wwPDB EM Validation Summary Report (i)

May 11, 2024 – 09:43 pm BST

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

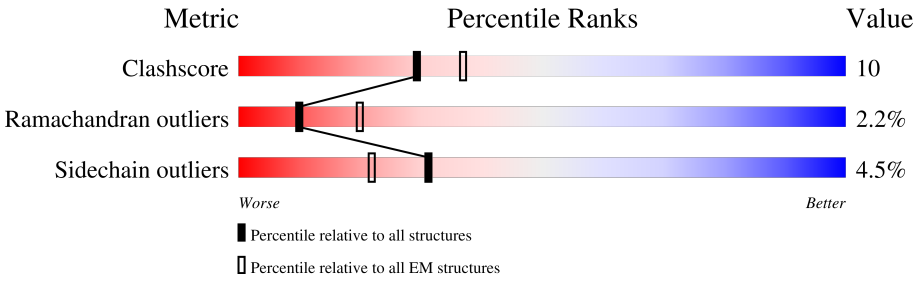
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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 <=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	100% 76% 21% ·
2	B	443	93% 63% 24% 6% 7%
3	C	403	100% 73% 23% ·
4	D	406	100% 78% 18% · ·
5	E	311	100% 71% 21% 7% ·
6	F	288	100% 74% 21% · ·
7	H	209	80% 60% 17% · 20%
8	G	208	100% 80% 15% · ·

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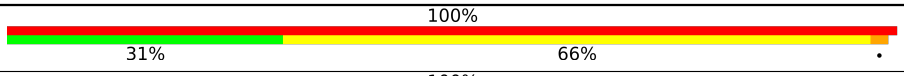
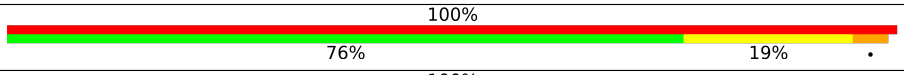
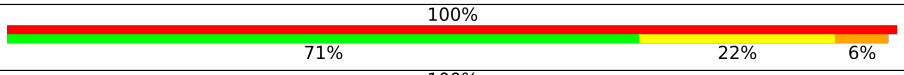
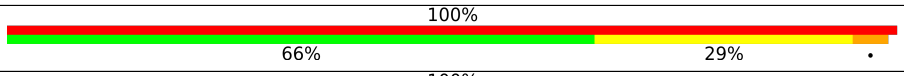
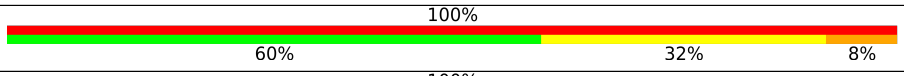
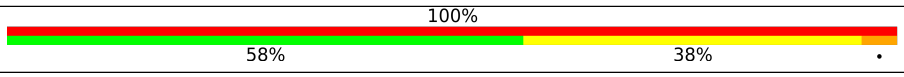
Mol	Chain	Length	Quality of chain
9	V	160	
10	P	118	
11	Q	112	
12	O	745	
13	R	90	
14	N	76	

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
7	H	168	Total	C	N	O	S	0	0
			1340	859	232	245	4		

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

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

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

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

- Molecule 10 is a protein called Elongin-B.

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

- Molecule 11 is a protein called Elongin-C.

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

- Molecule 12 is a protein called Cullin-2.

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

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

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

- Molecule 14 is a protein called NEDD8.

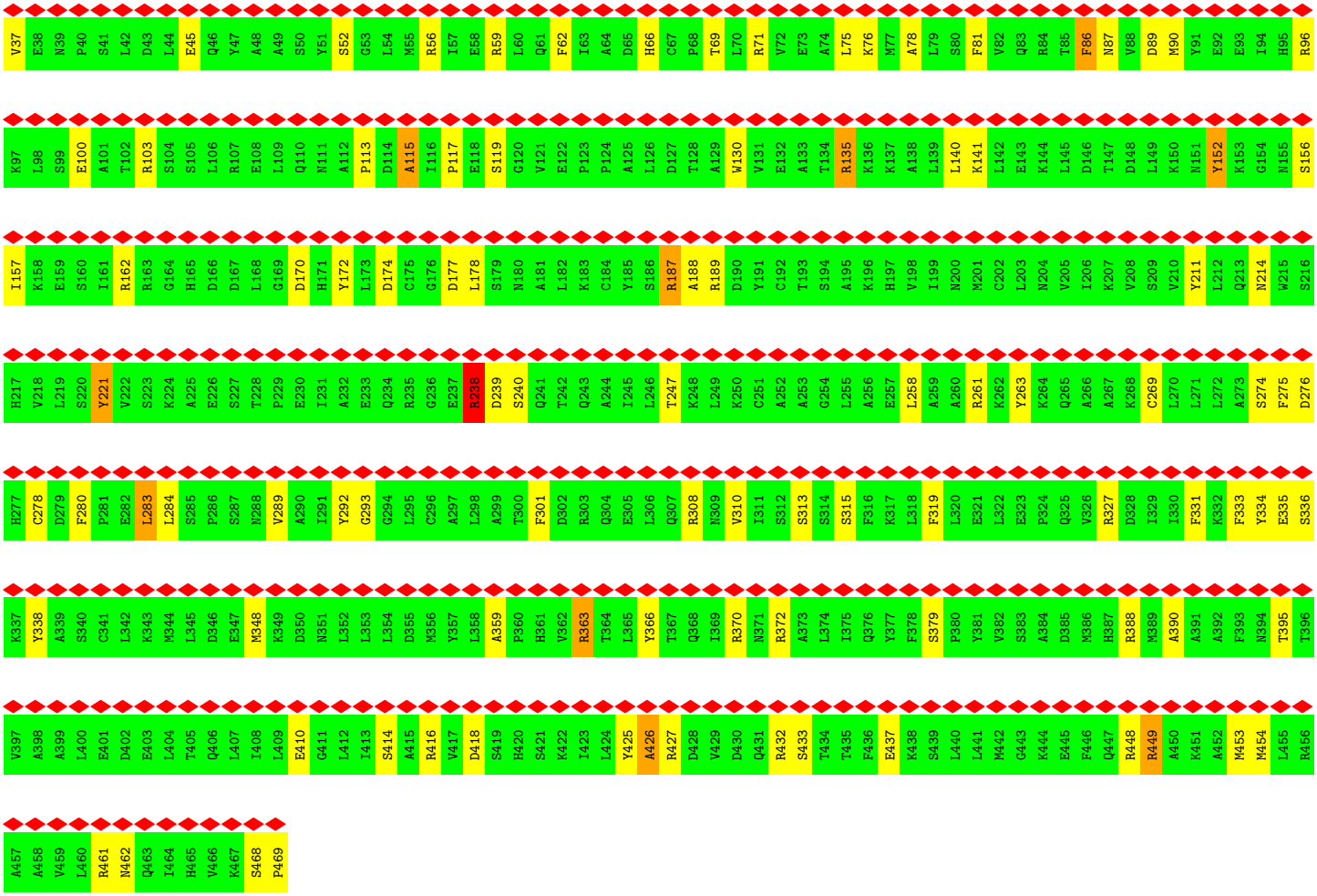
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	76	Total	C	N	O	S	0	0
			591	372	102	115	2		

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.

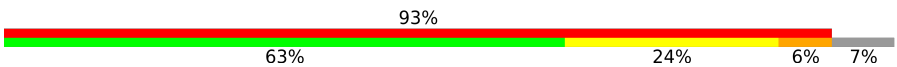
• Molecule 1: COP9 signalosome complex subunit 1

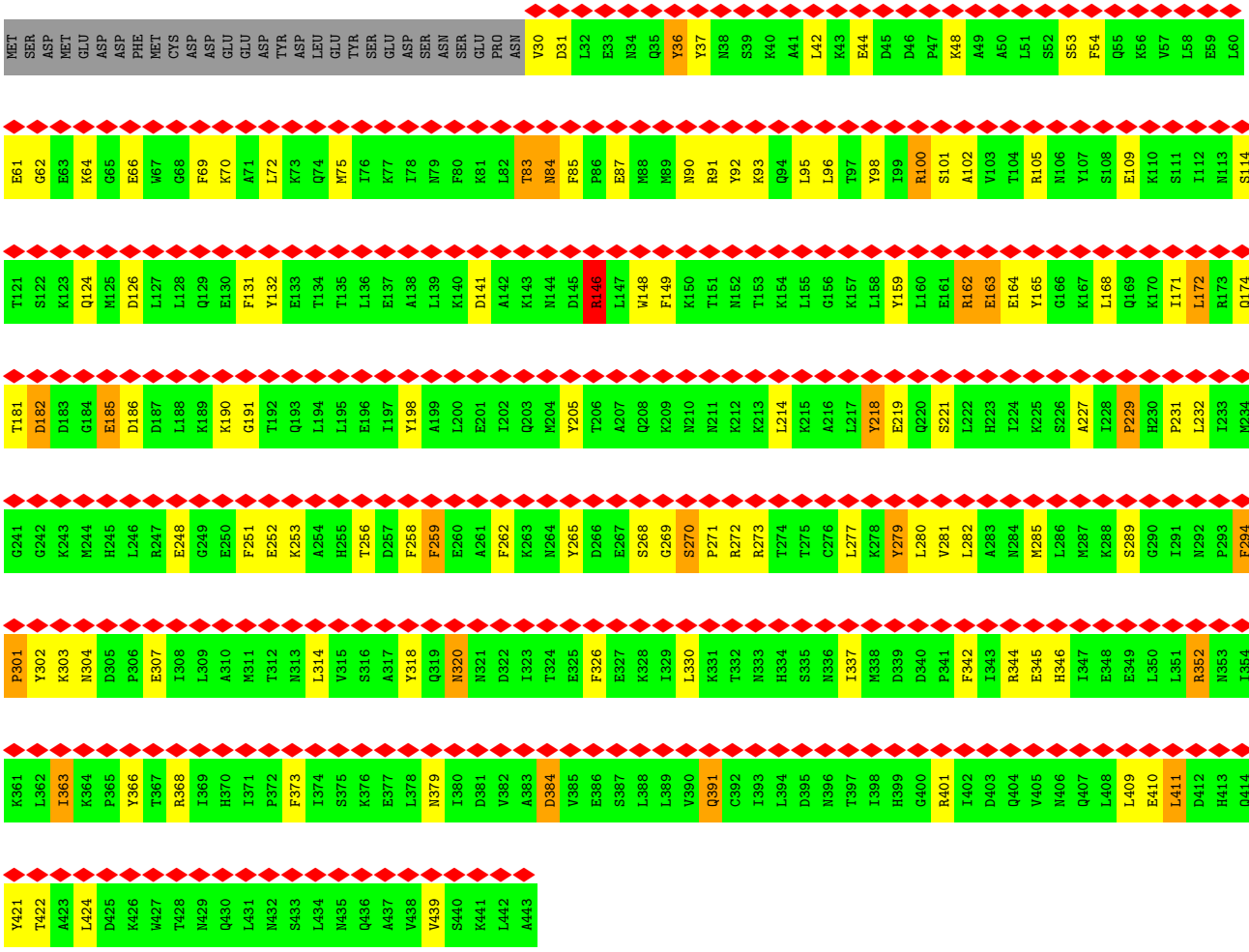
Chain A:



• Molecule 2: COP9 signalosome complex subunit 2

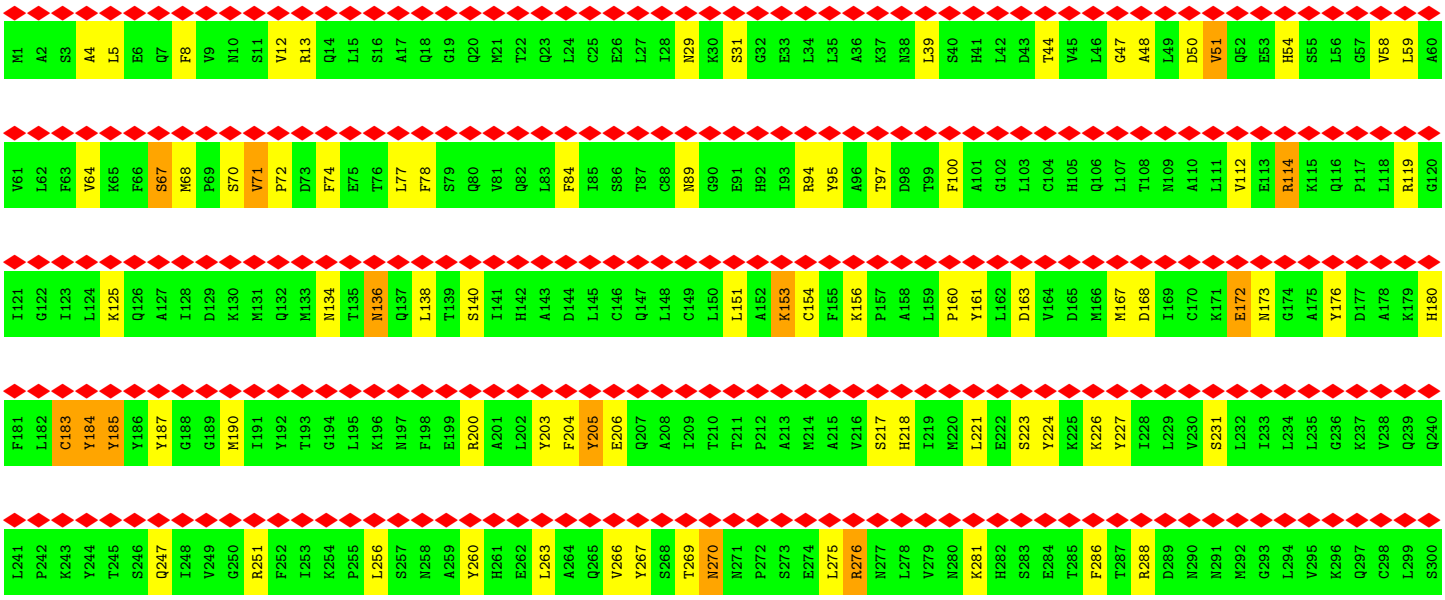
Chain B:

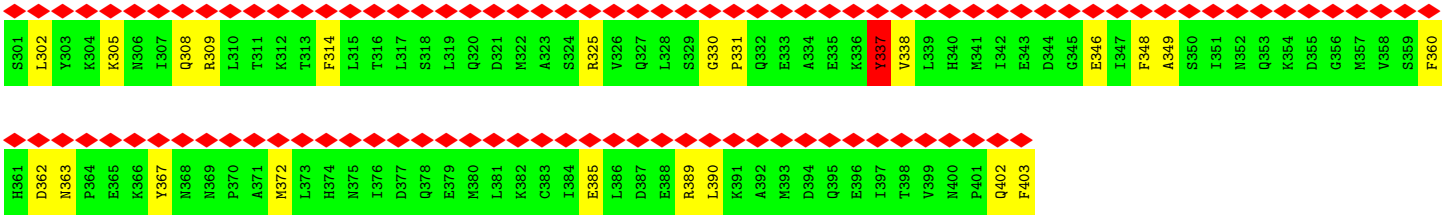




• Molecule 3: COP9 signalosome complex subunit 3

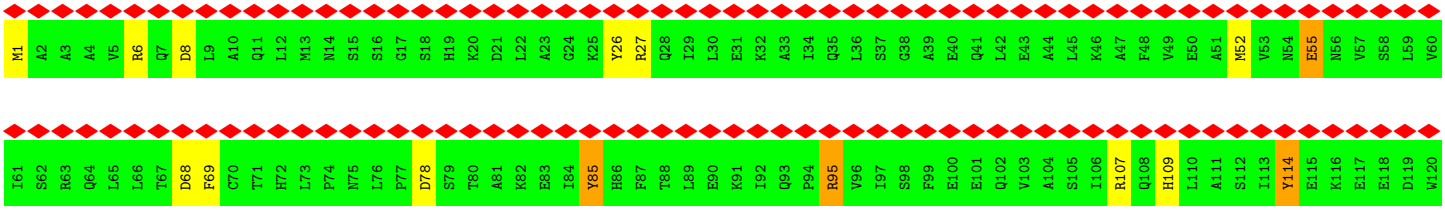
Chain C:





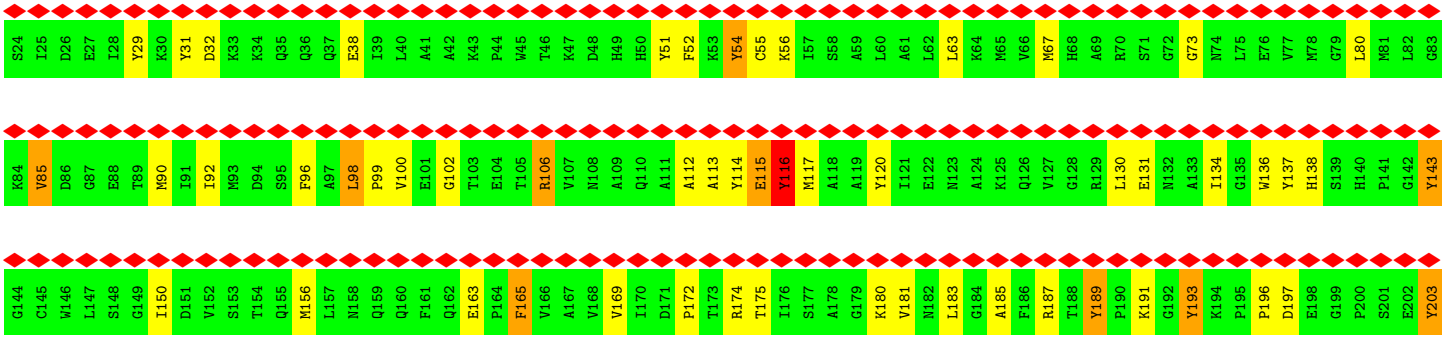
• Molecule 4: COP9 signalosome complex subunit 4

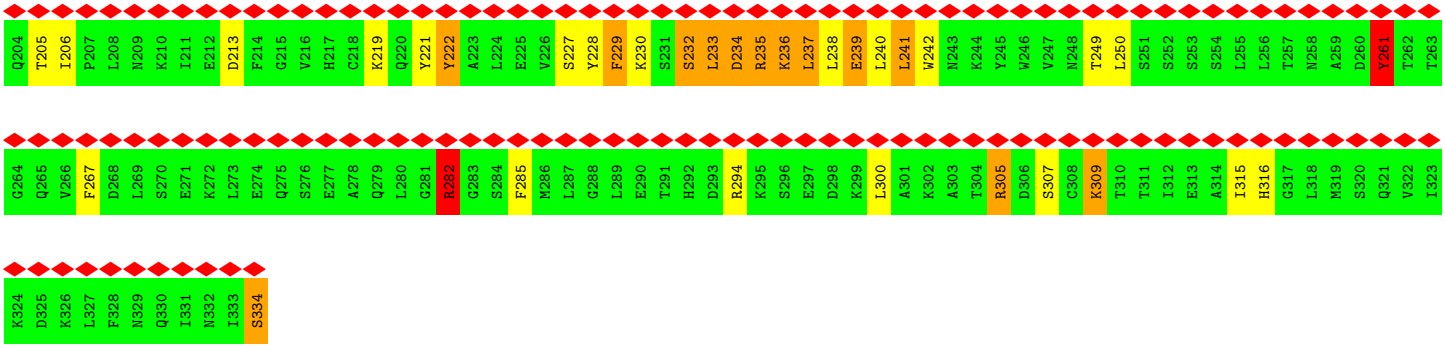
Chain D:



• Molecule 5: COP9 signalosome complex subunit 5

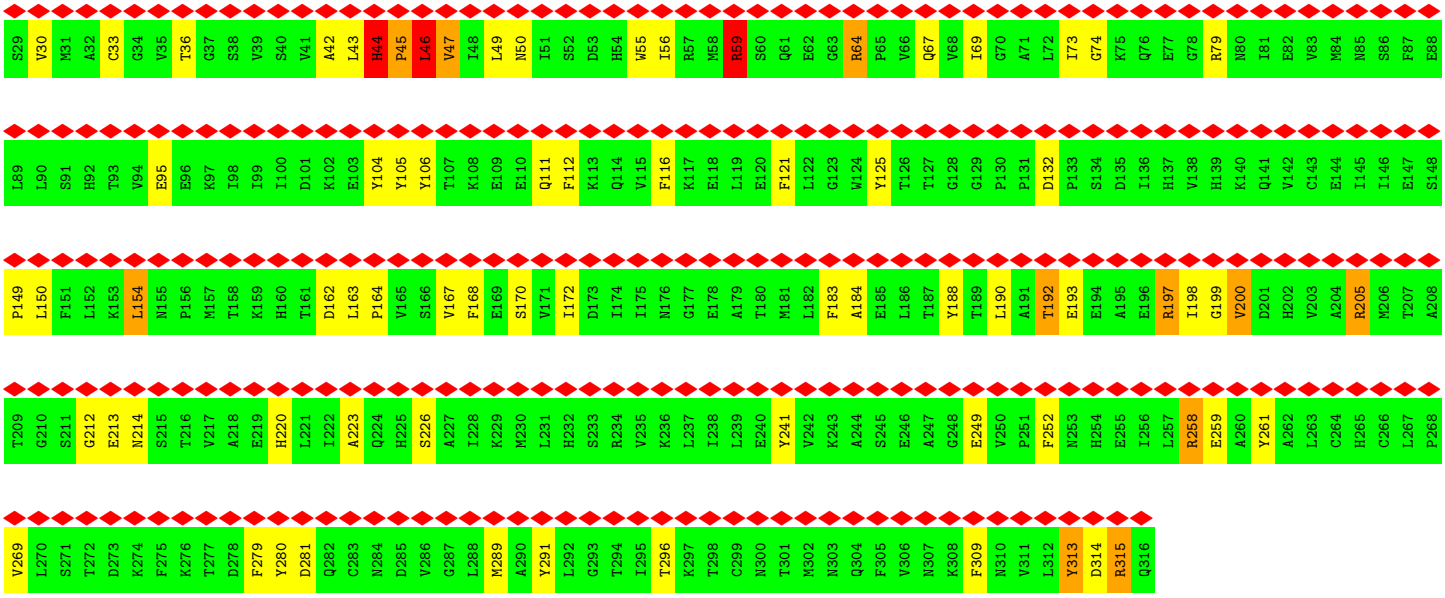
Chain E:





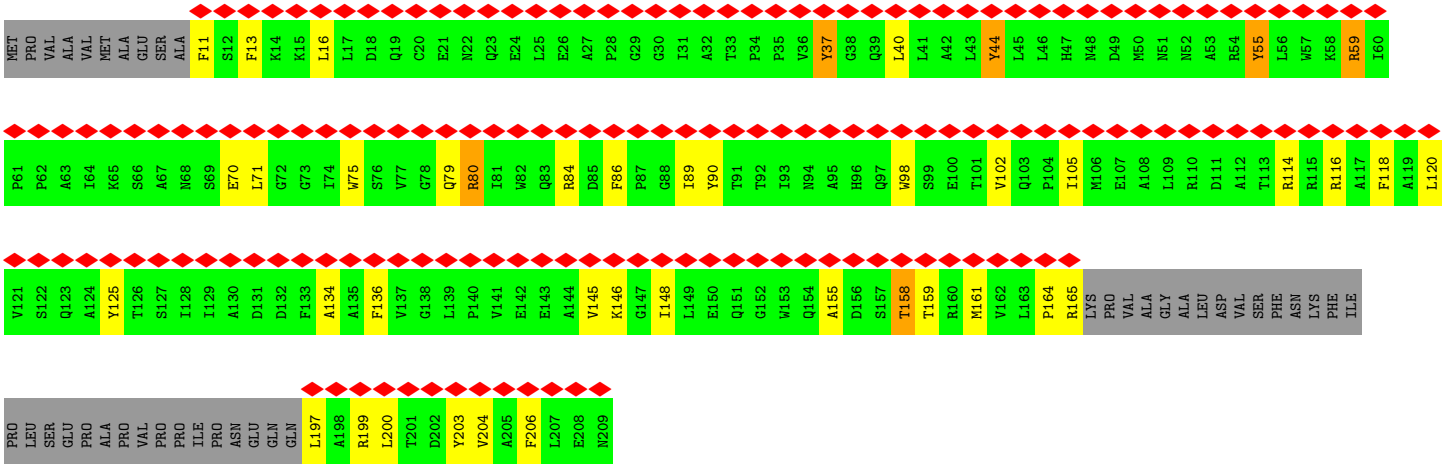
• Molecule 6: COP9 signalosome complex subunit 6

Chain F:



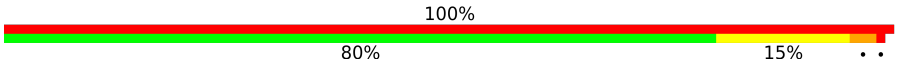
• Molecule 7: COP9 signalosome complex subunit 8

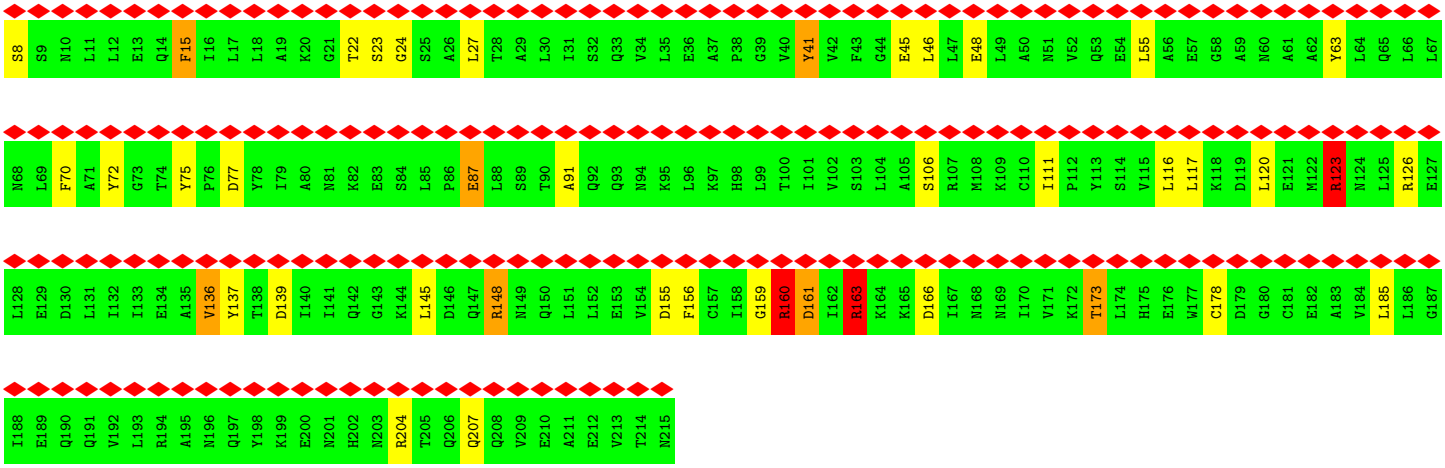
Chain H:



• Molecule 8: COP9 signalosome complex subunit 7b

Chain G:



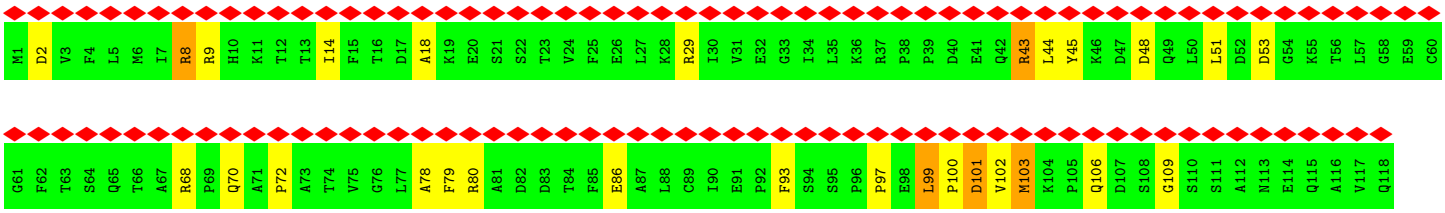


• Molecule 9: von Hippel-Lindau disease tumor suppressor

Chain V:

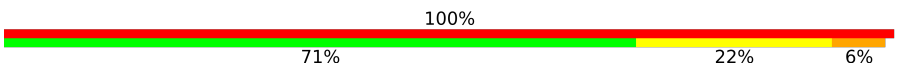
• Molecule 10: Elongin-B

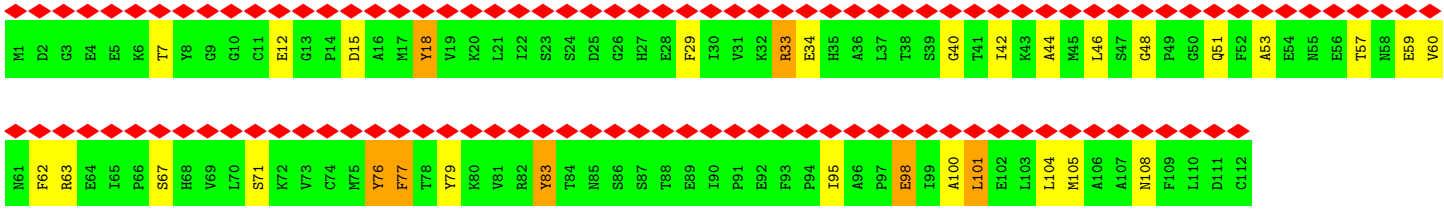
Chain P:



• Molecule 11: Elongin-C

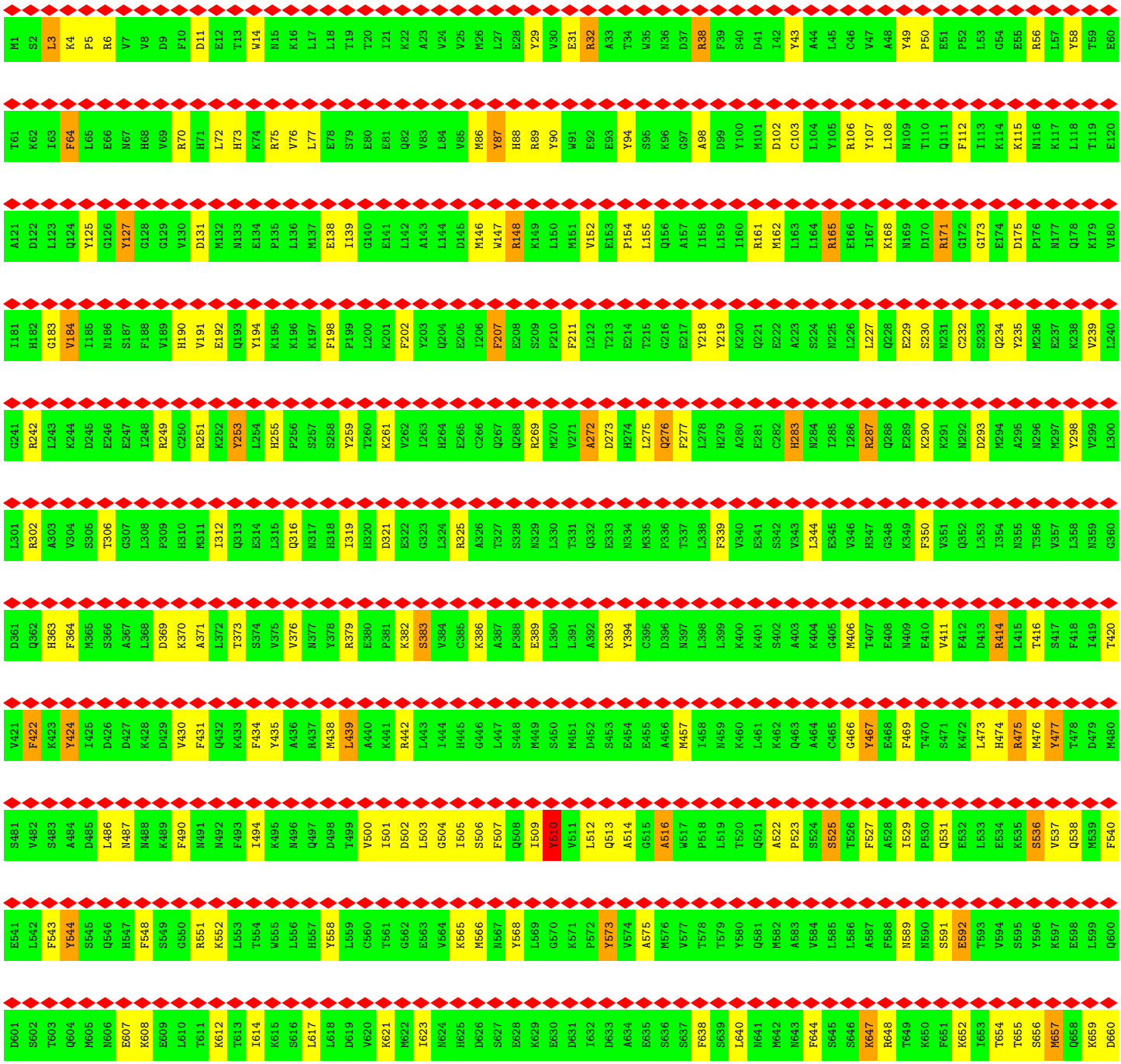
Chain Q:





• Molecule 12: Cullin-2

Chain O:



T661 P662 Q663 E664 M665 E666 Q667 T668 R669 S670 A671 V672 D673 E674 D675 R676 K677 M678 Y679 L680 Q681 A682 A683 I684 V685 R686 I687 M688 K689 A690 ARG K692 V693 L694 R695 H696 N697 A698 L699 I700 Q701 E702 V703 I704 S705 Q706 S707 R708 A709 R710 F711 N712 P713 S714 I715 S716 M717 I718 K719 K720

C721 I722 E723 V724 L725 I726 D727 K728 Q729 Y730 I731 E732 R733 S734 Q735 A736 S737 A738 D739 E740 Y741 S742 Y743 V744 A745

- Molecule 13: E3 ubiquitin-protein ligase RBX1

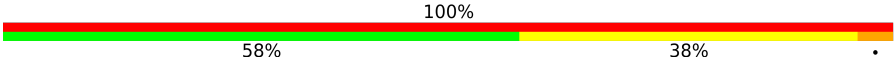
Chain R:

K19 K20 R21 F22 E23 V24 K25 K26 W27 N28 A29 V30 A31 L32 W33 A34 W35 D36 I37 V38 V39 D40 N41 C42 A43 I44 C45 R46 N47 H48 I49 M50 D51 L52 C53 I54 E55 C56 Q57 A58 N59 Q60 A61 S62 A63 T64 S65 E66 E67 C68 T69 V70 A71 W72 G73 V74 C75 N76 H77 A78

F79 H80 F81 H82 C83 I84 S85 R86 W87 L88 K89 T90 R91 Q92 V93 C94 P95 L96 D97 N98 R99 E100 W101 E102 F103 Q104 K105 Y106 G107 H108

- Molecule 14: NEDD8

Chain N:



M1 L2 I3 K4 V5 K6 T7 L8 T9 G10 K11 E12 I13 E14 I15 D16 I17 E18 P19 T20 D21 K22 V23 E24 R25 I26 K27 E28 R29 V30 E31 E32 K33 E34 G35 I36 P37 P38 Q39 Q40 Q41 R42 L43 I44 Y45 S46 G47 K48 Q49 M50 N51 D52 E53 K54 T55 A56 A57 D58 Y59 K60

I61 L62 G63 G64 S65 V66 L67 H68 L69 V70 L71 A72 L73 R74 G75 G76

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (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	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(^{o})	Ideal(^{o})
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 (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	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

Continued on next page...

Continued from previous page...

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

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

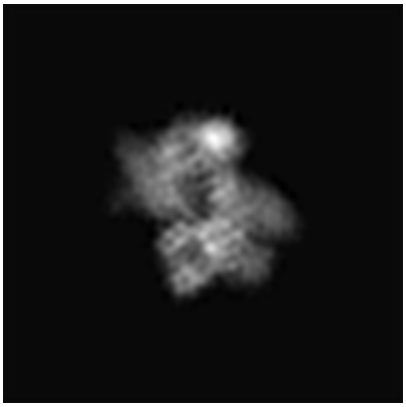
6 Map visualisation

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.

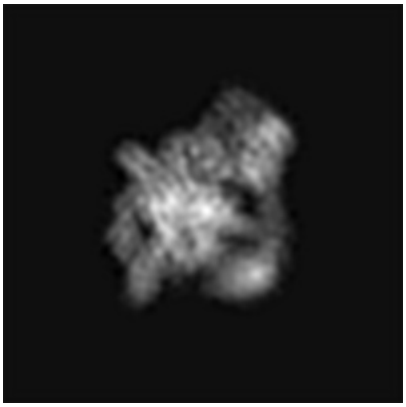
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

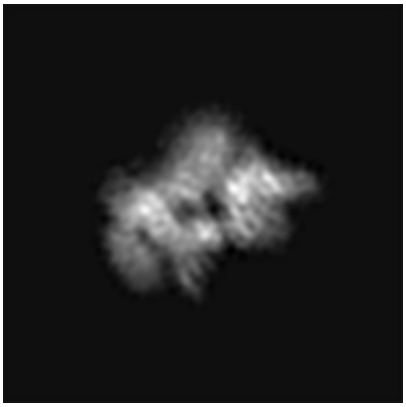
6.1.1 Primary map



X



Y

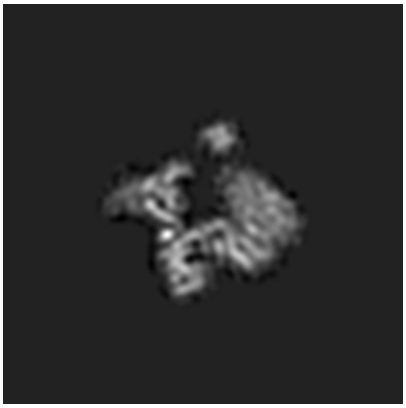


Z

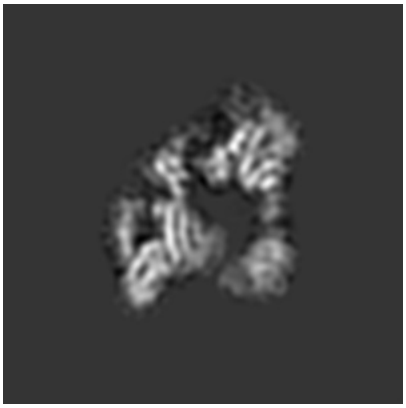
The images above show the map projected in three orthogonal directions.

6.2 Central slices

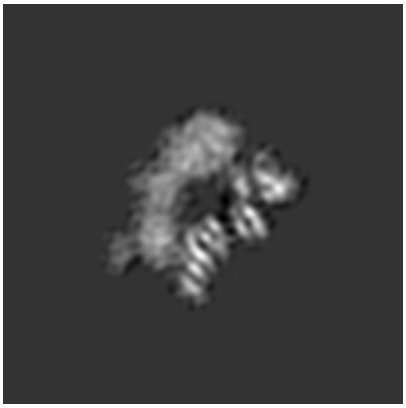
6.2.1 Primary map



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: 145

Y Index: 160

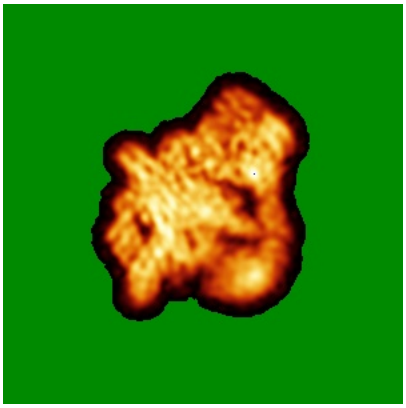
Z Index: 126

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

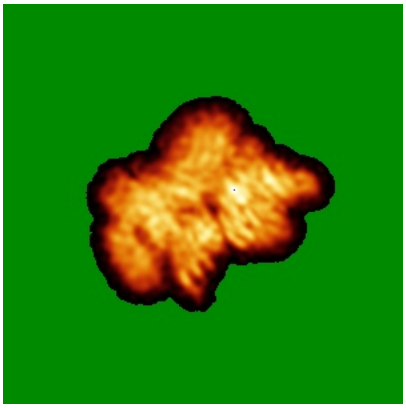
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

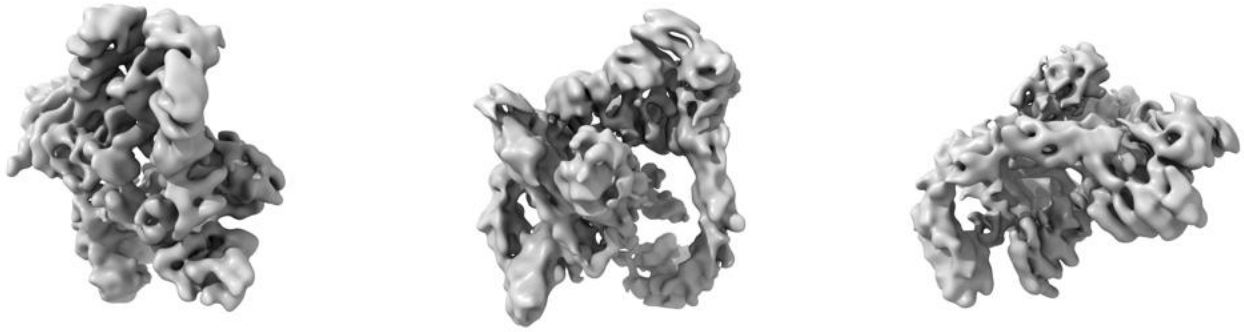


Z

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.

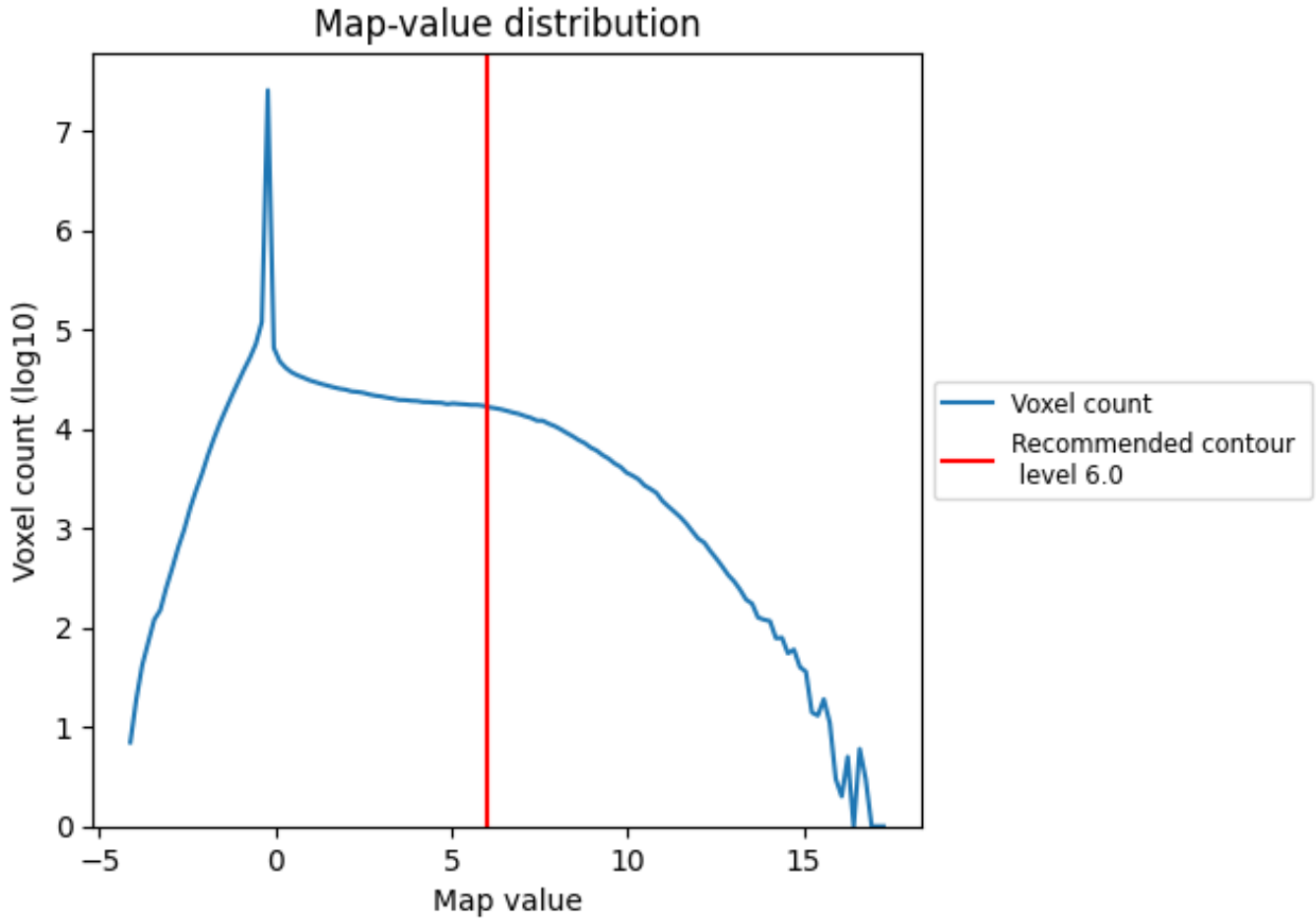
6.6 Mask visualisation (i)

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

7 Map analysis

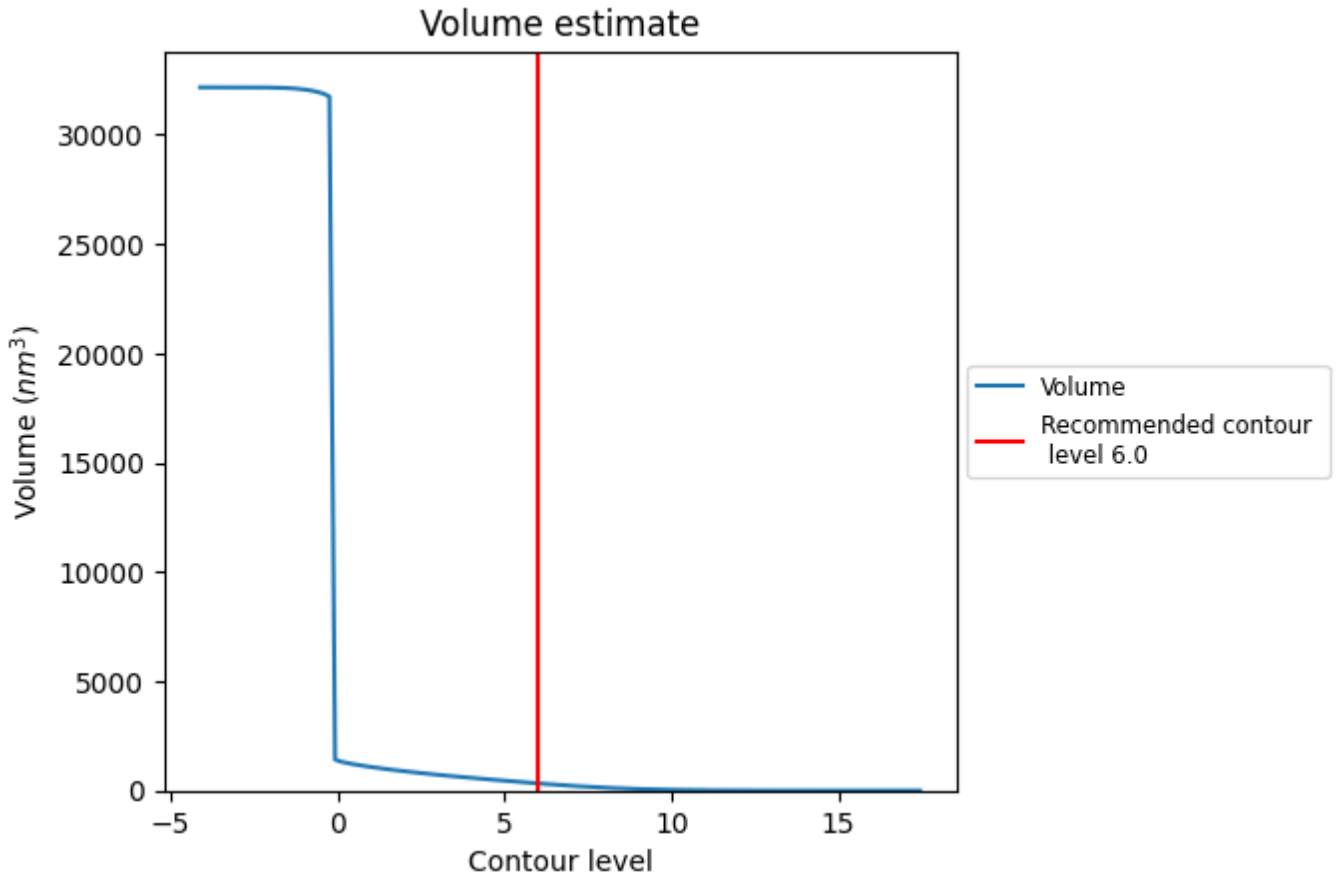
This section contains the results of statistical analysis of the map.

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.

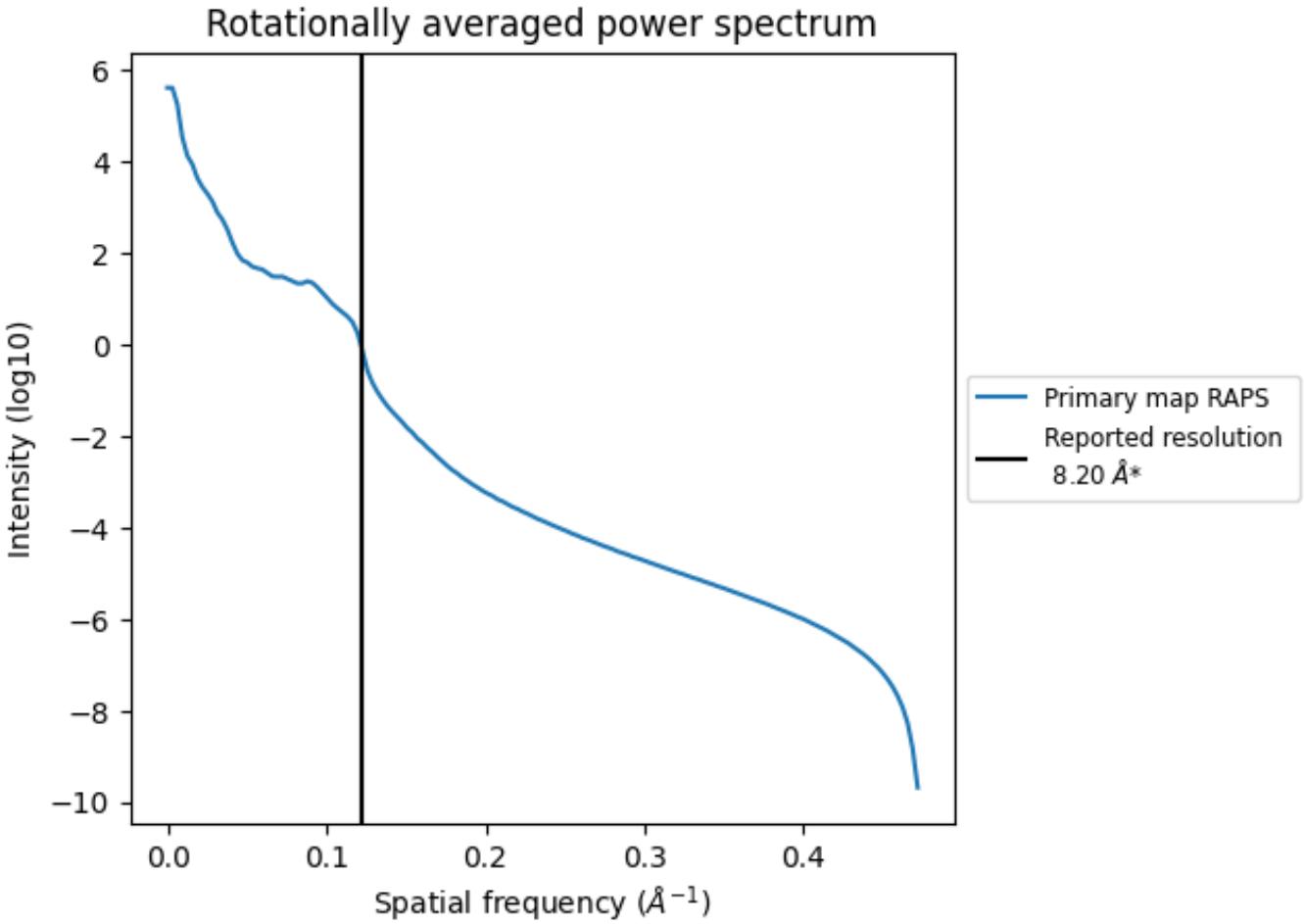
7.2 Volume estimate (i)



The volume at the recommended contour level is 327 nm^3; 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}

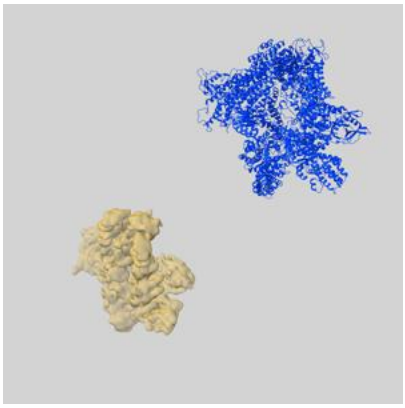
8 Fourier-Shell correlation (i)

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

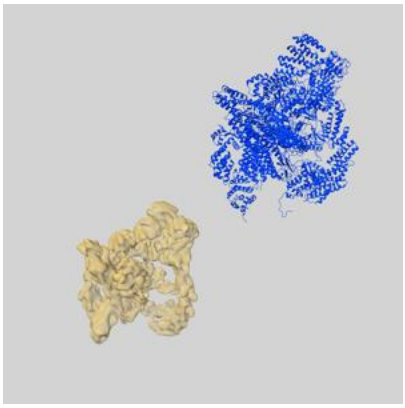
9 Map-model fit

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

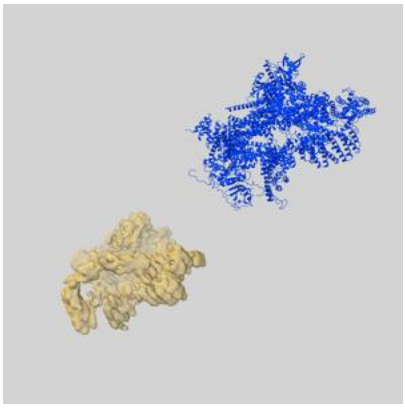
9.1 Map-model overlay



X



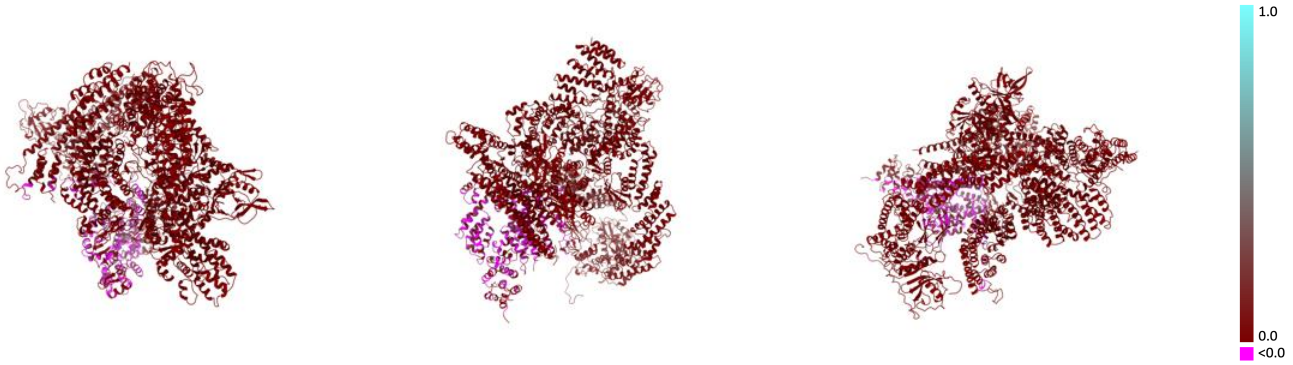
Y



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.

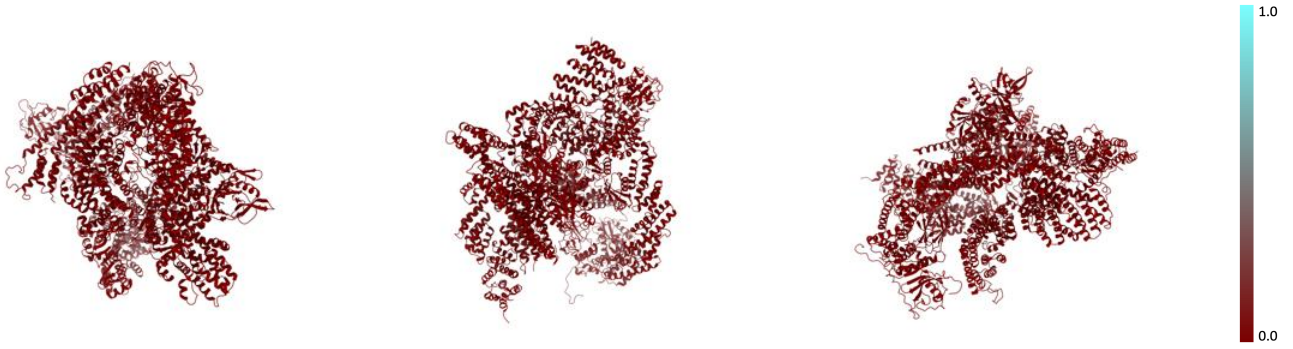
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

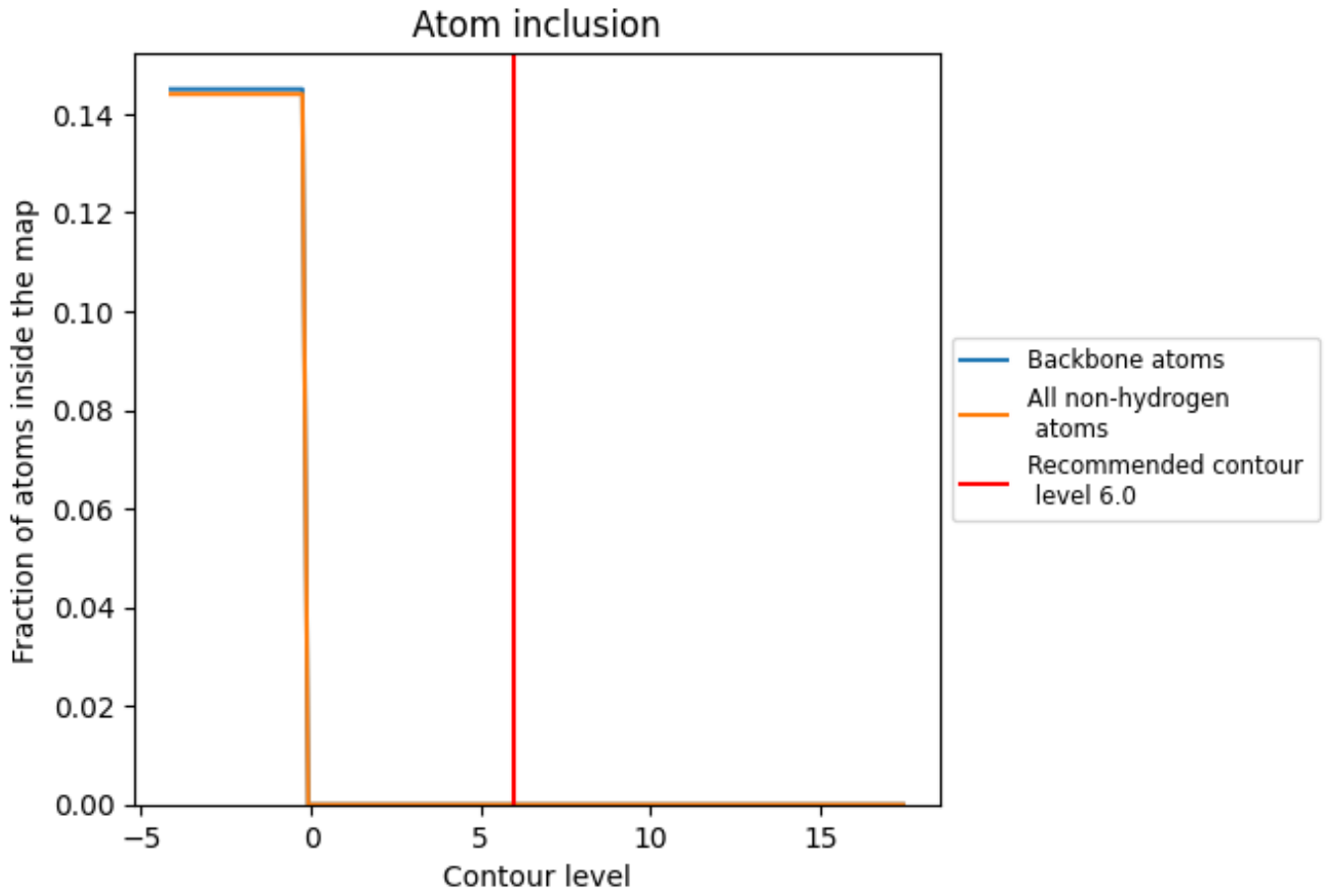
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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