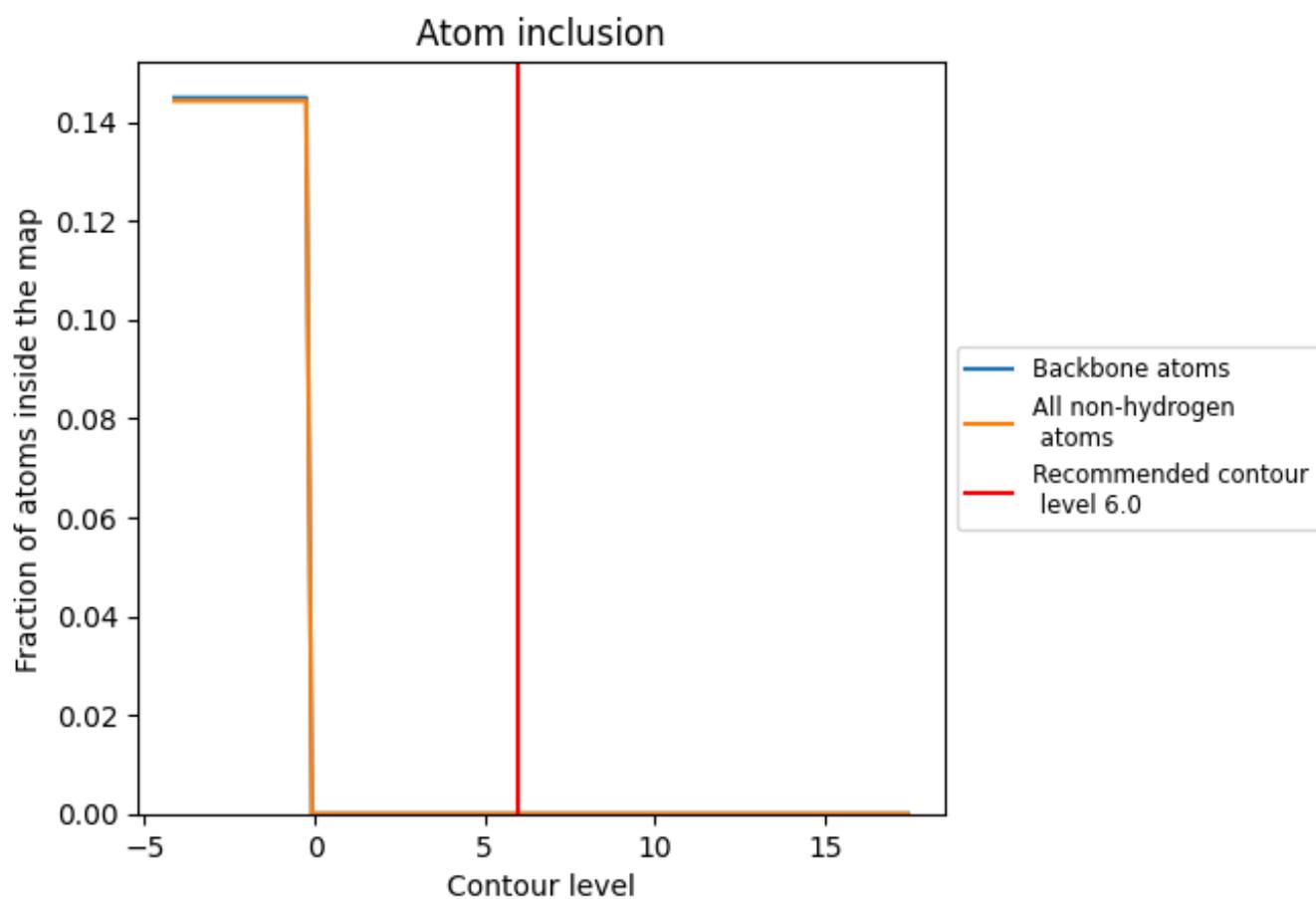
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0000	 0.0010
A	 0.0000	 0.0040
B	 0.0000	 0.0010
C	 0.0000	 0.0040
D	 0.0000	 0.0000
E	 0.0000	 -0.0010
F	 0.0000	 0.0030
G	 0.0000	 0.0000
H	 0.0000	 -0.0030
N	 0.0000	 0.0000
O	 0.0000	 0.0000
P	 0.0000	 0.0060
Q	 0.0000	 0.0000
R	 0.0000	 0.0000
V	 0.0000	 0.0070

