wwPDB EM Validation Summary Report

May 12, 2024 – 04:50 pm BST

PDB ID	:	6R6H
EMDB ID	:	EMD-4736
Title	:	Structural basis of Cullin-2 RING E3 ligase regulation by the COP9 signalosome
Authors	:	Morris, E.P.; Faull, S.V.; Lau, A.M.C.; Politis, A.; Beuron, F.; Cronin, N.
Deposited on	:	2019-03-27
Resolution	:	8.40 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:

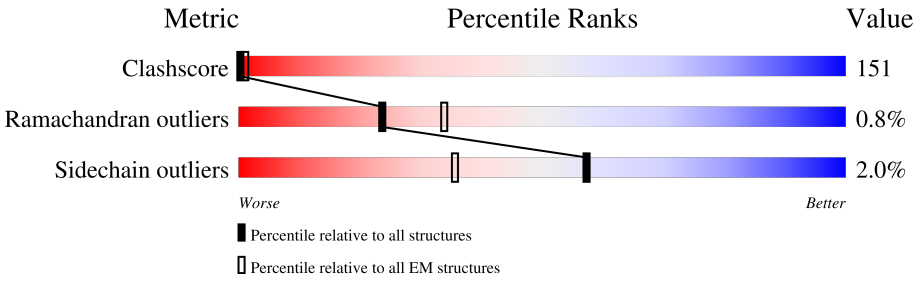
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 8.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	491	7% 10% 75% 15%
2	B	443	6% 11% 80% 5%
3	C	403	12% 86%
4	D	406	11% 88%
5	E	334	71% 10% 78% 7%
6	F	308	58% 15% 76% 9%
7	H	209	13% 69% 18%
8	O	745	21% 15% 80% 5%

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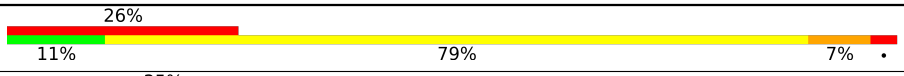
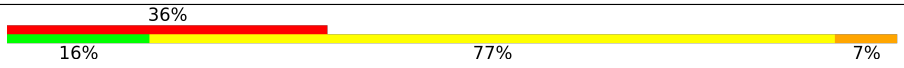
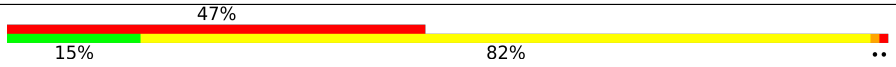
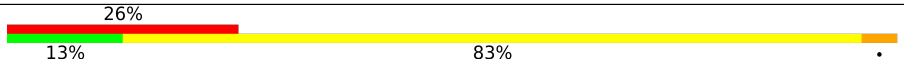
Mol	Chain	Length	Quality of chain
9	P	105	
10	Q	99	
11	R	86	
12	V	150	
13	G	206	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 32026 atoms, of which 1420 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	419	3348	2113	588	625	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	428	3512	2223	593	679	17	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	400	3183	2028	533	596	26	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	384	ILE	-	expression tag	UNP Q9UNS2
C	385	GLU	-	expression tag	UNP Q9UNS2
C	386	LEU	-	expression tag	UNP Q9UNS2
C	387	ASP	-	expression tag	UNP Q9UNS2
C	388	GLU	-	expression tag	UNP Q9UNS2
C	389	ARG	-	expression tag	UNP Q9UNS2
C	390	LEU	-	expression tag	UNP Q9UNS2
C	391	LYS	-	expression tag	UNP Q9UNS2
C	392	ALA	-	expression tag	UNP Q9UNS2
C	393	MET	-	expression tag	UNP Q9UNS2
C	394	ASP	-	expression tag	UNP Q9UNS2
C	395	GLN	-	expression tag	UNP Q9UNS2
C	396	GLU	-	expression tag	UNP Q9UNS2
C	397	ILE	-	expression tag	UNP Q9UNS2
C	398	THR	-	expression tag	UNP Q9UNS2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	399	VAL	-	expression tag	UNP Q9UNS2
C	400	ASN	-	expression tag	UNP Q9UNS2
C	401	PRO	-	expression tag	UNP Q9UNS2
C	402	GLN	-	expression tag	UNP Q9UNS2
C	403	PHE	-	expression tag	UNP Q9UNS2

- 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	3243	2041	565	621	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	310	2452	1562	411	466	13	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	281	2236	1429	371	421	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	172	1379	883	239	253	4	0	0

- Molecule 8 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	O	745	6508	3869	415	1032	1146	46	0	0

- Molecule 9 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	P	105	903	520	82	136	160	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	105	ALA	-	expression tag	UNP Q15370

- Molecule 10 is a protein called ELOC_HUMAN.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	Q	99	Total	C	H	N	O	S	0	0
			1577	505	782	121	165	4		

- Molecule 11 is a protein called RBX1_HUMAN.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	86	Total	C	N	O	S	0	0
			690	433	128	120	9		

- Molecule 12 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	V	150	Total	C	H	N	O	S	0	0
			1364	776	141	226	219	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	208	ALA	-	expression tag	UNP P40337
V	209	ALA	-	expression tag	UNP P40337

- Molecule 13 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	206	Total	C	N	O	S	0	0
			1630	1032	276	316	6		

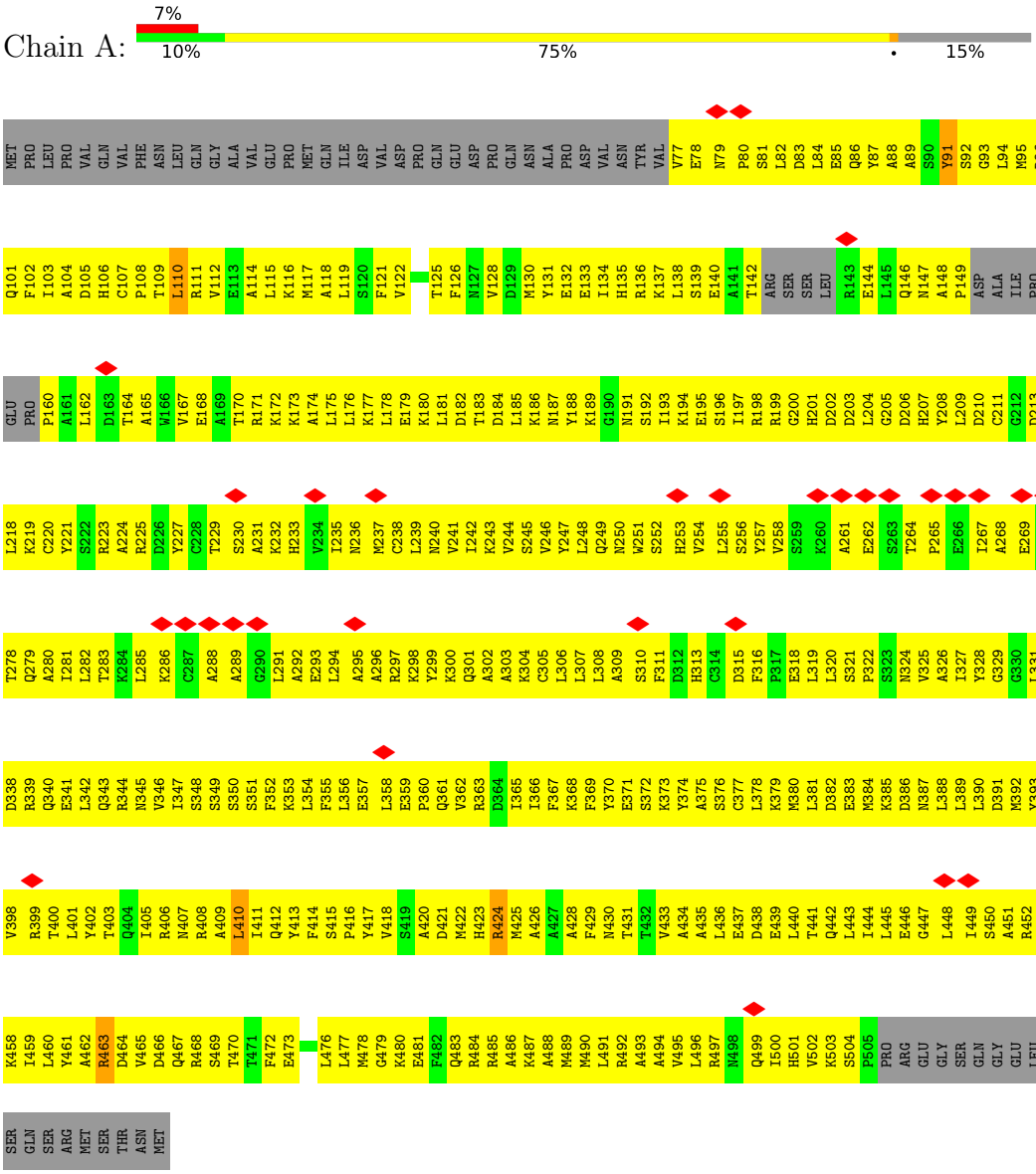
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	E	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

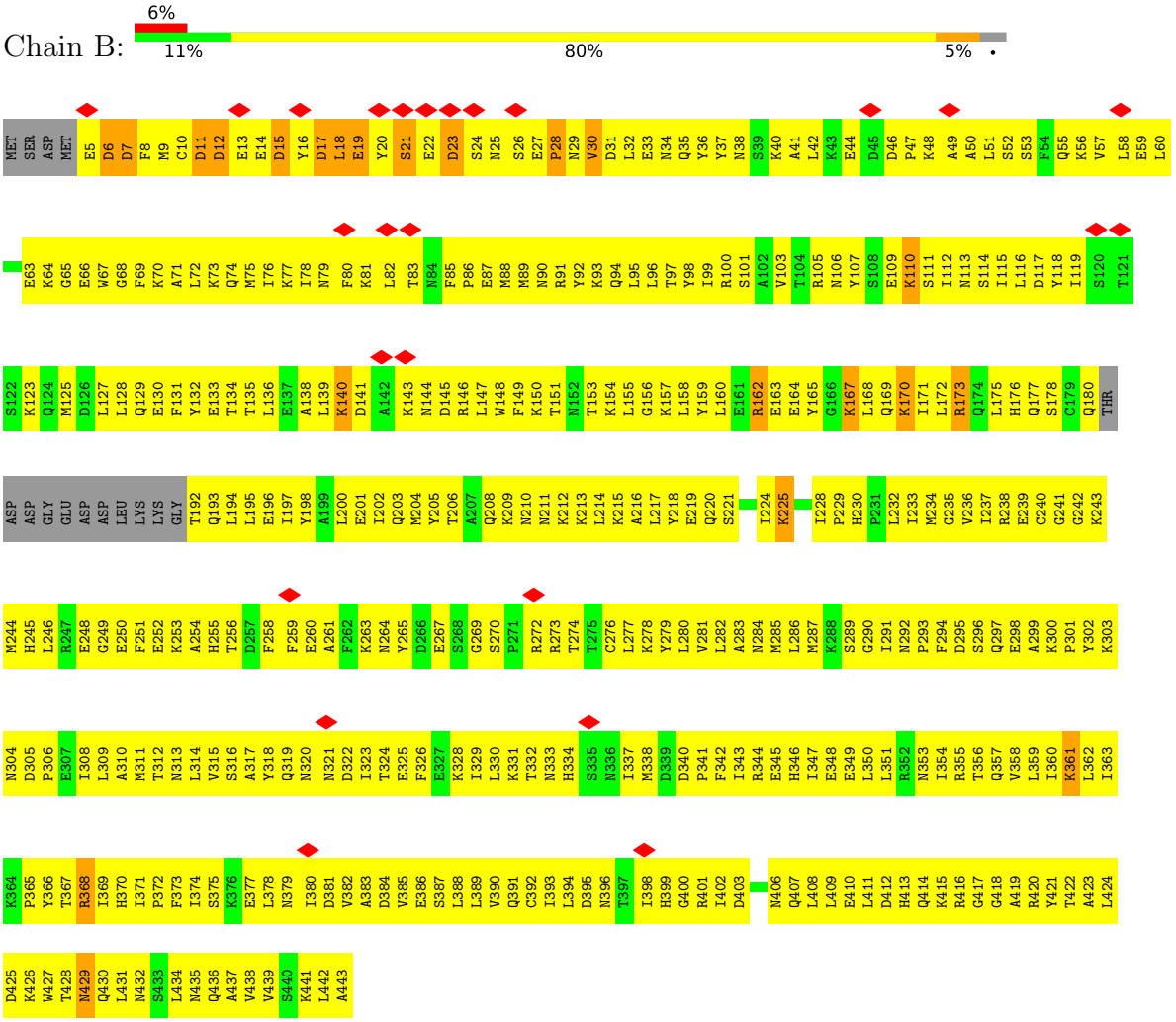
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



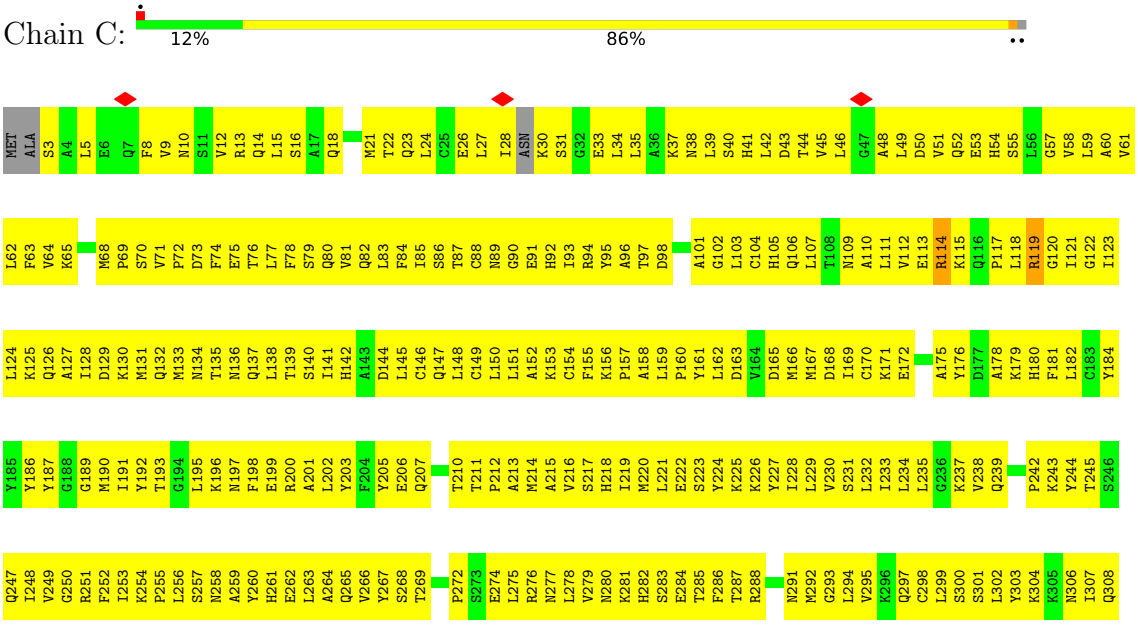
• Molecule 2: COP9 signalosome complex subunit 2

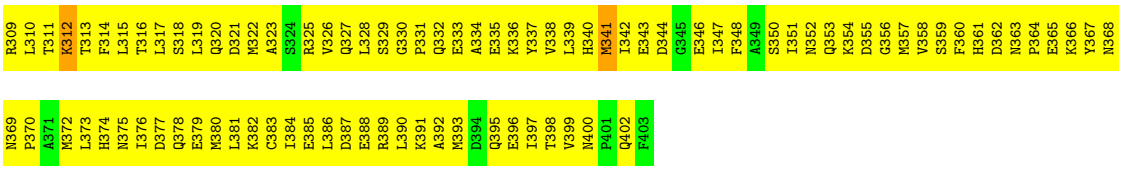
Chain B:



• Molecule 3: COP9 signalosome complex subunit 3

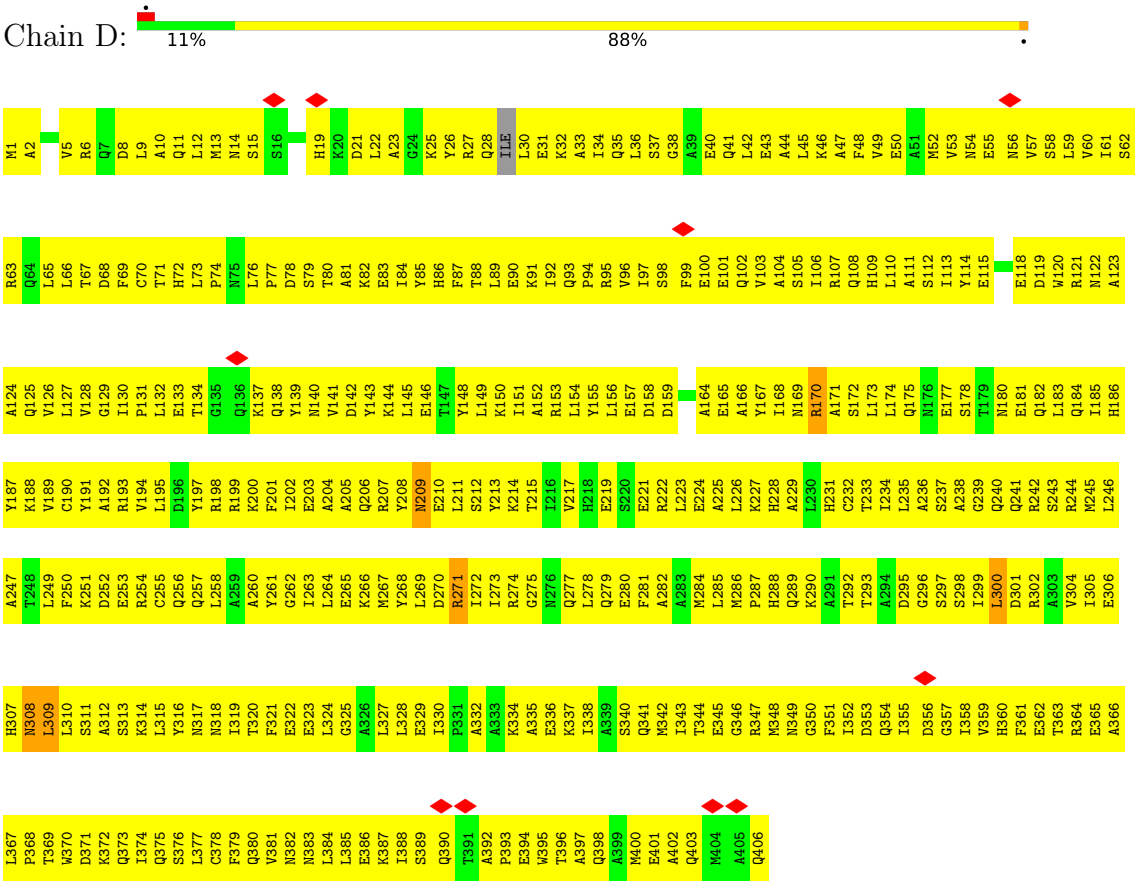
Chain C:





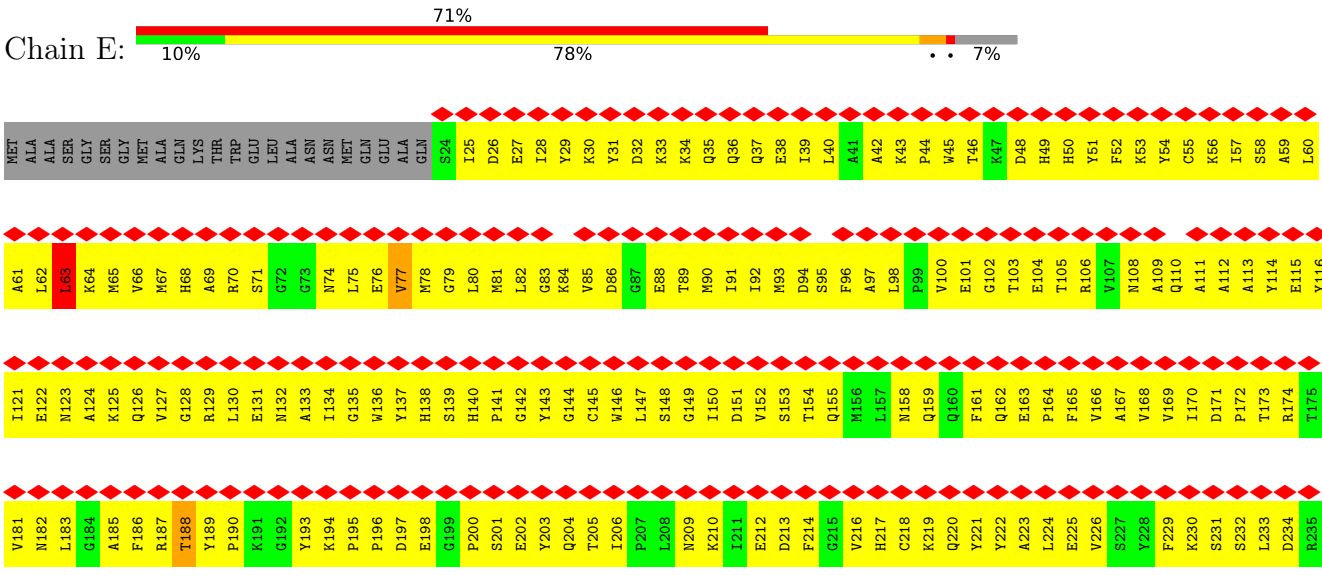
• Molecule 4: COP9 signalosome complex subunit 4

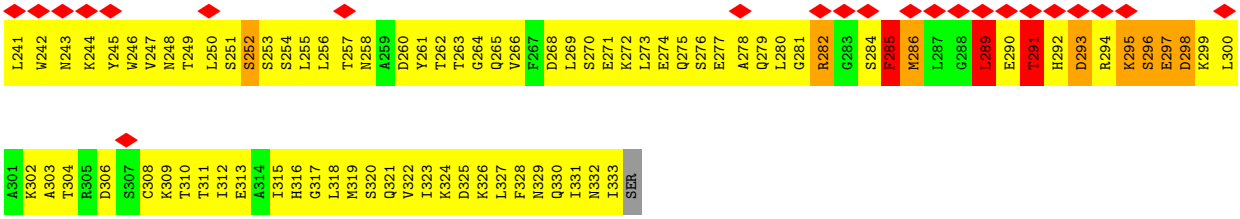
Chain D:



• Molecule 5: COP9 signalosome complex subunit 5

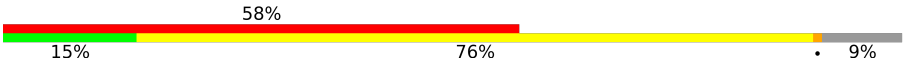
Chain E:





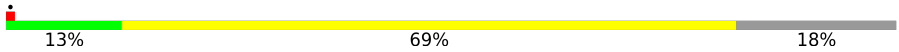
• Molecule 6: COP9 signalosome complex subunit 6

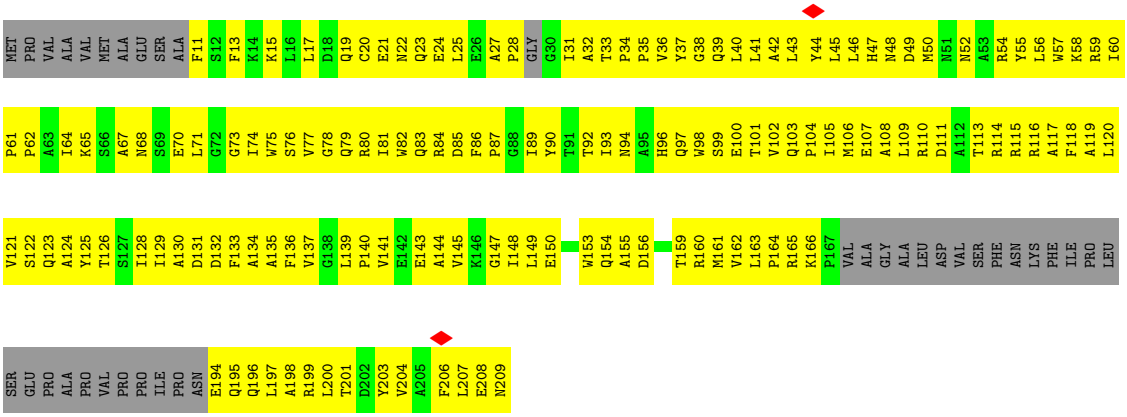
Chain F:



• Molecule 7: COP9 signalosome complex subunit 8

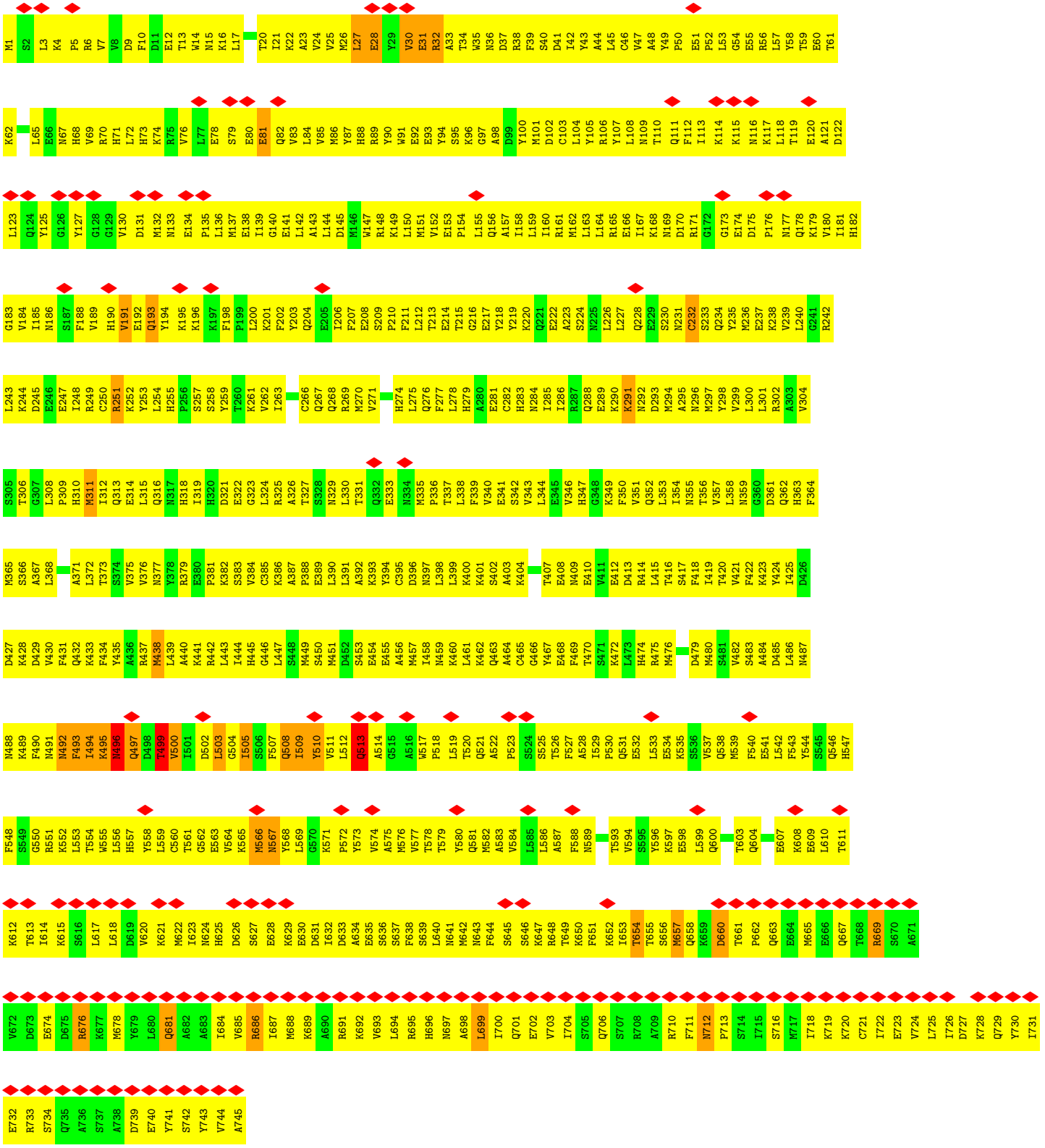
Chain H:



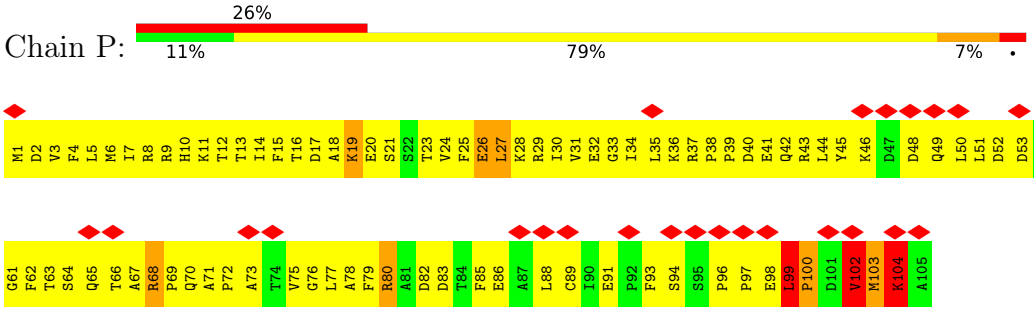


• Molecule 8: Cullin-2

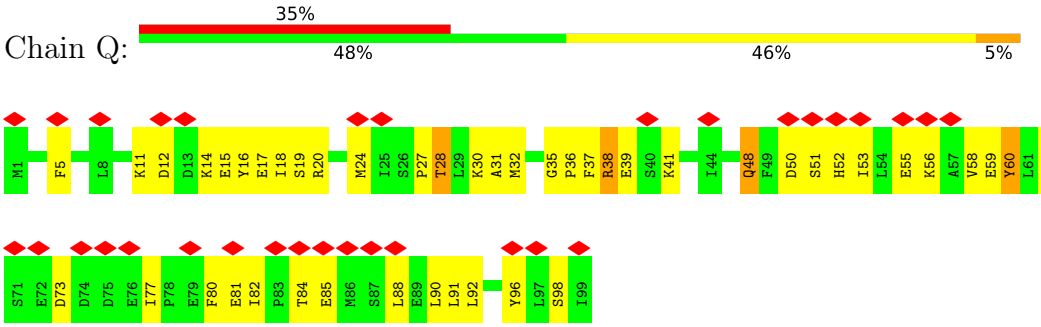
Chain O:



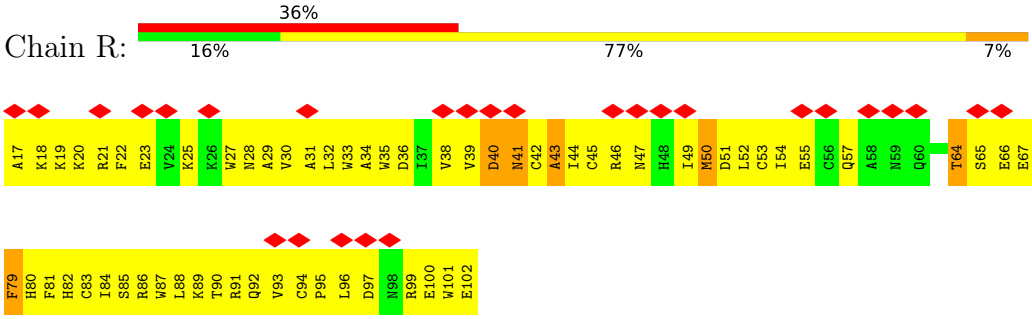
• Molecule 9: Elongin-B



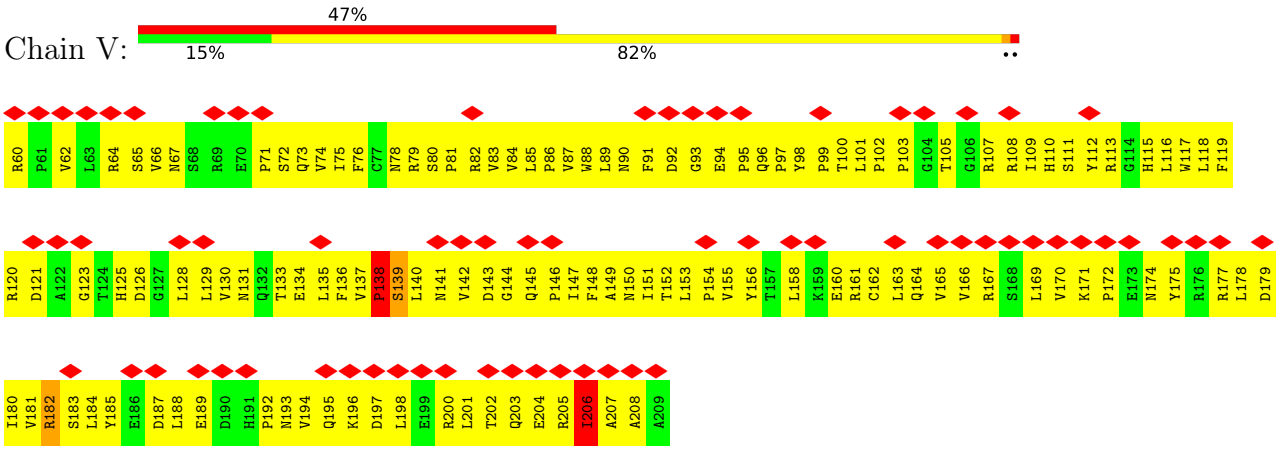
• Molecule 10: ELOC_HUMAN



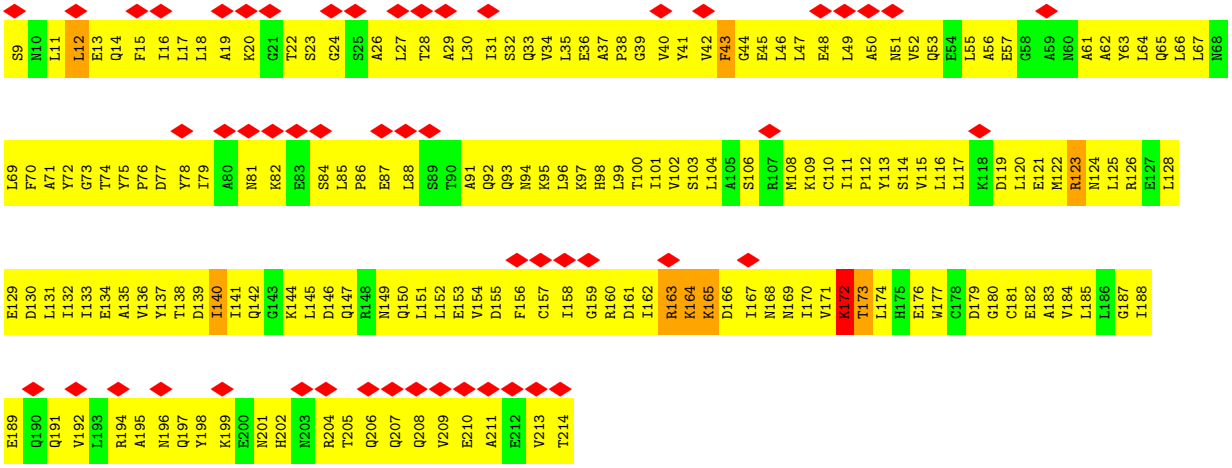
• Molecule 11: RBX1_HUMAN



• Molecule 12: von Hippel-Lindau disease tumor suppressor



• Molecule 13: COP9 signalosome complex subunit 7b


S9 M10 L11 L12 E13 Q14 F15 I16 L17 L18 A19 K20 G21 T22 S23 G24 S25 A26 L27 T28 A29 L30 I31 S32 Q33 V34 L35 E36 A37 P38 G39 V40 Y41 V42 F43 G44 E45 L46 L47 E48 L49 A50 N51 V52 Q53 E54 L55 A56 E57 G58 A59 N60 A61 A62 Y63 L64 Q65 L66 L67 N68
L69 F70 A71 Y72 G73 T74 Y75 P76 D77 Y78 I79 A80 N81 K82 E83 S84 L85 P86 E87 L88 S89 T90 A91 Q92 Q93 N94 K95 L96 K97 H98 L99 T100 I101 V102 S103 L104 A105 S106 R107 M108 K109 C110 I111 P112 Y113 S114 V115 L116 L117 K118 D119 L120 E121 M122 R123 N124 L125 R126 E127 L128
E129 D130 L131 I132 I133 E134 A135 V136 Y137 T138 D139 I140 I141 Q142 G143 K144 L145 D146 Q147 R148 N149 Q150 L151 L152 E153 V154 D155 F156 C157 I158 G159 R160 D161 I162 R163 K164 K165 D166 I167 N168 N169 I170 V171 K172 T173 L174 H175 E176 W177 C178 D179 G180 C181 E182 A183 V184 L185 L186 G187 I188
E189 Q190 Q191 V192 L193 R194 A195 N196 Q197 Y198 K199 E200 N201 H202 N203 R204 T205 Q206 Q207 Q208 V209 E210 A211 E212 V213 T214

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24040	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47170	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	20.682	Depositor
Minimum map value	-5.749	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

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	0.34	0/3404	0.53	1/4588 (0.0%)
2	B	0.32	0/3572	0.57	8/4807 (0.2%)
3	C	0.33	0/3241	0.52	0/4376
4	D	0.33	0/3291	0.50	1/4437 (0.0%)
5	E	0.46	3/2503 (0.1%)	1.21	10/3378 (0.3%)
6	F	0.34	0/2279	0.61	1/3083 (0.0%)
7	H	0.31	0/1411	0.48	0/1916
8	O	0.75	6/6206 (0.1%)	0.96	11/8350 (0.1%)
9	P	1.00	3/836 (0.4%)	1.84	8/1129 (0.7%)
10	Q	0.55	0/808	0.87	1/1087 (0.1%)
11	R	0.40	0/706	0.66	0/955
12	V	0.39	1/1252 (0.1%)	1.33	5/1705 (0.3%)
13	G	0.95	1/1650 (0.1%)	1.31	4/2234 (0.2%)
All	All	0.53	14/31159 (0.0%)	0.86	50/42045 (0.1%)

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	2
2	B	0	1
3	C	0	1
4	D	0	1
5	E	0	4
6	F	0	1
8	O	0	9
9	P	0	4
10	Q	0	2
11	R	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	V	0	4
13	G	0	2
All	All	0	37

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	499	THR	C-N	-37.18	0.48	1.34
9	P	102	VAL	C-N	-21.83	0.83	1.34
9	P	99	LEU	C-N	14.17	1.61	1.34
5	E	252	SER	C-N	10.99	1.59	1.34
13	G	172	LYS	C-N	-10.44	1.10	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	499	THR	O-C-N	-52.98	37.93	122.70
12	V	138	PRO	CA-C-N	-42.65	23.38	117.20
5	E	252	SER	C-N-CA	-39.14	23.84	121.70
9	P	104	LYS	O-C-N	-35.51	65.89	122.70
9	P	102	VAL	CA-C-N	-31.27	48.40	117.20

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	LEU	Peptide
1	A	91	TYR	Peptide
2	B	83	THR	Peptide
3	C	114	ARG	Peptide
4	D	309	LEU	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	A	3348	0	3381	866	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3512	0	3490	1227	0
3	C	3183	0	3201	848	0
4	D	3243	0	3231	992	0
5	E	2452	0	2389	1178	0
6	F	2236	0	2216	1002	0
7	H	1379	0	1362	380	0
8	O	6093	415	6048	2116	0
9	P	821	82	807	469	0
10	Q	795	782	776	444	0
11	R	690	0	648	560	0
12	V	1223	141	1221	427	0
13	G	1630	0	1650	712	0
14	E	1	0	0	0	0
All	All	30606	1420	30420	9193	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 151.

The worst 5 of 9193 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:P:15:PHE:CD2	10:Q:16:TYR:HB3	1.15	1.66
2:B:14:GLU:HB3	2:B:18:LEU:CD1	1.20	1.65
10:Q:91:LEU:HD23	12:V:184:LEU:CD1	1.19	1.65
8:O:49:TYR:CE1	10:Q:92:LEU:HD11	1.26	1.64
9:P:93:PHE:CE1	10:Q:16:TYR:HE2	1.10	1.63

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	415/491 (84%)	340 (82%)	75 (18%)	0	100 100
2	B	423/443 (96%)	367 (87%)	52 (12%)	4 (1%)	17 57
3	C	396/403 (98%)	328 (83%)	68 (17%)	0	100 100
4	D	395/406 (97%)	337 (85%)	58 (15%)	0	100 100
5	E	302/334 (90%)	240 (80%)	56 (18%)	6 (2%)	7 38
6	F	271/308 (88%)	224 (83%)	47 (17%)	0	100 100
7	H	166/209 (79%)	147 (89%)	19 (11%)	0	100 100
8	O	733/745 (98%)	588 (80%)	135 (18%)	10 (1%)	11 46
9	P	101/105 (96%)	76 (75%)	21 (21%)	4 (4%)	3 23
10	Q	97/99 (98%)	81 (84%)	14 (14%)	2 (2%)	7 36
11	R	82/86 (95%)	59 (72%)	22 (27%)	1 (1%)	13 50
12	V	144/150 (96%)	118 (82%)	25 (17%)	1 (1%)	22 63
13	G	204/206 (99%)	190 (93%)	11 (5%)	3 (2%)	10 46
All	All	3729/3985 (94%)	3095 (83%)	603 (16%)	31 (1%)	24 60

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	30	VAL
5	E	290	GLU
5	E	297	GLU
8	O	500	VAL
8	O	513	GLN

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	365/429 (85%)	363 (100%)	2 (0%)	88 93
2	B	392/405 (97%)	381 (97%)	11 (3%)	43 65
3	C	357/359 (99%)	354 (99%)	3 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	346/347 (100%)	342 (99%)	4 (1%)	71 83
5	E	262/283 (93%)	256 (98%)	6 (2%)	50 70
6	F	251/270 (93%)	251 (100%)	0	100 100
7	H	144/173 (83%)	143 (99%)	1 (1%)	84 90
8	O	679/681 (100%)	654 (96%)	25 (4%)	34 58
9	P	91/92 (99%)	88 (97%)	3 (3%)	38 61
10	Q	90/90 (100%)	84 (93%)	6 (7%)	16 41
11	R	73/75 (97%)	73 (100%)	0	100 100
12	V	138/138 (100%)	136 (99%)	2 (1%)	67 80
13	G	179/179 (100%)	174 (97%)	5 (3%)	43 65
All	All	3367/3521 (96%)	3299 (98%)	68 (2%)	57 74

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	Q	38	ARG
10	Q	64	ASN
13	G	140	ILE
5	E	296	SER
5	E	295	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	49	HIS
11	R	76	ASN
6	F	232	HIS
10	Q	62	ASN
13	G	206	GLN

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)

Of 1 ligands modelled in this entry, 1 is 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	O	6
5	E	4
4	D	3
9	P	3
6	F	3
12	V	3
2	B	1
11	R	1
13	G	1

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	315:LEU	C	316:TYR	N	14.37
1	B	192:THR	C	193:GLN	N	11.96
1	O	693:VAL	C	694:LEU	N	4.82
1	P	29:ARG	C	30:ILE	N	4.76
1	D	389:SER	C	390:GLN	N	3.72

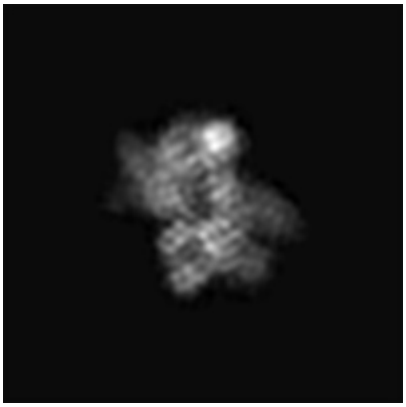
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4736. These allow visual inspection of the internal detail of the map and identification of artifacts.

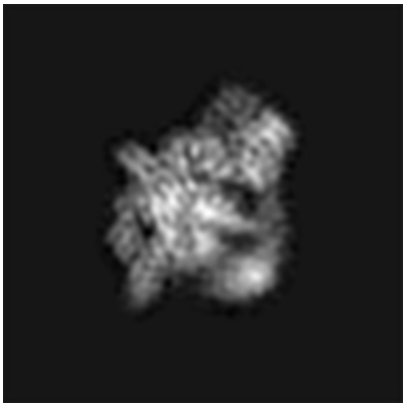
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

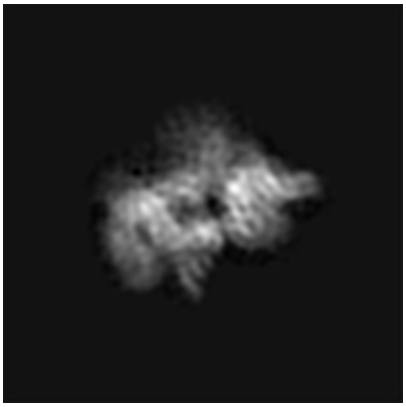
6.1.1 Primary map



X



Y



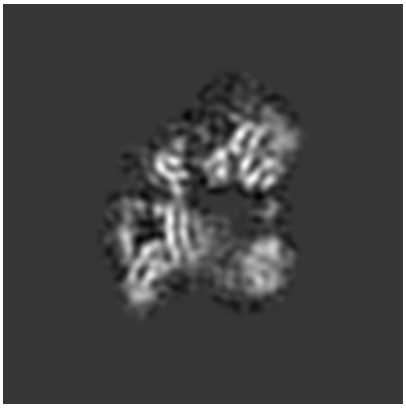
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 150



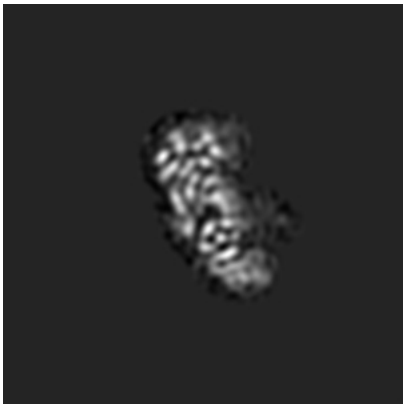
Y Index: 150

Z Index: 150

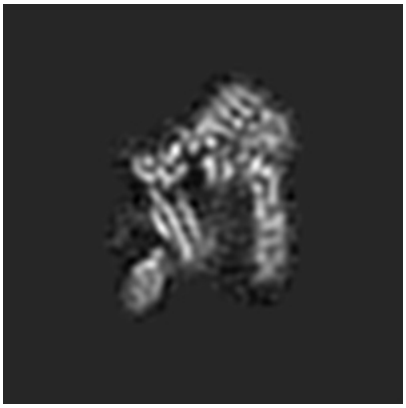
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 179



Y Index: 159

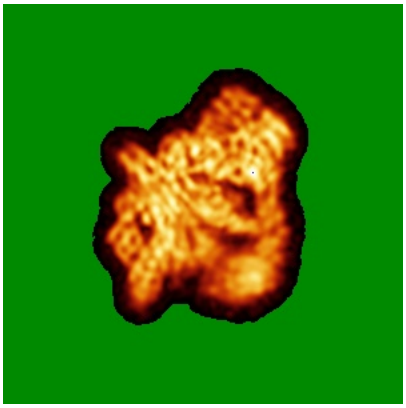
Z Index: 191

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



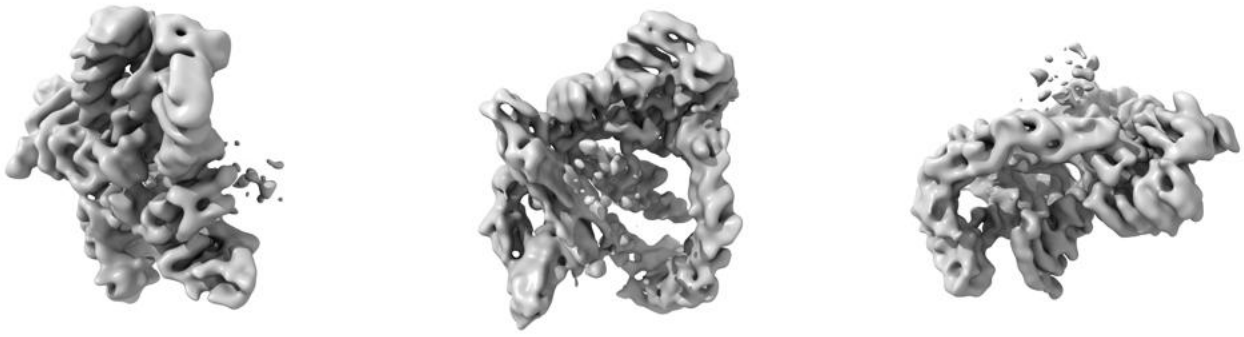
Y

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

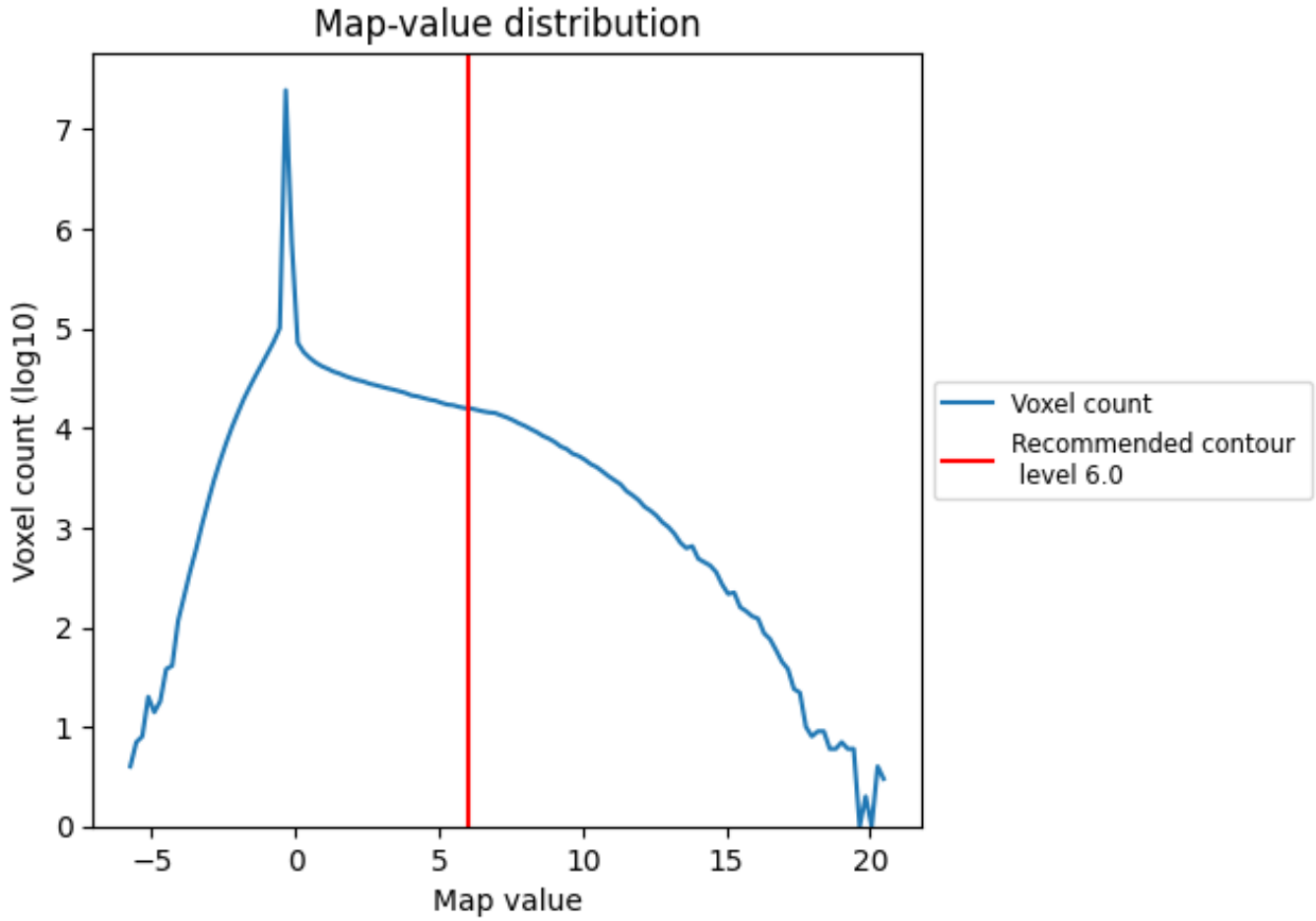
6.6 Mask visualisation (i)

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

7 Map analysis

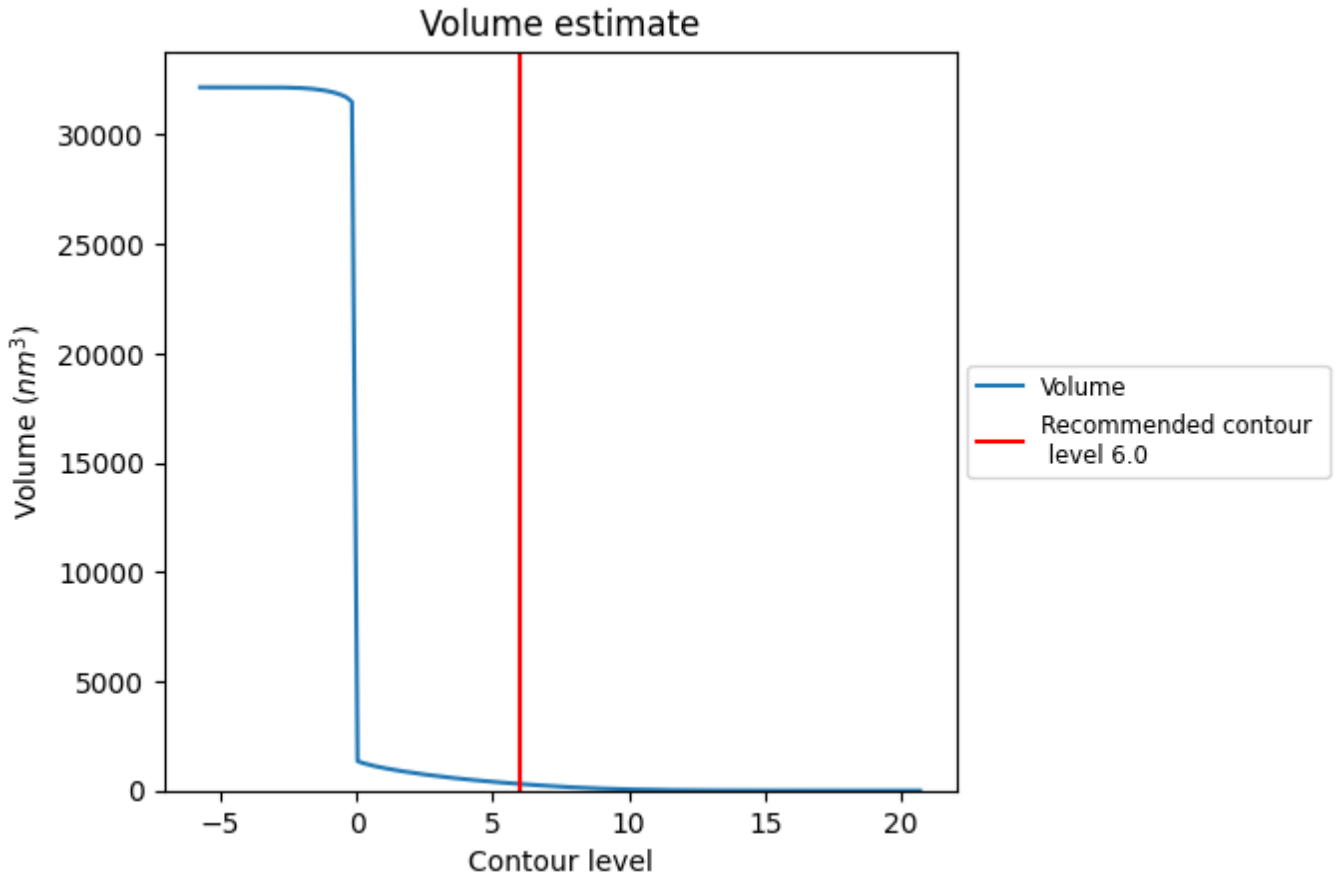
This section contains the results of statistical analysis of the map.

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.

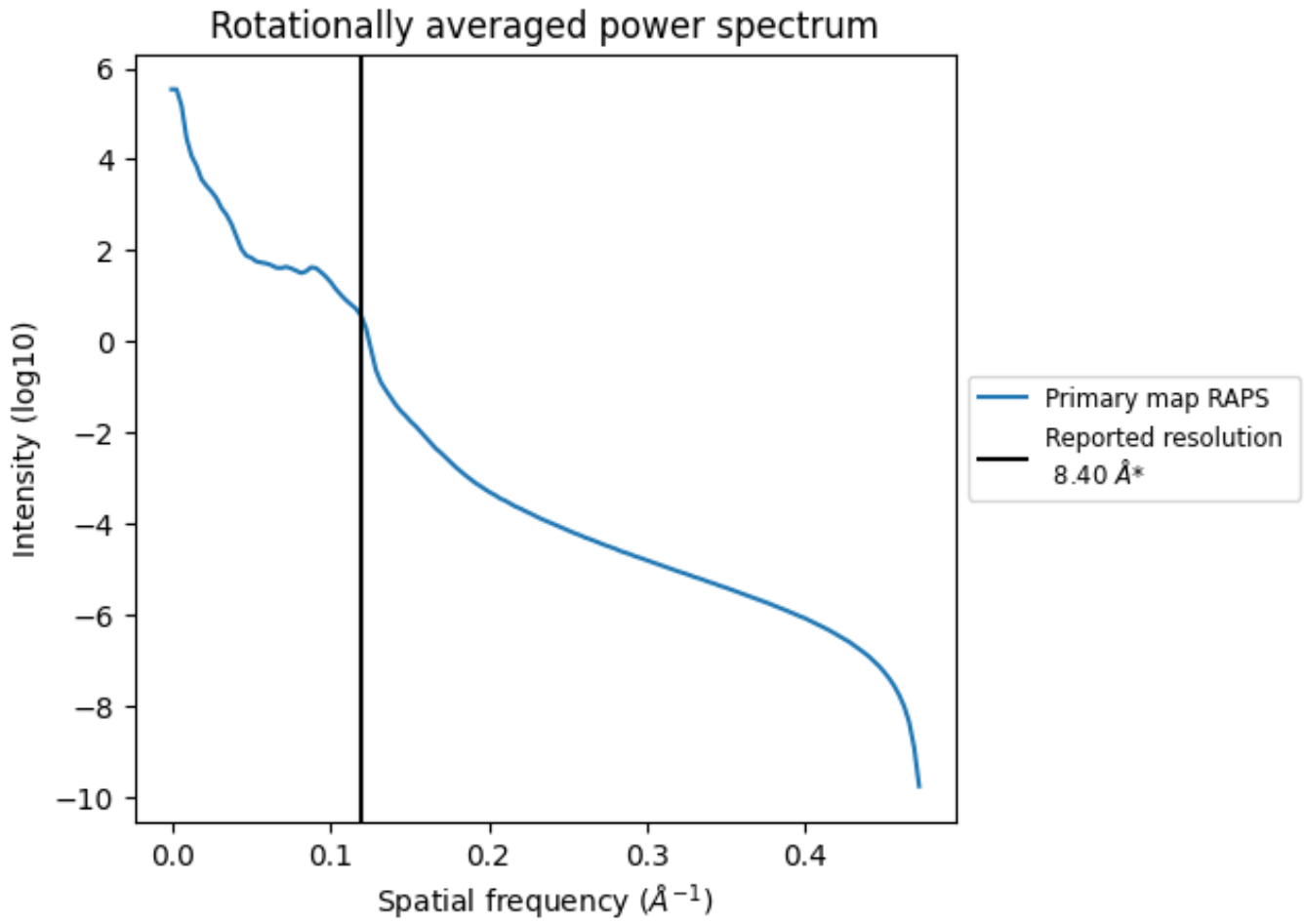
7.2 Volume estimate (i)



The volume at the recommended contour level is 302 nm^3; this corresponds to an approximate mass of 273 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 0.119 Å^{-1}

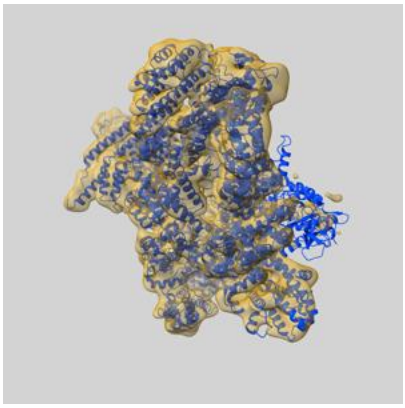
8 Fourier-Shell correlation (i)

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

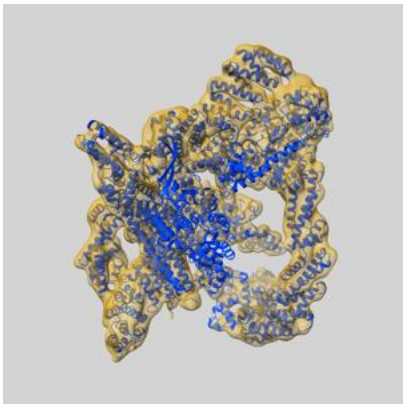
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4736 and PDB model 6R6H. Per-residue inclusion information can be found in section 3 on page 7.

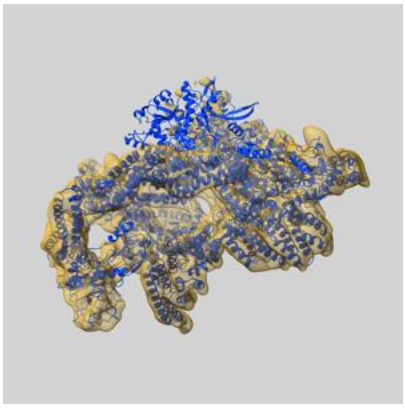
9.1 Map-model overlay



X



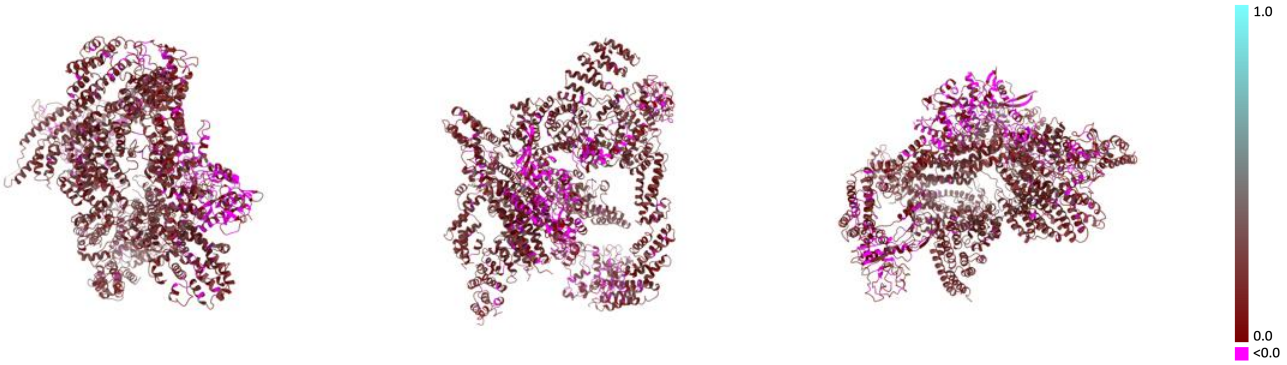
Y



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.

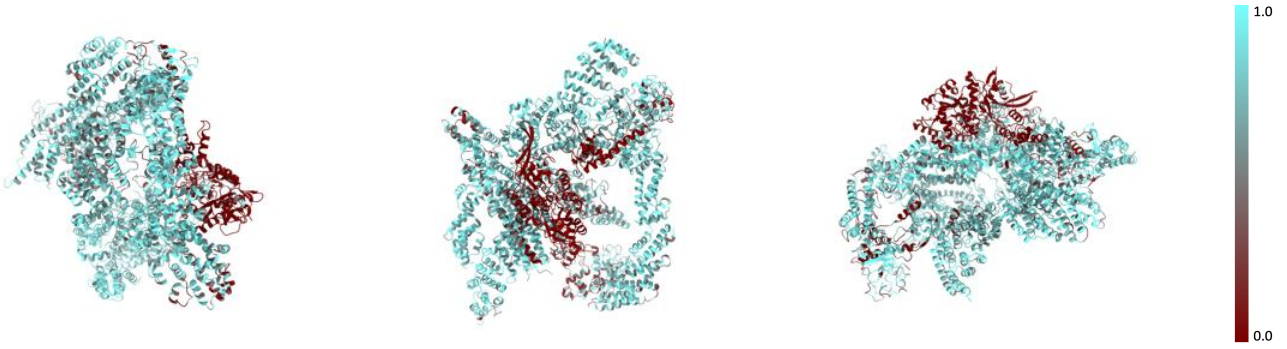
9.2 Q-score mapped to coordinate model



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.

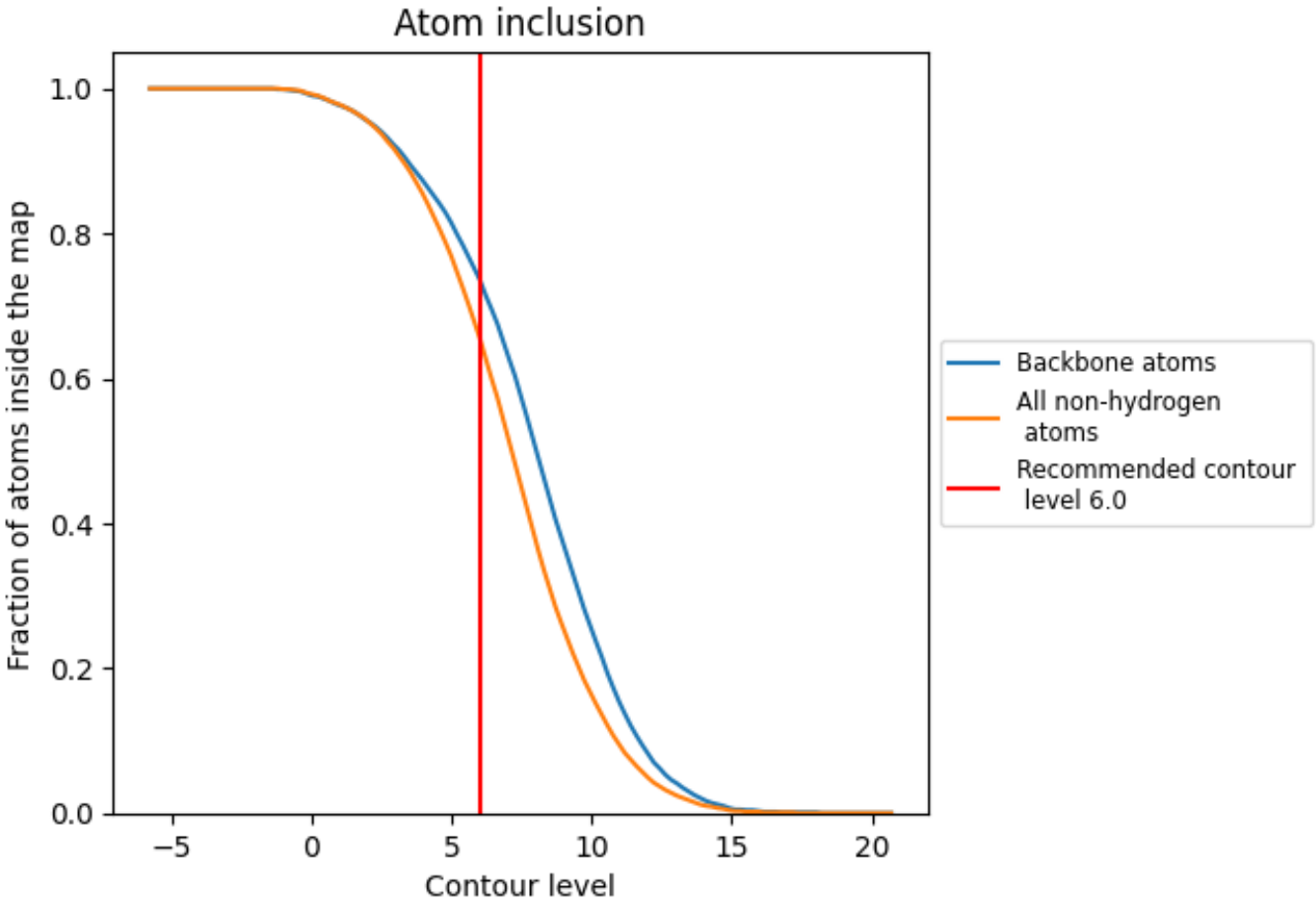
9.3 Atom inclusion mapped to coordinate model



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 (i)



At the recommended contour level, 74% of all backbone atoms, 66% 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	0.6570	0.1460
A	0.7590	0.1950
B	0.7650	0.1810
C	0.8520	0.1870
D	0.8290	0.1940
E	0.1980	0.0600
F	0.3110	0.0510
G	0.6110	0.1550
H	0.8720	0.1880
O	0.6740	0.1360
P	0.6710	0.1300
Q	0.5680	0.0640
R	0.6130	0.0940
V	0.4750	0.1140