W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 11:54 pm GMT

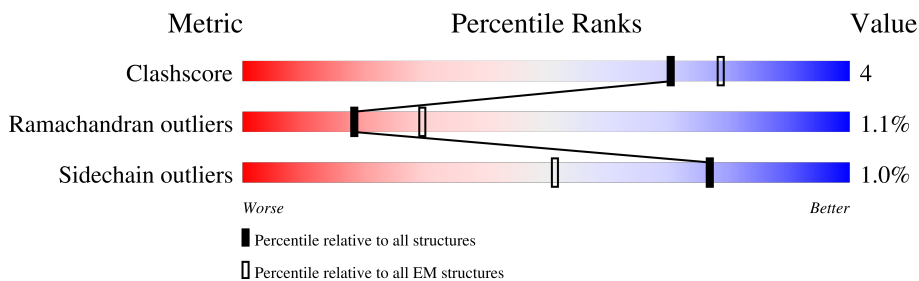|		
PDB ID	:	6R7H
EMDB ID	:	EMD-4741
Title	:	Structural basis of Cullin-2 RING E3 ligase regulation by the COP9 signalosome
Authors	:	Faull, S.V.; Lau, A.M.C.; Beuron, F.; Cronin, N.B.; Morris, E.P.; Politis, A.
Deposited on	:	2019-03-28
Resolution	:	8.80 Å(reported)

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 8.80 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	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		1.1%
Sidechain outliers		1.0%

Worse   *Better*

■ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	433	56% / 93% ... 7% •
2	Q	112	42% / 93% ... 6% •
3	O	654	34% / 87% ... 12% •
4	R	90	51% / 86% ... 13% •
5	B	414	38% / 89% ... 10% •
6	C	403	41% / 90% ... 9%
7	D	406	53% / 92% ... 8%
8	E	311	41% / 94% ... 5% •

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	288	53% ████ 85% ████ 15%
10	G	208	49% ████ 85% ████ 15%
11	H	199	30% ████ 75% ████ 10% · 15%
12	P	104	68% ████ 91% ████ 9%

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 28843 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
1	A	433	Total 3450	C 2174	N 605	O 649	S 22	0	0

- Molecule 2 is a protein called Elongin-C.

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

- Molecule 3 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	654	Total 5364	C 3419	N 899	O 1006	S 40	0	0

- Molecule 4 is a protein called E3 ubiquitin-protein ligase RBX1.

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

- Molecule 5 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	414	Total 3386	C 2149	N 579	O 643	S 15	0	0

- Molecule 6 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	403	Total 3205	C 2040	N 537	O 601	S 27	0	0

• Molecule 7 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	406	Total 3251	C 2047	N 566	O 622	S 16	0	0

• Molecule 8 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	311	Total 2472	C 1575	N 412	O 471	S 14	0	0

• Molecule 9 is a protein called COP9 signalosome complex subunit 6.

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

• Molecule 10 is a protein called COP9 signalosome complex subunit 7b.

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

• Molecule 11 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	169	Total 1349	C 864	N 234	O 247	S 4	0	0

• Molecule 12 is a protein called Elongin-B.

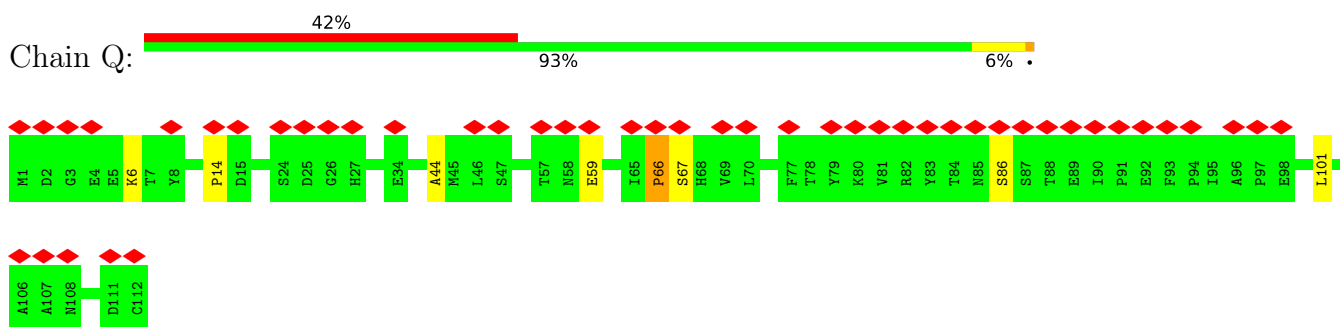| Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	104	Total 822	C 520	N 138	O 159	S 5	0	0

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.
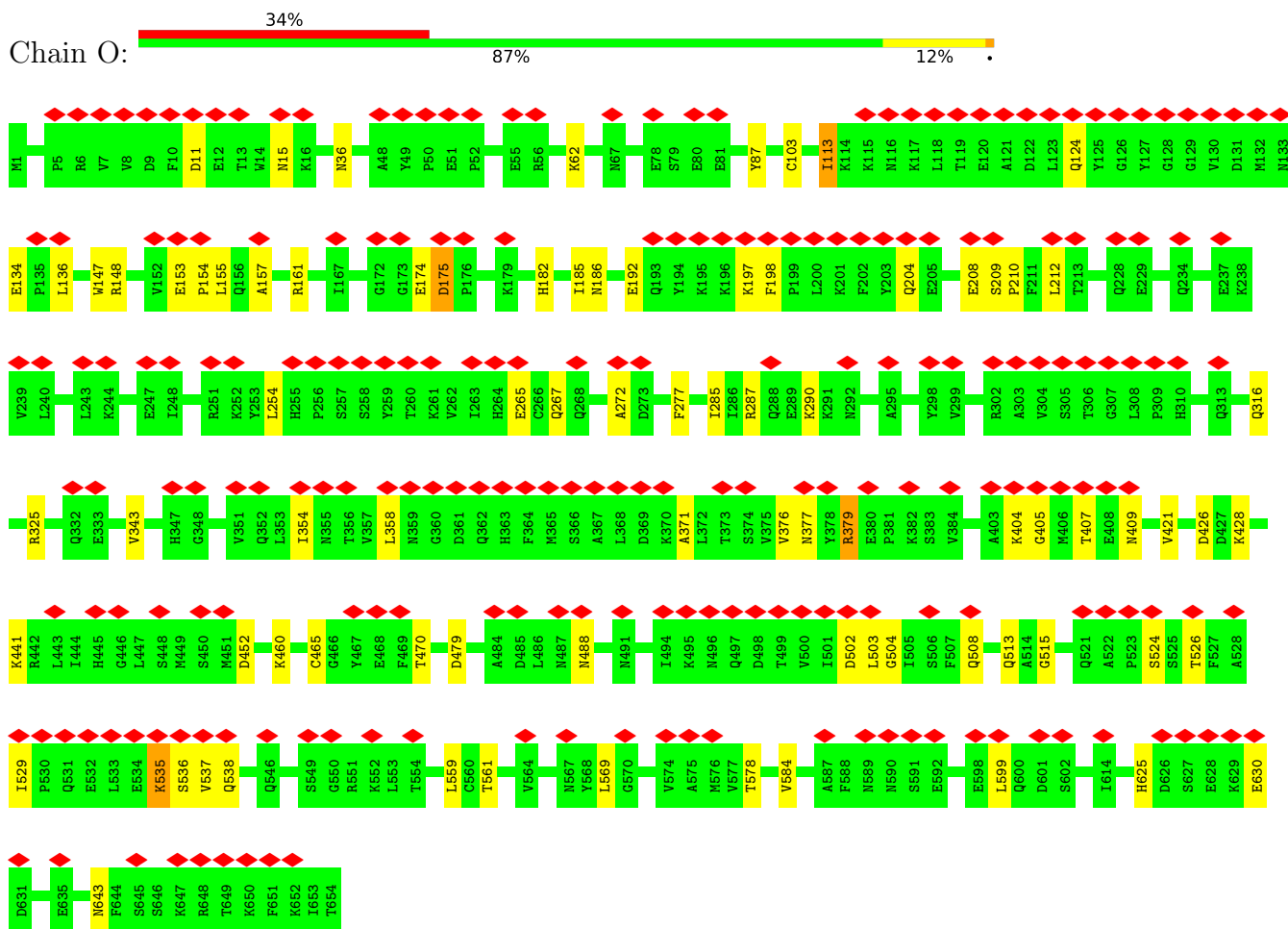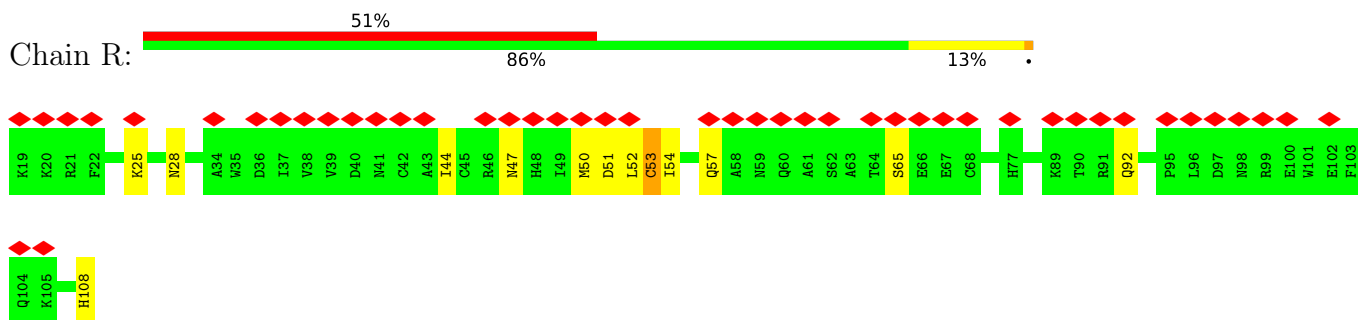
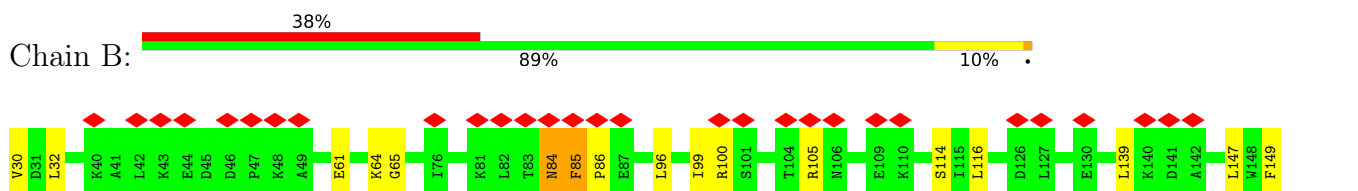• Molecule 1: COP9 signalosome complex subunit 1

Chain A:

• Molecule 2: Elongin-C

Chain Q:

• Molecule 3: Cullin-2

Chain O:
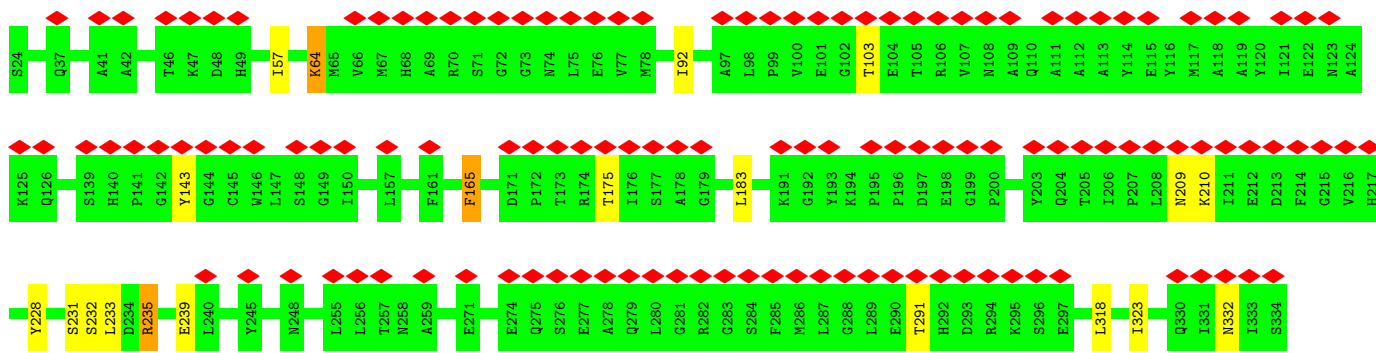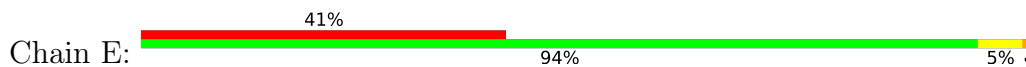
34%

87%

12%

• Molecule 4: E3 ubiquitin-protein ligase RBX1

Chain R:

51%

86%

13%

• Molecule 5: COP9 signalosome complex subunit 2

Chain B:

38%

89%

10%

K154 Y159 L160 E161 R162 E163 E164 Y165 G166 K167 L168 Q169 K170 I171 L172 R173 Q174 L175 H176 Q177 S178 C179 Q180 G184 E185 D186 G191 L194 L195 E196 I197 Y198 Y205 T206 A207 Q208 K209 N210 N211 K212 K213 L214 K215 A216 L217 Y218 E219 Q220 S221 L222 H223 I224 K225 S226

A227 I228 P229 H230 P231 M234 I237 R238 G241 M244 H245 L246 R247 E248 G249 E250 F251 E252 K253 A254 H255 T256 D257 E260 K263 S270 P271 L282 L286 M287 K288 S289 G290 I291 Q319 I323 E327 K328 I329 L330 K331 T332 N333 H334 S335 N336 I337 M338

D339 D340 P341 F342 I343 R344 E345 H346 I347 E348 E349 R352 N353 L359 T367 R368 I371 L378 D381 V382 A383 S387 V390 Q391 C392 I393 L394 D395 N396 T397 I398 H399 V405 N406 Q407 L408 L409 E410 L411 D412 H413 Q414 K415 R416 G417 G418 A419 T422 A423 L424
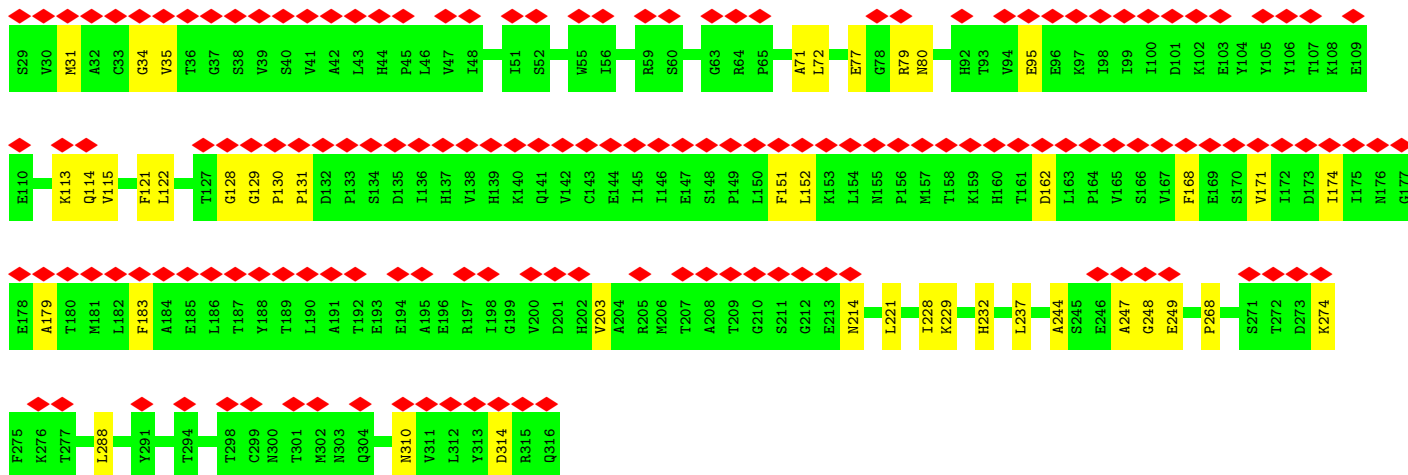
D425 K426 W427 T428 N429 Q430 L431 N432 S433 L434 N435 Q436 K441 L442 A443

• Molecule 6: COP9 signalosome complex subunit 3

Chain C:

41%

90%　　　　9%

M1 A2 S3 A4 L5 E6 Q7 Q14 A17 Q18 G19 Q20 I28 G32 E33 L34 L35 A36 K37 N38 L39 S40 H41 L42 D43 T44 V45 L46 G47 A48 L49 D50 V51 Q52 E53 H54 S55 L56 V64 K65 F66 S67 M68 P69 S70 V71 P72 D73 F74 E75 T76 L77 F78 S79 Q80

V81 Q82 L83 S86 T87 C88 N89 T97 D98 T99 F100 N109 A110 L111 V112 E113 R114 K115 Q116 P117 L118 R119 G120 I121 G122 Q132 M133 N134 Q137 L138 T139 S140 I141 L159 P160 Y161 L162 D163 V164 D165 M166 M167 D168 I169 A178 K179 Y192 K196 N197 F198

F204 A213 M214 A215 V216 S217 H218 I219 M220 L221 E222 K226 L229 Q239 Q240 L241 P242 K243 R251 F252 I253 K254 P255 L256 S257 N258 A259 Y260 S273 E274 L275 R276 N277 L278 V279 N280 K281 H282 S283 E284 T285 F286 T287 R288 D289 N290 N291 M292 G293 L294 V295 T311 K312

L315 Q320 A323 S324 Q327 L328 S329 G330 P331 Q332 E333 I342 E343 D344 Q353 K354 D355 G356 F360 N363 P364 E365 K366 Y367 N368 N369 P370 A371 M372 L373 H374 N375 Q378 E379 M380 L381 K382 C383 I384 E385 L386 D387 E388 R389 L390 K391 A392 M393 D394 Q395 E396

I397 T398 V399 N400 P401 Q402 F403

• Molecule 7: COP9 signalosome complex subunit 4

Chain D:

53%

92%　　　　8%

M1 A2 A3 A4 V5 R6 Q7 D8 L9 A10 Q11 L12 M13 N14 S15 S16 G17 S18 H19 K20 D21 L22 A23 G24 K25 Y26 R27 Q28 I29 L30 E31 K32 A33 I34 Q35 L36 S37 G38 A39 E40 Q41 L42 E43 A44 L45 K46 A47 F48 V49 E50 A51 M52 V53 N54 E55 N56 V57 S58 L59 V60

I61 S62 R63 Q64 L65 L66 T67 D68 F69 C70 T71 H72 L73 P74 N75 L76 P77 D78 S79 T80 A81 K82 E83 I84 Y85 H86 F87 T88 L89 E90 K91 I92 Q93 P94 R95 V96 I97 S98 F99 E100 E101 Q102 V103 A104 S105 I106 R107 Q108 H109 L110 I113 Y114 E115 K116 E117 E118 M122

Q125 V128 G129 I130 P131 L132 E133 T134 G135 Q136 K137 Q138 Y139 N140 V141 D142 Y143 E146 R153 N176 E177 S178 T179 N180 E181 Q182 L183 Q184 I185 H186 Y187 K188 Y191 R198 R199 K200 F201 I202 E203 N209 E210 L211 S212 Y213 K214 T215 I216 V217 H218 E219 S220 E221 R222

L223 I234 L235 A236 S237 A238 G239 Q240 Q241 R242 S243 R244 M245 L246 A247 T248 L249 F250 K251 D252 E253 R254 C255 Q256 E265 K266 M267 Y268 L269 D270 R274 G275 N276 M286 P287 H288 Q289 A294 L300 L309 L310 Y316 T320 F321 E322 A332 G346 R347 M348

N349 G350 F351 I352 D353 Q354 I355 D356 G357 I358 V359 H360 R364 E365 A366 L367 P368 T369 E386 S389 P393 E394 A397 Q398 A399 M400 E401 A402 Q403 M404 A405 Q406

• Molecule 8: COP9 signalosome complex subunit 5

Chain E:

41%
94% 5% •

S24 Q37 A41 A42 T46 K47 D48 H49 I57 K64 M65 V66 M67 H68 A69 R70 S71 G72 G73 N74 L75 E76 V77 M78 I92 A97 L98 P99 V100 E101 G102 T103 E104 T105 R106 V107 N108 A109 Q110 A111 A112 A113 Y114 E115 Y116 M117 A118 A119 Y120 I121 E122 N123 A124

K125 Q126 S139 H140 P141 G142 Y143 G144 C145 W146 L147 S148 G149 I150 L157 F161 F165 D171 P172 T173 R174 T175 I176 S177 A178 G179 L183 K191 G192 Y193 K194 P195 P196 D197 E198 G199 P200 Y203 Q204 T205 I206 P207 L208 N209 K210 I211 E212 D213 F214 G215 V216 H217

Y228 S231 S232 L233 D234 R235 E239 L240 Y245 N248 L255 L256 T257 N258 A259 E271 E274 Q275 S276 E277 A278 Q279 L280 G281 R282 G283 S284 F285 M286 L287 G288 L289 E290 T291 H292 D293 R294 K295 S296 E297 L318 I323 Q330 I331 N332 I333 S334

• Molecule 9: COP9 signalosome complex subunit 6

Chain F:

53%
85% 15%

S29 V30 M31 A32 C33 G34 V35 T36 G37 S38 V39 S40 V41 A42 L43 H44 P45 L46 V47 I48 I51 S52 W55 I56 R59 S60 G63 R64 P65 A71 L72 E77 G78 R79 N80 H92 T93 V94 E95 E96 K97 I98 I99 I100 D101 K102 E103 Y104 Y105 Y106 T107 K108 E109

E110 K113 Q114 V115 F121 L122 T127 G128 G129 P130 P131 D132 P133 S134 D135 I136 H137 V138 H139 K140 Q141 V142 C143 E144 I145 I146 E147 S148 P149 L150 F151 L152 K153 L154 N155 P156 M157 T158 K159 H160 T161 D162 L163 P164 V165 S166 V167 F168 E169 S170 V171 I172 D173 I174 I175 N176 G177

E178 A179 T180 M181 L182 F183 A184 E185 L186 T187 Y188 L189 L190 A191 T192 E193 E194 A195 E196 R197 I198 G199 V200 D201 H202 V203 A204 R205 M206 T207 A208 T209 G210 S211 G212 E213 N214 L221 I228 K229 H232 L237 A244 S245 E246 A247 G248 E249 P268 S271 T272 D273 K274

F275 K276 T277 L288 Y291 T294 T298 C299 N300 T301 M302 N303 Q304 N310 V311 L312 Y313 D314 R315 Q316

• Molecule 10: COP9 signalosome complex subunit 7b

Chain G:

49%
85% 15%

S8 S9 N10 L17 L18 A19 K20 G21 T22 S23 G24 S25 L47 E48 L49 A50 N51 V52 Q53 E54 L55 A56 E57 G58 A59 N60 A61 A62 Y63 L64 Q65 N68 L69 F70 A71 Y72 G73 T74 Y75 P76 D77 Y78 I79 A80 N81 K82 E83 S84 L85 P86 E87 L88 S89 T90 V102 S103

L104 A105 S106 R107 M108 K109 C110 I111 P112 Y113 S114 V115 L116 L117 K118 D119 M122 R123 N124 L125 R126 E127 L128 A135 V136 Y137 I140 I141 Q142 D146 Q147 R148 N149 Q150 L151 F156 C157 I158 G159 R160 R163 K164 K165 D166 I167 N168 N169 K172 T173 L174 H175 E176 W177

C178 D179 G180 C181 E182 A183 L186 Q190 Q191 V192 L193 R194 Q197 Y198 K199 E200 N201 H202 N203 R204 T205 Q206 Q207 Q208 V209 E210 A211 E212 V213 T214 N215

• Molecule 11: COP9 signalosome complex subunit 8

Chain H:

F11 Q23 E24 L25 E26 A27 P28 G29 G30 I31 A32 T33 P34 P35 L45 P61 P62 A63 I64 K65 S66 A67 N68 S69 E70 L71 G72 G73 S76 I81 W82 Q83 R84 D85 F86 P87 G88 T91 T92 I93 N94 A95 H96 Q97 W98 S99 E100 T101 V102 Q103 P104 A124

I129 A130 D131 D132 L139 P140 V141 E142 E143 K146 E150 D156 S157 T158 T159 R160 P164 R165 LYS PRO VAL ALA GLY ALA LEU ASP VAL SER PHE ASN LYS PHE ILE PRO LEU SER GLU PRO ALA PRO VAL PRO PRO ILE PRO ASN GLU GLN Q196 L197 A198 R199 L200 T201 D202

Y203 V204 A205 F206 N209

• Molecule 12: Elongin-B

Chain P:

M1 D2 V3 F4 L5 M6 I7 R8 R9 H10 K11 I14 K19 E20 S21 E32 G33 K36 D40 E41 Q42 R43 L44 Y45 K46 D47 D48 Q49 L50 L51 D52 D53 G54 K55 T56 L57 G58 E59 C60 G61 F62 T63 S64 Q65 T66 A67 R68 P69 Q70 A71 P72 A73 T74 V75 G76

L77 A78 F79 R80 A81 D82 D83 T84 F85 E86 A87 L88 C89 I90 E91 P92 F93 S94 S95 P96 P97 E98 L99 P100 D101 V102 M103 K104

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17191	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 $(e^-/\text{Å}^2)$	83	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	10.037	Depositor
Minimum map value	-1.471	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.23	0/3509	0.37	0/4733
2	Q	0.24	0/892	0.39	0/1204
3	O	0.23	0/5475	0.36	0/7379
4	R	0.23	0/767	0.41	0/1037
5	B	0.23	0/3444	0.36	0/4634
6	C	0.23	0/3264	0.36	0/4407
7	D	1.36	6/3303 (0.2%)	0.36	0/4460
8	E	0.23	0/2526	0.37	0/3411
9	F	0.23	0/2327	0.38	0/3153
10	G	1.68	1/1665 (0.1%)	0.42	2/2253 (0.1%)
11	H	0.23	0/1381	0.37	0/1877
12	P	0.24	0/838	0.40	0/1132
All	All	0.64	7/29391 (0.0%)	0.37	2/39680 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	126	ARG	CG-CD	67.75	3.21	1.51
7	D	316	TYR	CD2-CE2	39.91	1.99	1.39
7	D	316	TYR	CD1-CE1	39.88	1.99	1.39
7	D	316	TYR	CE1-CZ	29.09	1.76	1.38
7	D	316	TYR	CE2-CZ	28.93	1.76	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	126	ARG	CB-CG-CD	8.17	132.85	111.60
10	G	126	ARG	CG-CD-NE	6.49	125.43	111.80

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	3450	0	3482	20	0
2	Q	873	0	845	7	0
3	O	5364	0	5334	45	0
4	R	746	0	706	13	0
5	B	3386	0	3424	27	0
6	C	3205	0	3225	24	0
7	D	3251	0	3253	46	0
8	E	2472	0	2444	12	0
9	F	2280	0	2263	24	0
10	G	1645	0	1667	42	0
11	H	1349	0	1332	12	0
12	P	822	0	824	5	0
All	All	28843	0	28799	210	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 4.

The worst 5 of 210 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)
7:D:316:TYR:CZ	7:D:316:TYR:CE2	1.76	1.71
7:D:316:TYR:CZ	7:D:316:TYR:CE1	1.76	1.70
7:D:316:TYR:CE2	7:D:316:TYR:CD2	1.99	1.49
7:D:316:TYR:CE1	7:D:316:TYR:CD1	1.99	1.48
7:D:316:TYR:CZ	10:G:126:ARG:CG	2.36	1.09

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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%)	396 (92%)	33 (8%)	2 (0%)	29	69
2	Q	110/112 (98%)	101 (92%)	7 (6%)	2 (2%)	8	40
3	O	652/654 (100%)	592 (91%)	54 (8%)	6 (1%)	17	57
4	R	87/90 (97%)	68 (78%)	18 (21%)	1 (1%)	14	52
5	B	412/414 (100%)	378 (92%)	27 (7%)	7 (2%)	9	42
6	C	401/403 (100%)	364 (91%)	34 (8%)	3 (1%)	22	63
7	D	404/406 (100%)	392 (97%)	9 (2%)	3 (1%)	22	63
8	E	309/311 (99%)	280 (91%)	26 (8%)	3 (1%)	15	55
9	F	286/288 (99%)	254 (89%)	26 (9%)	6 (2%)	7	36
10	G	206/208 (99%)	197 (96%)	8 (4%)	1 (0%)	29	69
11	H	165/199 (83%)	152 (92%)	9 (6%)	4 (2%)	6	33
12	P	102/104 (98%)	91 (89%)	10 (10%)	1 (1%)	15	55
All	All	3565/3622 (98%)	3265 (92%)	261 (7%)	39 (1%)	18	52

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	229	PRO
5	B	231	PRO
11	H	164	PRO
2	Q	66	PRO
3	O	524	SER

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/377 (100%)	373 (99%)	4 (1%)	73	84
2	Q	96/96 (100%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	599/599 (100%)	592 (99%)	7 (1%)	71	83
4	R	79/79 (100%)	77 (98%)	2 (2%)	47	68
5	B	376/376 (100%)	374 (100%)	2 (0%)	88	93
6	C	359/359 (100%)	356 (99%)	3 (1%)	81	89
7	D	347/347 (100%)	344 (99%)	3 (1%)	78	87
8	E	267/267 (100%)	262 (98%)	5 (2%)	57	75
9	F	255/255 (100%)	254 (100%)	1 (0%)	91	94
10	G	181/181 (100%)	176 (97%)	5 (3%)	43	65
11	H	140/166 (84%)	139 (99%)	1 (1%)	84	90
12	P	92/92 (100%)	92 (100%)	0	100	100
All	All	3168/3194 (99%)	3135 (99%)	33 (1%)	77	86

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	G	126	ARG
10	G	164	LYS
11	H	156	ASP
4	R	108	HIS
4	R	92	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
6	C	291	ASN
7	D	318	ASN
10	G	147	GLN
6	C	352	ASN
7	D	102	GLN

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
4	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	107:GLY	C	108:HIS	N	3.75

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4741. 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 |
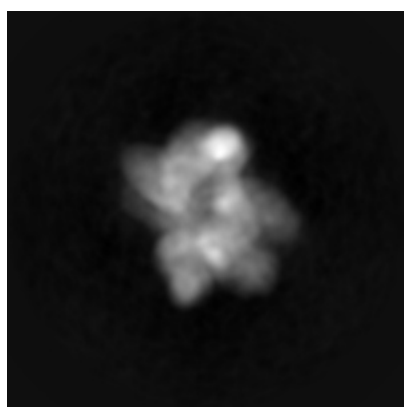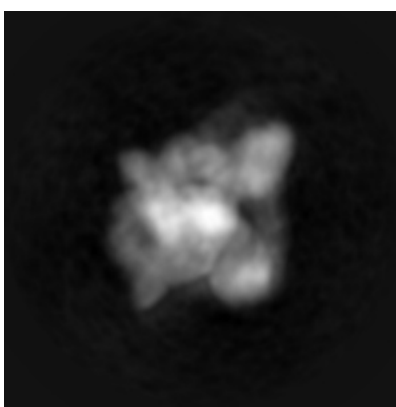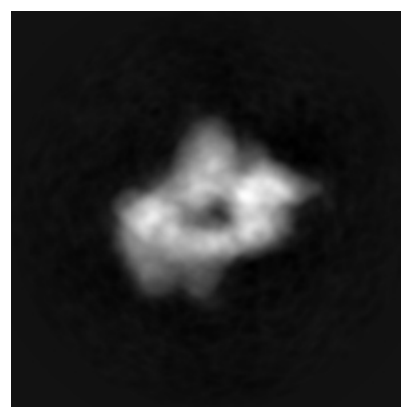
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
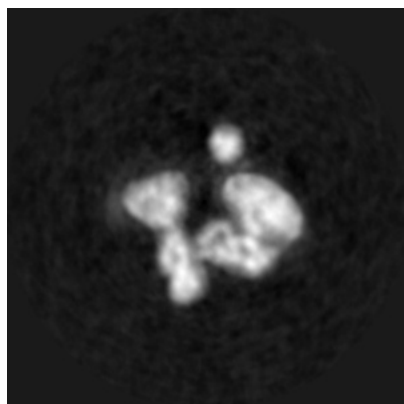
6.2.1 Primary map
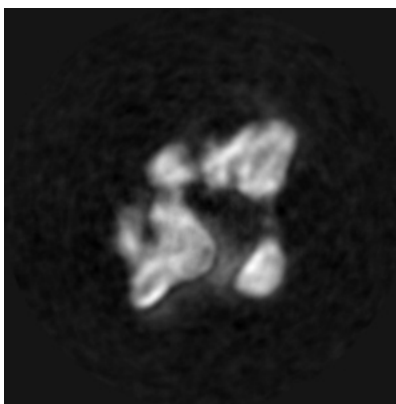
| X Index: 150 | Y Index: 150 | Z Index: 150 |
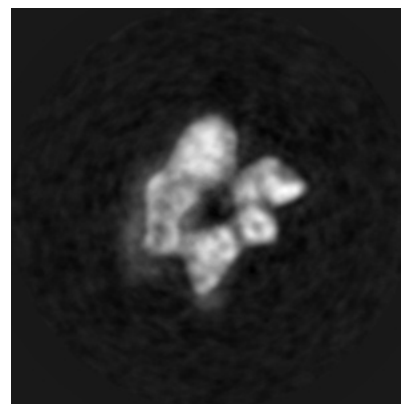
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
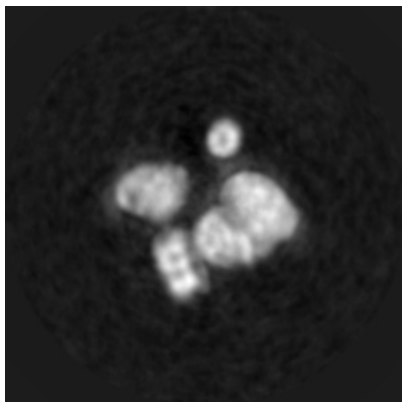
6.3.1 Primary map
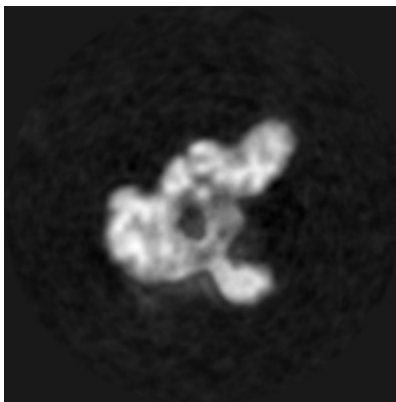
| X Index: 142 | Y Index: 132 | Z Index: 156 |
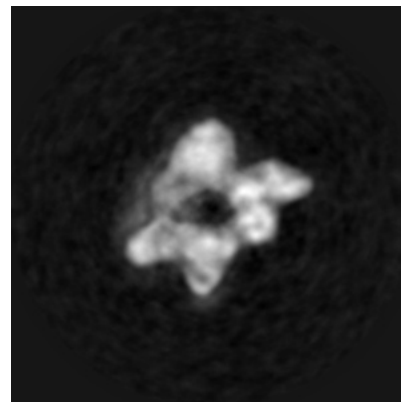
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

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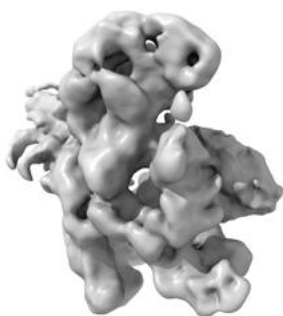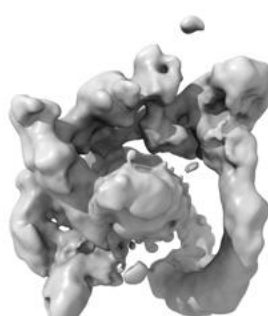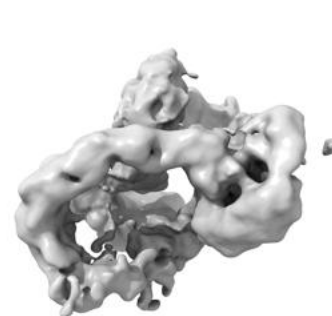
The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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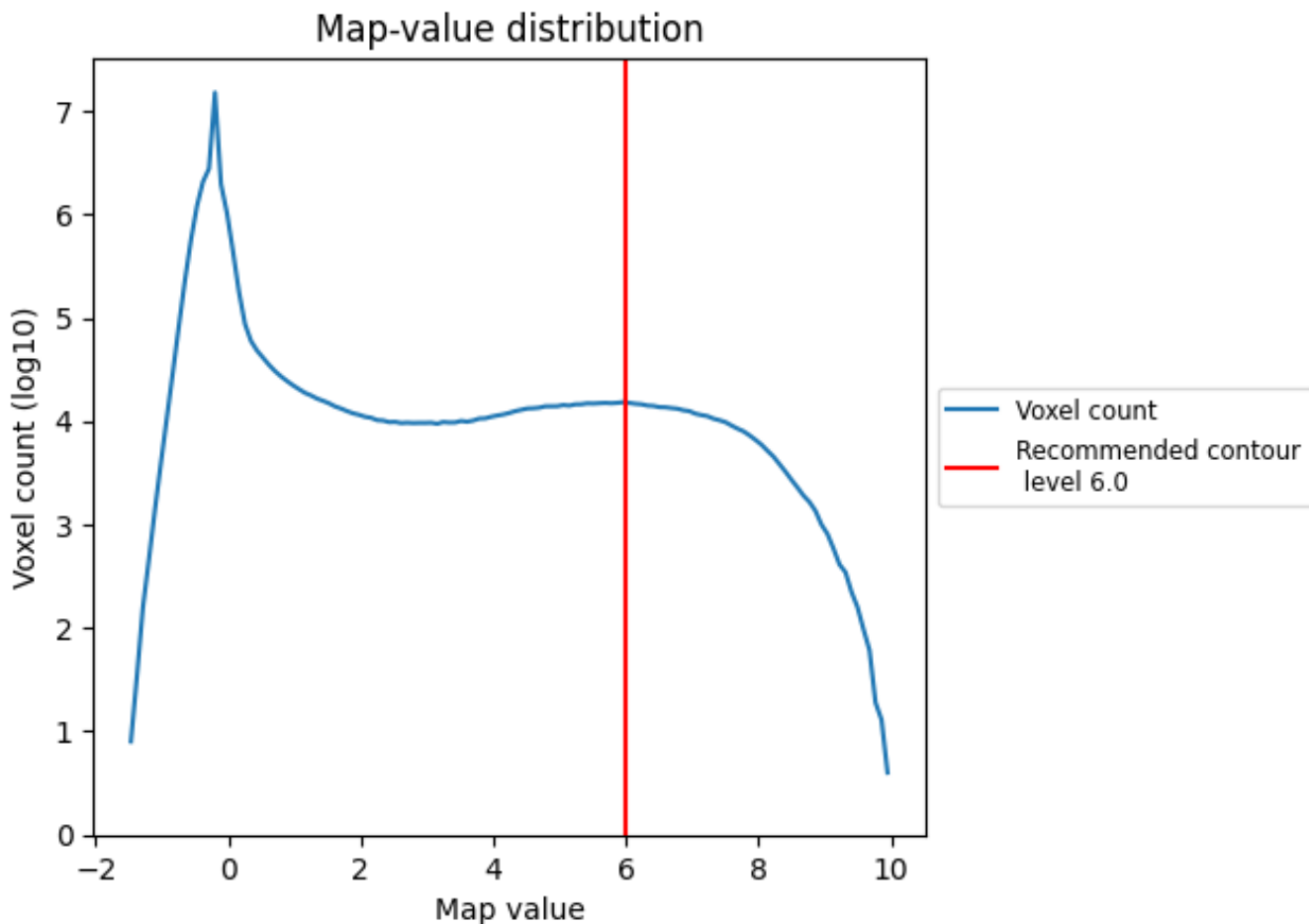
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
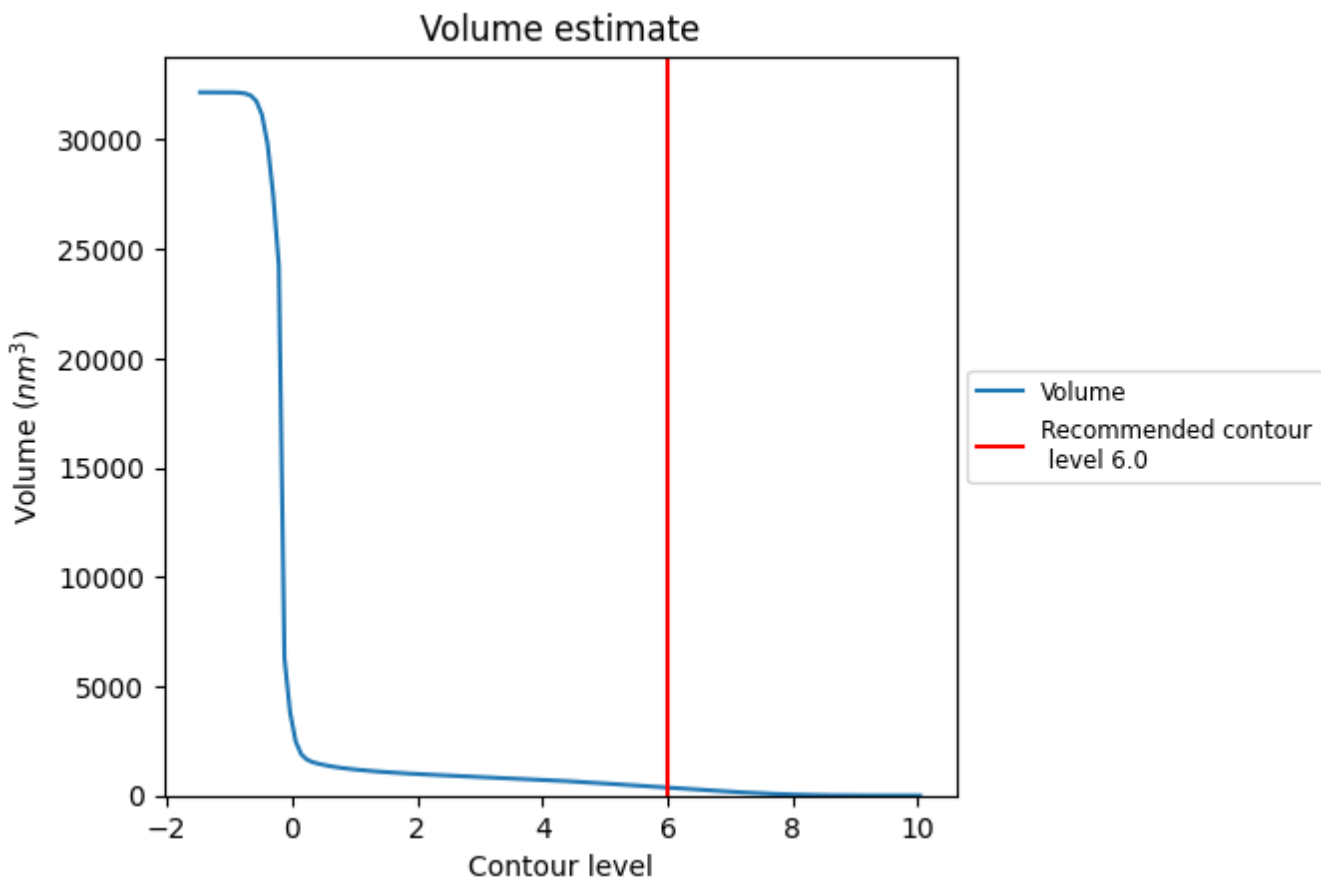
The volume at the recommended contour level is 359 nm^3; this corresponds to an approximate mass of 324 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ
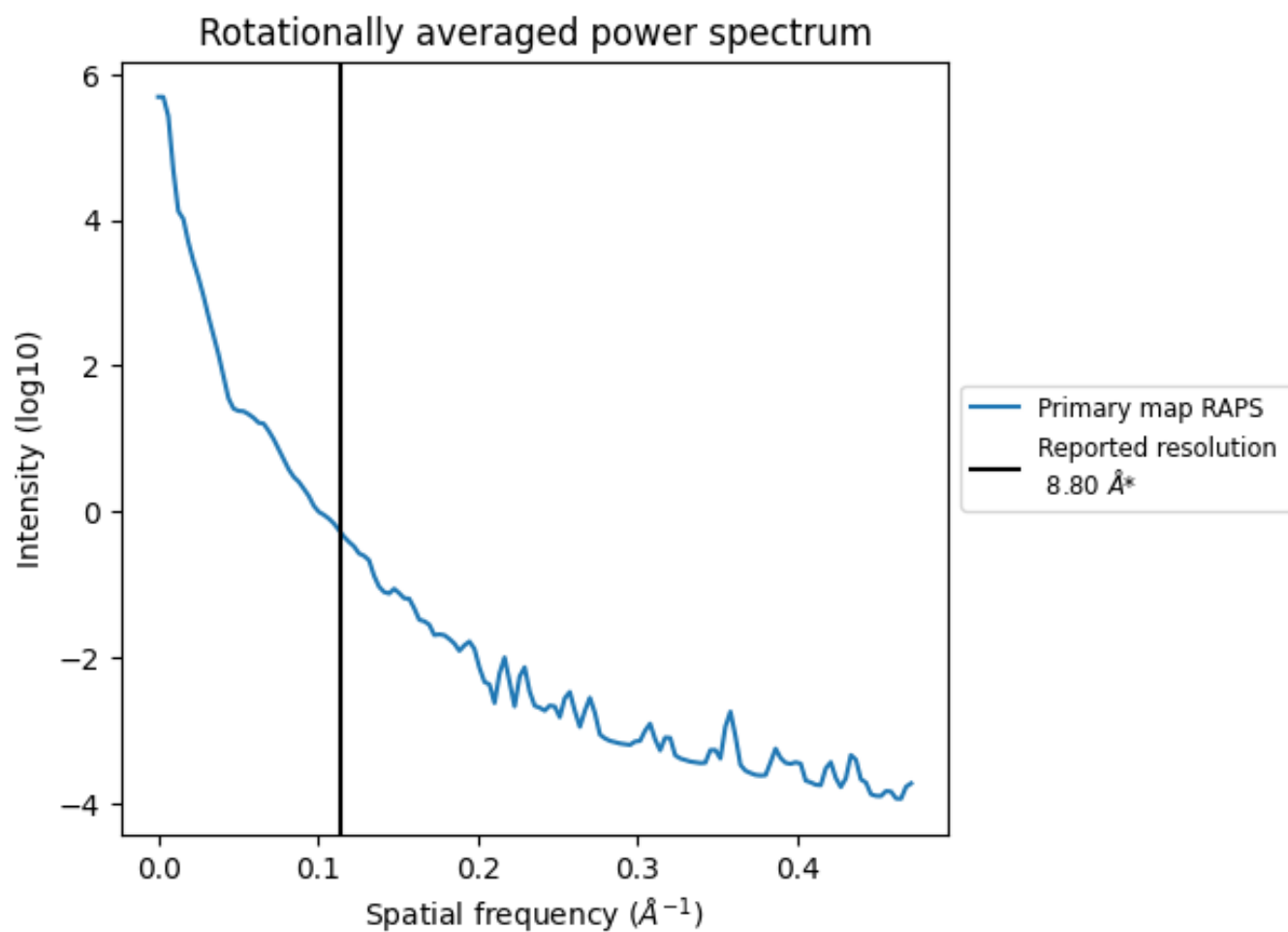
*Reported resolution corresponds to spatial frequency of 0.114 Å^{-1}

8 Fourier-Shell correlation (i)

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-4741 and PDB model 6R7H. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)

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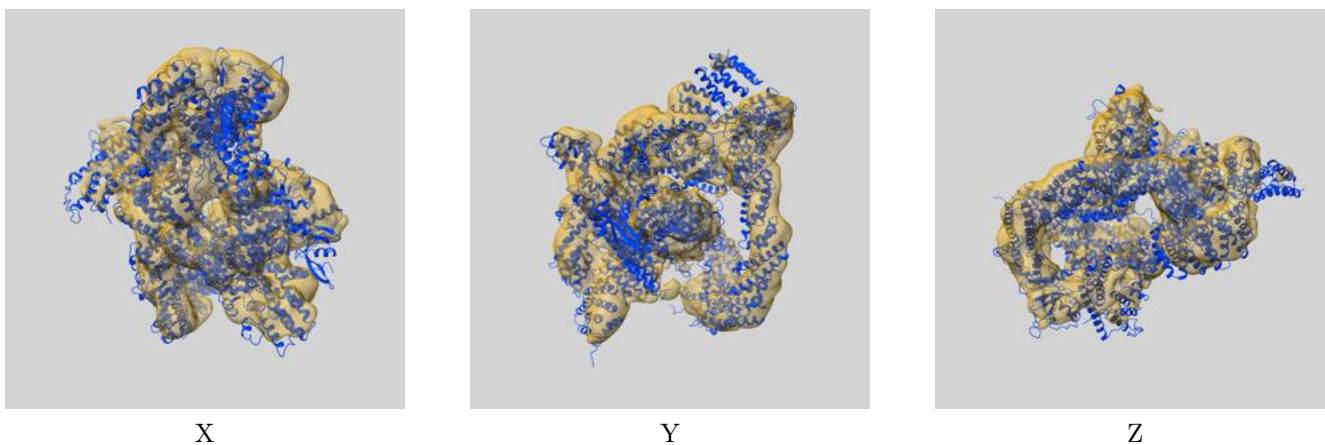
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
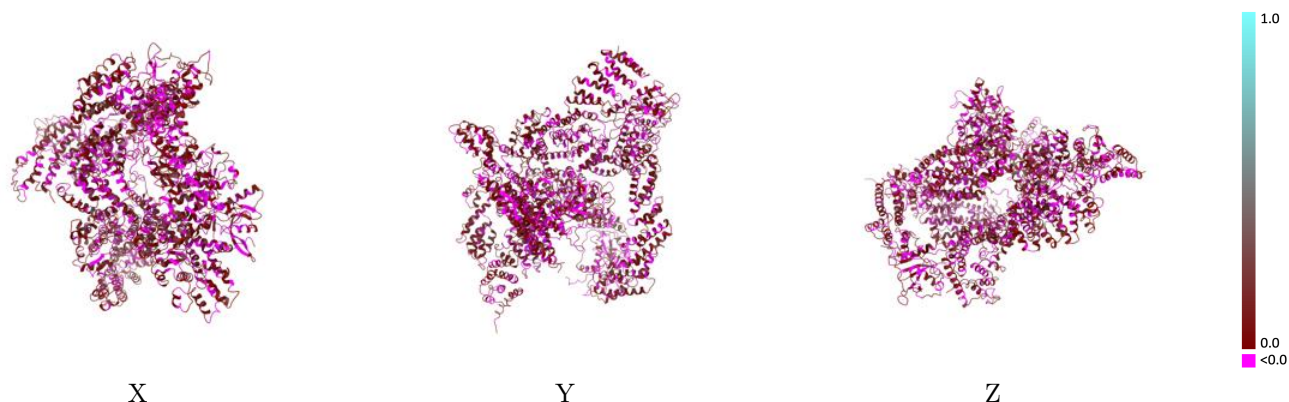
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
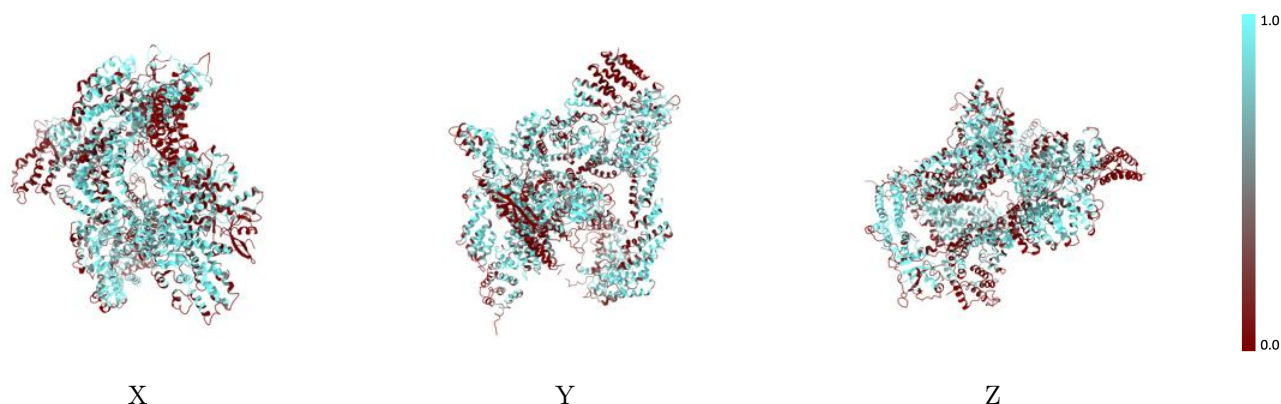
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).

9.4 Atom inclusion ⓘ
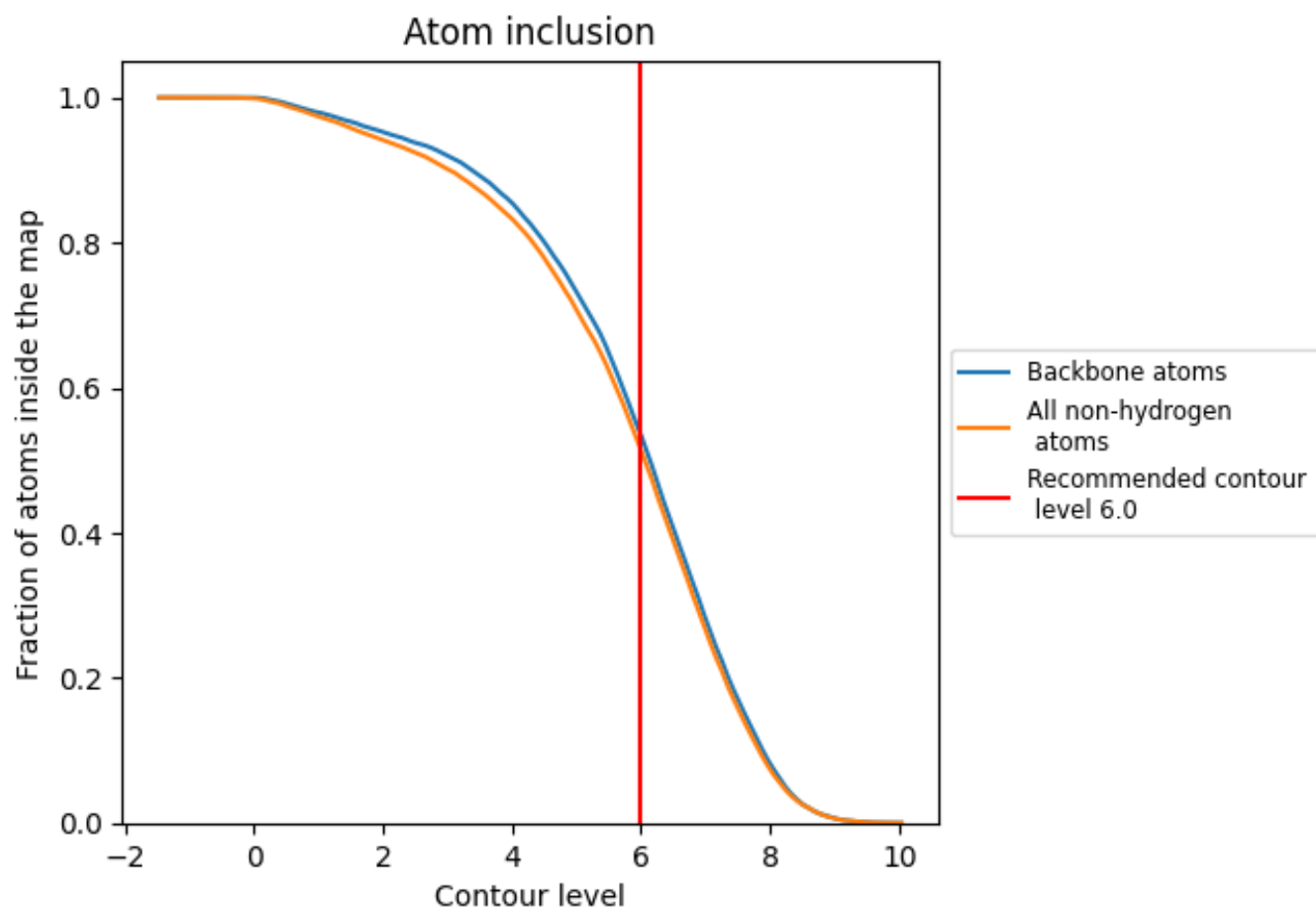
At the recommended contour level, 53% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.5138	0.0500
A	0.3983	0.0520
B	0.5707	0.0450
C	0.5425	0.0590
D	0.4317	0.0550
E	0.5576	0.0360
F	0.4391	0.0210
G	0.4772	0.0460
H	0.6239	0.0750
O	0.6101	0.0620
P	0.2949	0.0380
Q	0.5441	0.0510
R	0.4993	0.0090

1.0

0.0
<0.0