



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 04:11 pm GMT

PDB ID : 6R7I
EMDB ID : EMD-4742
Title : Structural basis of Cullin-2 RING E3 ligase regulation by the COP9 signalosome
Authors : Faull, S.F.; Lau, A.M.C.; Beuron, F.; Cronin, N.B.; Morris, E.P.; Politis, A.
Deposited on : 2019-03-28
Resolution : 5.90 Å(reported)

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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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

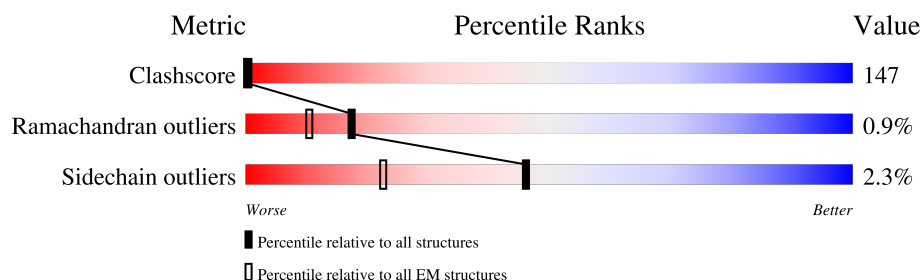
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	462	<div> <div>7%</div> <div>10%</div> <div>80%</div> <div>8%</div> </div>
2	B	443	<div> <div>13%</div> <div>14%</div> <div>79%</div> <div>•</div> </div>
3	C	401	<div> <div>8%</div> <div>10%</div> <div>88%</div> <div>•</div> </div>
4	D	407	<div> <div>8%</div> <div>46%</div> <div>53%</div> <div>•</div> </div>
5	E	334	<div> <div>61%</div> <div>11%</div> <div>77%</div> <div>•</div> <div>11%</div> </div>
6	F	327	<div> <div>43%</div> <div>13%</div> <div>69%</div> <div>•</div> <div>14%</div> </div>
7	G	215	<div> <div>18%</div> <div>15%</div> <div>82%</div> <div>•</div> </div>
8	H	209	<div> <div>•</div> <div>11%</div> <div>70%</div> <div>•</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
9	N	78	<div><div></div><div>96%</div><div>10%</div><div>87%</div><div></div></div>
10	O	745	<div><div></div><div>33%</div><div>14%</div><div>78%</div><div>7%</div><div></div></div>
11	P	106	<div><div></div><div>26%</div><div>9%</div><div>88%</div><div></div></div>
12	Q	99	<div><div></div><div>26%</div><div>30%</div><div>53%</div><div>14%</div><div></div></div>
13	R	85	<div><div></div><div>41%</div><div>5%</div><div>89%</div><div>6%</div><div></div></div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 34171 atoms, of which 4049 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	426	Total	C	N	O	S	0	0
			3382	2133	595	632	22		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	LYS	-	expression tag	UNP Q13098
A	71	VAL	-	expression tag	UNP Q13098
A	72	TYR	-	expression tag	UNP Q13098
A	73	ILE	-	expression tag	UNP Q13098
A	74	GLU	-	expression tag	UNP Q13098
A	75	LYS	-	expression tag	UNP Q13098
A	76	ASP	-	expression tag	UNP Q13098

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	428	Total	C	N	O	S	0	0
			3429	2177	591	646	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	400	Total	C	N	O	S	0	0
			3183	2028	533	596	26		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	407	Total	C	H	N	O	S	8	0
			6249	2075	2959	572	623	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ARG	-	expression tag	UNP Q9BT78

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	298	Total	C	N	O	S	0	0
			2366	1510	393	450	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	281	Total	C	N	O	S	0	0
			2236	1429	371	421	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	215	Total	C	N	O	S	0	0
			1678	1060	283	328	7		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	167	LEU	ILE	conflict	UNP Q9H9Q2
G	168	SER	ASN	conflict	UNP Q9H9Q2
G	169	ALA	ASN	conflict	UNP Q9H9Q2
G	171	ALA	VAL	conflict	UNP Q9H9Q2
G	172	ARG	LYS	conflict	UNP Q9H9Q2
G	175	GLN	HIS	conflict	UNP Q9H9Q2
G	179	VAL	ASP	conflict	UNP Q9H9Q2
G	183	VAL	ALA	conflict	UNP Q9H9Q2
G	186	SER	LEU	conflict	UNP Q9H9Q2
G	190	GLU	GLN	conflict	UNP Q9H9Q2
G	193	SER	LEU	conflict	UNP Q9H9Q2
G	198	HIS	TYR	conflict	UNP Q9H9Q2
G	201	GLN	ASN	conflict	UNP Q9H9Q2
G	202	GLN	HIS	conflict	UNP Q9H9Q2
G	203	LEU	ASN	conflict	UNP Q9H9Q2
G	204	GLY	ARG	conflict	UNP Q9H9Q2
G	205	LEU	THR	conflict	UNP Q9H9Q2
G	206	LYS	GLN	conflict	UNP Q9H9Q2
G	209	ILE	VAL	conflict	UNP Q9H9Q2
G	211	SER	ALA	conflict	UNP Q9H9Q2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	214	ALA	THR	conflict	UNP Q9H9Q2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	172	Total	C	N	O	S	0	0
			1379	883	239	253	4		

- Molecule 9 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	78	Total	C	N	O	Se	0	0
			609	382	106	118	3		

- Molecule 10 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	744	Total	C	H	N	O	S	
			6393	3865	308	1031	1143	46	0

- Molecule 11 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	106	Total	C	N	O	S	0	0
			831	526	140	161	4		

- Molecule 12 is a protein called Elongin-C.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	85	Total	C	N	O	S	0	0
			686	431	127	119	9		

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

Mol	Chain	Residues	Atoms		AltConf
14	E	1	Total 1	Zn 1	0
14	R	3	Total 3	Zn 3	0

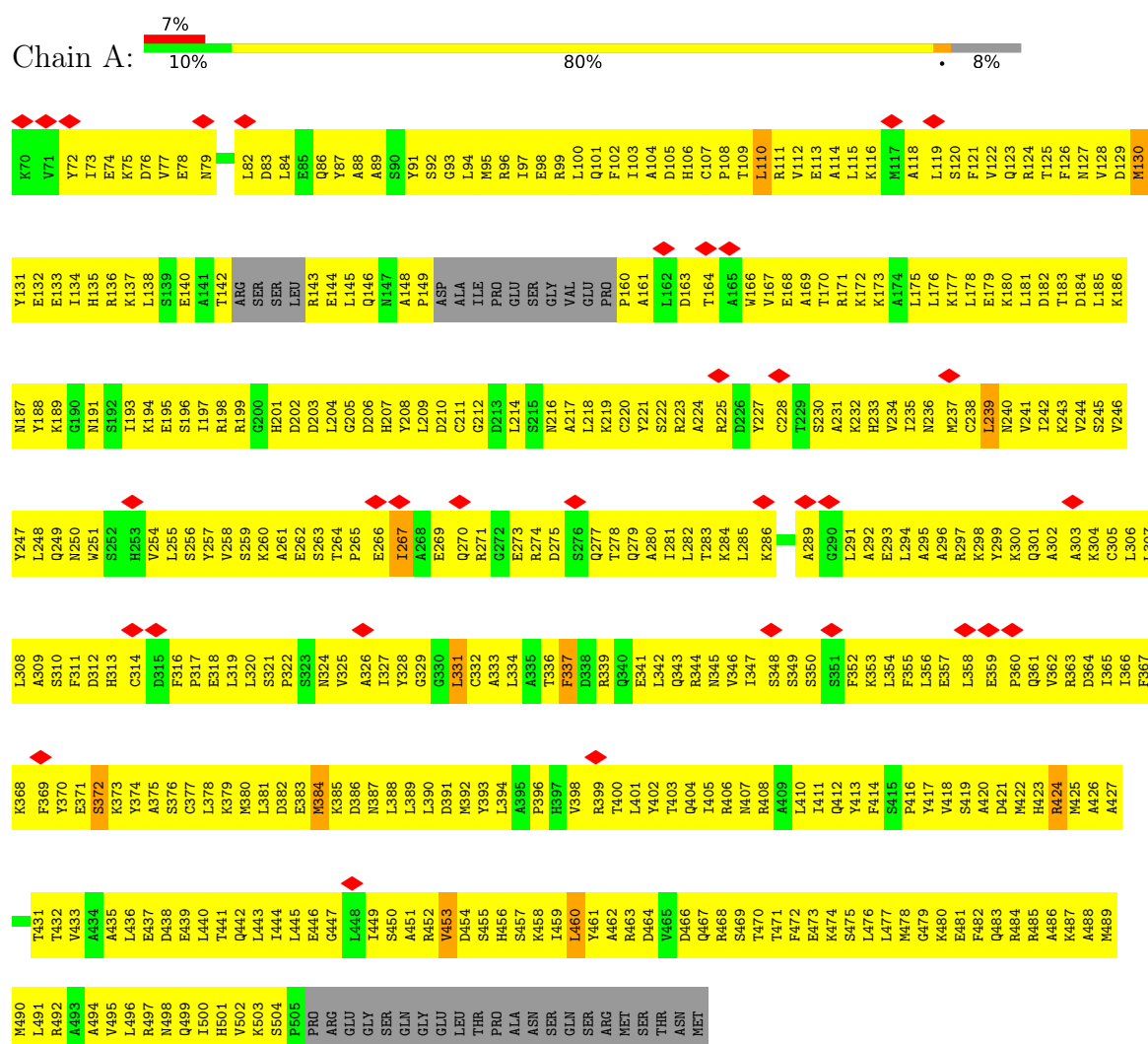
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	9	Total 9	O 9	0
15	P	144	Total 144	O 144	0
15	Q	16	Total 16	O 16	0

3 Residue-property plots

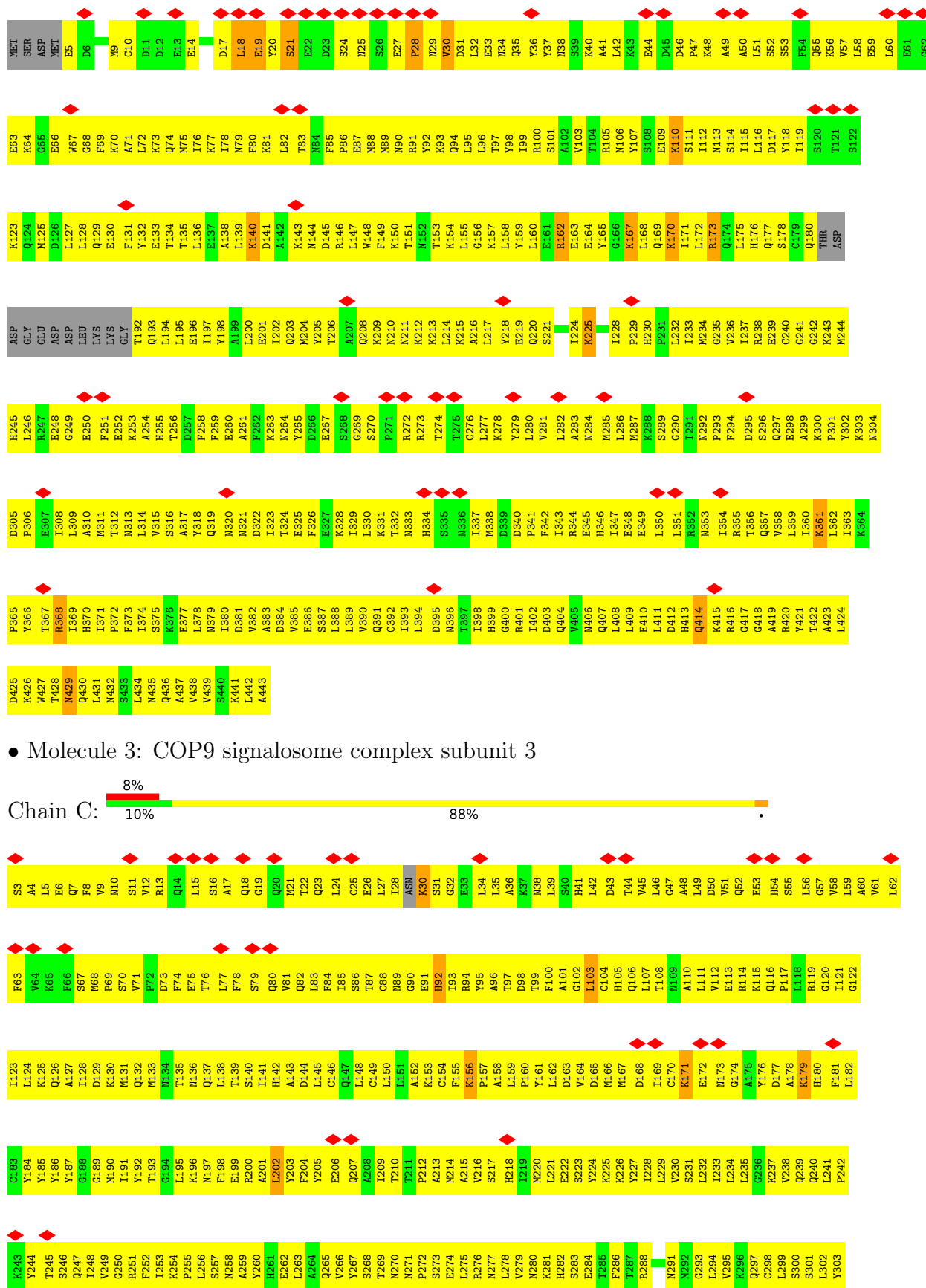
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

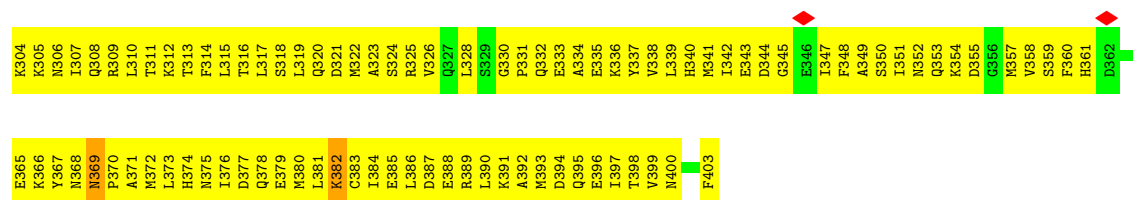
• Molecule 1: COP9 signalosome complex subunit 1



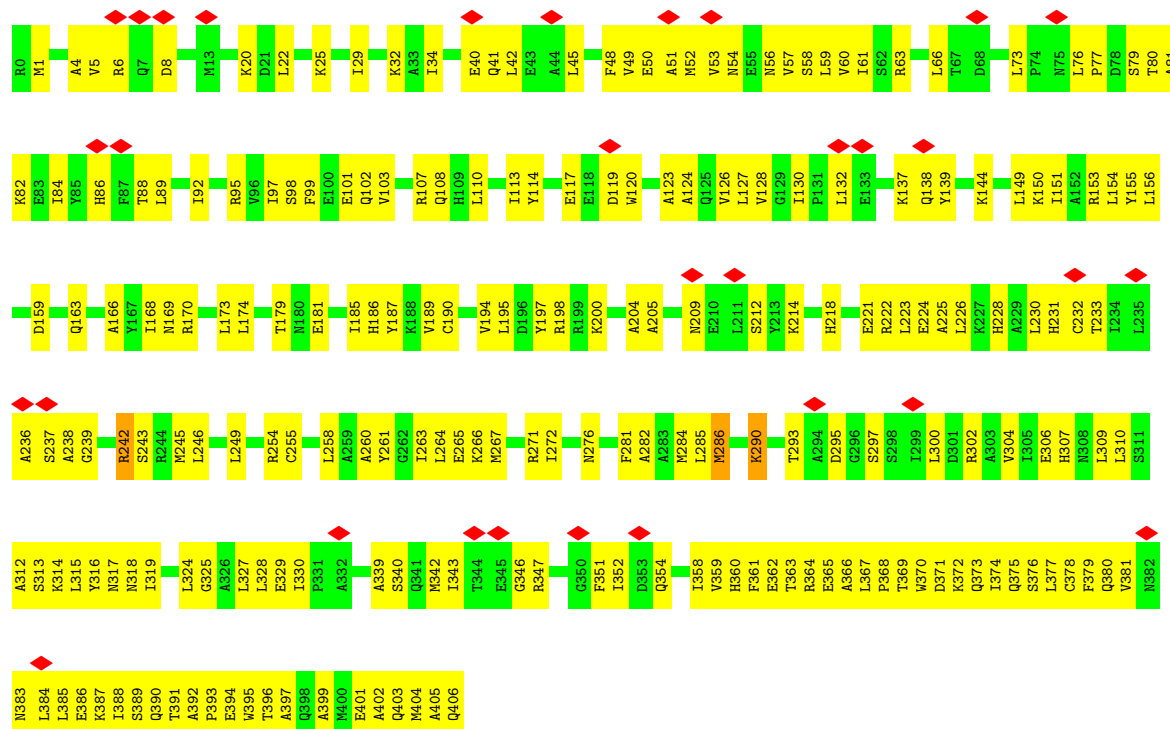
• Molecule 2: COP9 signalosome complex subunit 2







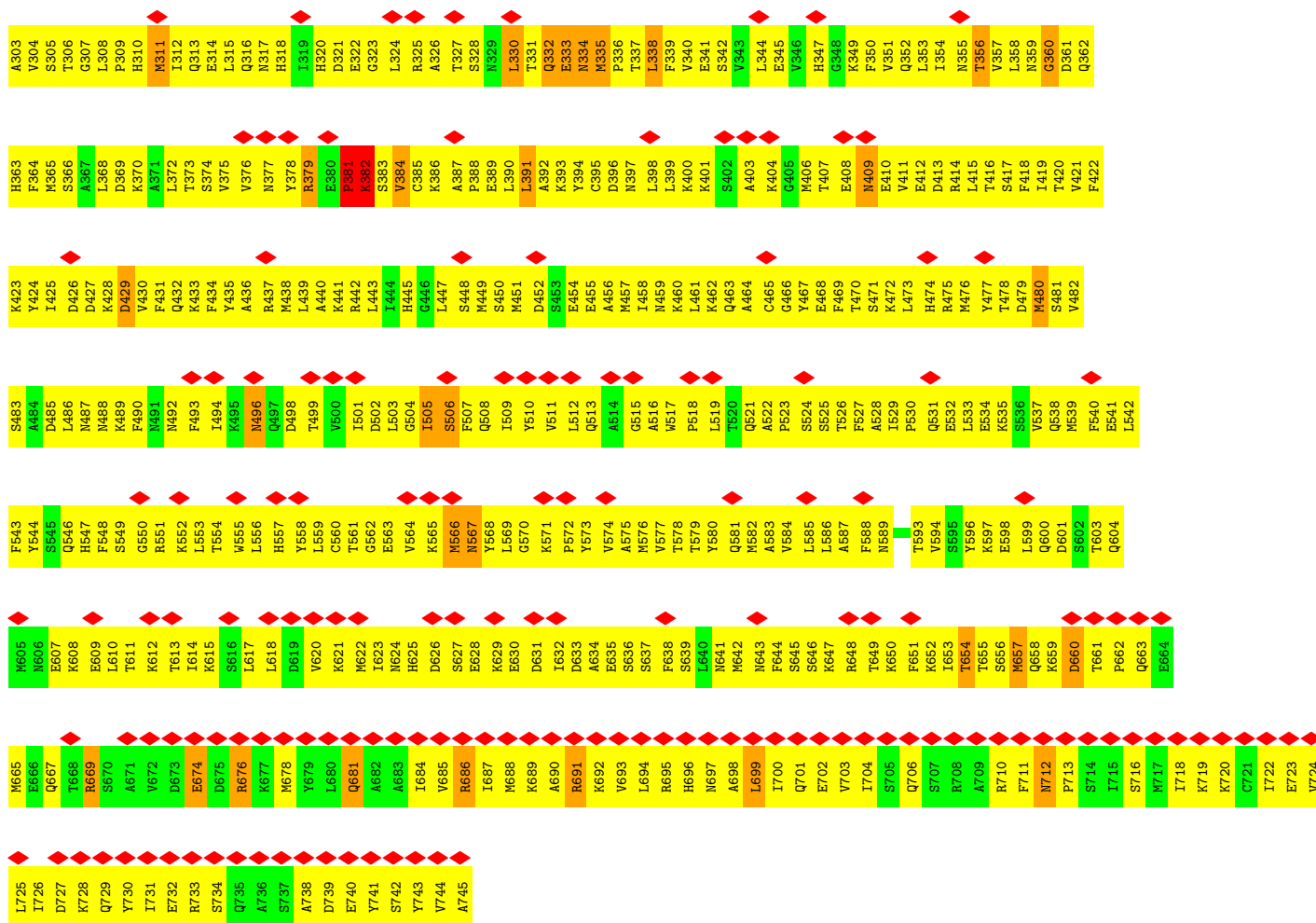
• Molecule 4: COP9 signalosome complex subunit 4



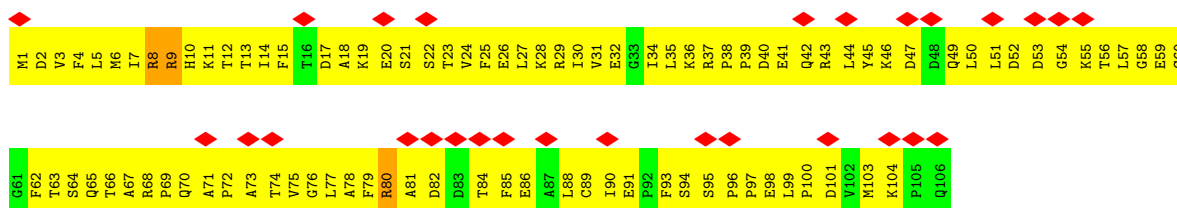
• Molecule 5: COP9 signalosome complex subunit 5



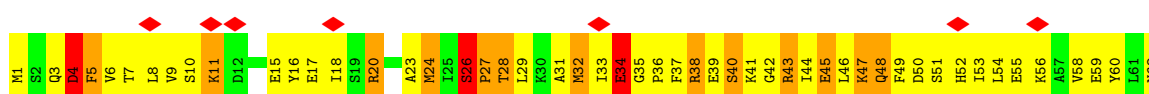




• Molecule 11: Elongin-B

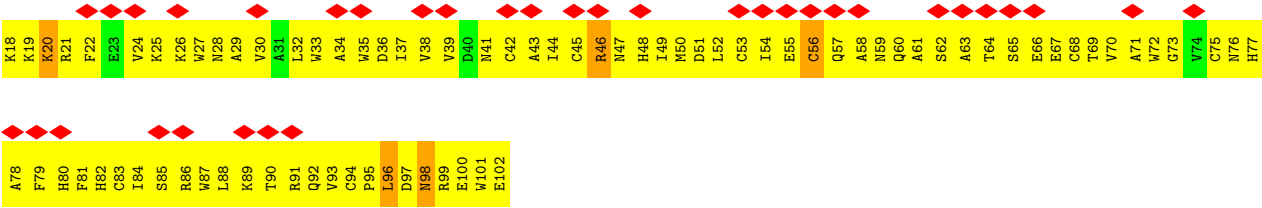


• Molecule 12: Elongin-C





• Molecule 13: E3 ubiquitin-protein ligase RBX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	316921	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.966	Depositor
Minimum map value	-12.318	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6	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 [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/3437	0.84	3/4632 (0.1%)
2	B	0.40	1/3485 (0.0%)	0.54	2/4694 (0.0%)
3	C	0.40	0/3241	0.59	2/4376 (0.0%)
4	D	0.54	0/3354	0.73	2/4523 (0.0%)
5	E	0.38	1/2417 (0.0%)	0.61	3/3266 (0.1%)
6	F	0.67	3/2282 (0.1%)	1.12	6/3092 (0.2%)
7	G	0.34	0/1697	0.63	4/2293 (0.2%)
8	H	0.36	0/1411	0.50	0/1916
9	N	0.29	0/610	0.54	0/808
10	O	0.93	15/6193 (0.2%)	1.56	41/8323 (0.5%)
11	P	0.33	0/848	0.53	0/1148
12	Q	1.09	2/804 (0.2%)	2.07	7/1075 (0.7%)
13	R	0.39	0/702	0.68	0/950
All	All	0.60	22/30481 (0.1%)	1.00	70/41096 (0.2%)

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	6
2	B	0	1
3	C	0	3
4	D	0	3
5	E	0	2
6	F	0	3
7	G	0	2
10	O	0	17
11	P	0	2
12	Q	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	R	0	4
All	All	0	49

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	256	PRO	C-N	-37.88	0.47	1.34
12	Q	26	SER	C-N	26.39	1.84	1.34
6	F	293	GLY	C-N	25.80	1.93	1.34
10	O	48	ALA	C-N	24.04	1.89	1.34
10	O	265	GLU	C-N	20.19	1.80	1.34

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Q	4	ASP	O-C-N	-54.73	35.14	122.70
10	O	274	HIS	O-C-N	-47.18	47.21	122.70
10	O	265	GLU	O-C-N	-39.51	59.49	122.70
10	O	254	LEU	C-N-CA	-38.18	26.25	121.70
10	O	254	LEU	CA-C-N	-37.19	35.38	117.20

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	LEU	Peptide
1	A	267	ILE	Peptide
1	A	337	PHE	Peptide
1	A	372	SER	Peptide
1	A	453	VAL	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	3382	0	3394	895	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3429	0	3396	954	0
3	C	3183	0	3201	886	0
4	D	3290	2959	3301	434	0
5	E	2366	0	2334	957	0
6	F	2236	0	2211	1106	0
7	G	1678	0	1709	625	0
8	H	1379	0	1361	459	0
9	N	609	0	632	404	0
10	O	6085	308	6016	2453	0
11	P	831	0	825	418	0
12	Q	795	782	764	437	0
13	R	686	0	651	384	0
14	E	1	0	0	0	0
14	R	3	0	0	0	0
15	A	9	0	0	10	0
15	P	144	0	0	95	0
15	Q	16	0	0	19	0
All	All	30122	4049	29795	8756	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 147.

The worst 5 of 8756 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)
4:D:404:MET:SD	6:F:161:THR:HG21	1.26	1.67
11:P:34:ILE:HG12	12:Q:5:PHE:CE2	1.18	1.67
10:O:211:PHE:CE2	10:O:262:VAL:HG11	1.30	1.66
2:B:443:ALA:HB1	3:C:244:TYR:CD2	1.24	1.64
10:O:211:PHE:CE2	10:O:259:TYR:HD2	1.14	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	420/462 (91%)	338 (80%)	82 (20%)	0	100	100
2	B	423/443 (96%)	367 (87%)	52 (12%)	4 (1%)	14	51
3	C	396/401 (99%)	308 (78%)	87 (22%)	1 (0%)	37	73
4	D	407/407 (100%)	346 (85%)	61 (15%)	0	100	100
5	E	294/334 (88%)	237 (81%)	56 (19%)	1 (0%)	37	73
6	F	277/327 (85%)	237 (86%)	38 (14%)	2 (1%)	19	57
7	G	213/215 (99%)	185 (87%)	27 (13%)	1 (0%)	25	65
8	H	166/209 (79%)	147 (89%)	19 (11%)	0	100	100
9	N	74/78 (95%)	66 (89%)	8 (11%)	0	100	100
10	O	722/745 (97%)	579 (80%)	128 (18%)	15 (2%)	5	30
11	P	104/106 (98%)	91 (88%)	13 (12%)	0	100	100
12	Q	89/99 (90%)	73 (82%)	9 (10%)	7 (8%)	1	9
13	R	81/85 (95%)	51 (63%)	29 (36%)	1 (1%)	11	44
All	All	3666/3911 (94%)	3025 (82%)	609 (17%)	32 (1%)	17	51

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	30	VAL
6	F	258	ARG
10	O	256	PRO
10	O	265	GLU
10	O	266	CYS

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	365/403 (91%)	361 (99%)	4 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/405 (91%)	356 (97%)	11 (3%)	36	55
3	C	357/358 (100%)	353 (99%)	4 (1%)	70	80
4	D	352/348 (101%)	347 (99%)	5 (1%)	62	75
5	E	255/283 (90%)	255 (100%)	0	100	100
6	F	251/276 (91%)	245 (98%)	6 (2%)	44	62
7	G	184/184 (100%)	182 (99%)	2 (1%)	70	80
8	H	144/173 (83%)	142 (99%)	2 (1%)	62	75
9	N	67/64 (105%)	65 (97%)	2 (3%)	36	55
10	O	678/681 (100%)	650 (96%)	28 (4%)	26	47
11	P	92/94 (98%)	91 (99%)	1 (1%)	70	80
12	Q	90/90 (100%)	78 (87%)	12 (13%)	3	13
13	R	73/75 (97%)	72 (99%)	1 (1%)	62	75
All	All	3275/3434 (95%)	3197 (98%)	78 (2%)	46	62

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	O	566	MET
12	Q	43	ARG
10	O	660	ASP
12	Q	24	MET
12	Q	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	204	GLN
11	P	49	GLN
6	F	282	GLN
11	P	42	GLN
10	O	513	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	O	18
12	Q	5
4	D	3
2	B	2
13	R	1
9	N	1
1	A	1
6	F	1

The worst 5 of 32 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	192:THR	C	193:GLN	N	11.96
1	O	693:VAL	C	694:LEU	N	4.82
1	D	362:GLU	C	363:THR	N	4.17
1	R	33:TRP	C	34:ALA	N	4.13
1	O	175:ASP	C	176:PRO	N	3.97

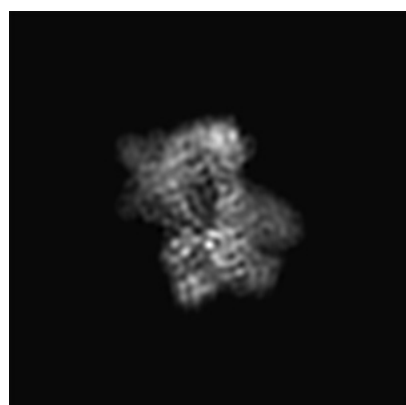
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4742. These allow visual inspection of the internal detail of the map and identification of artifacts.

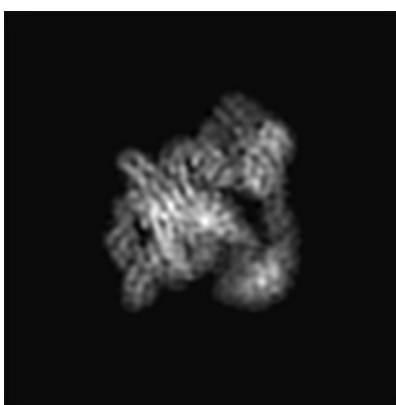
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

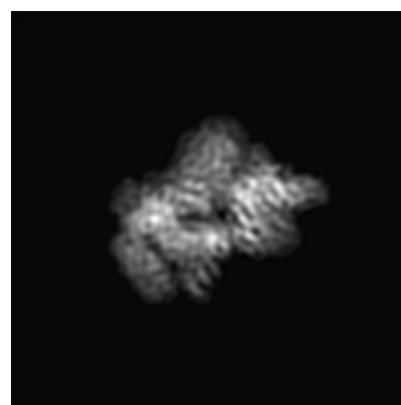
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

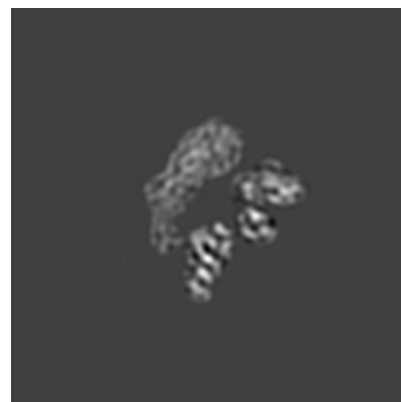
6.2.1 Primary map



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: 179



Y Index: 159



Z Index: 124

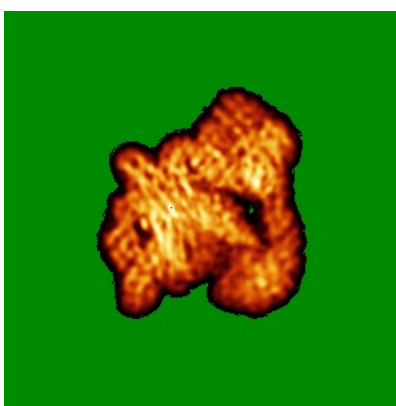
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

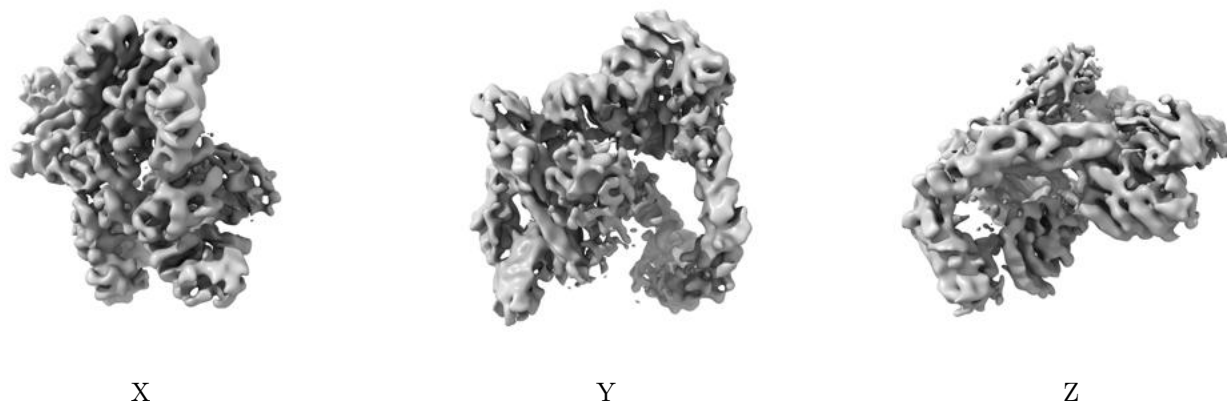


Z

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



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.

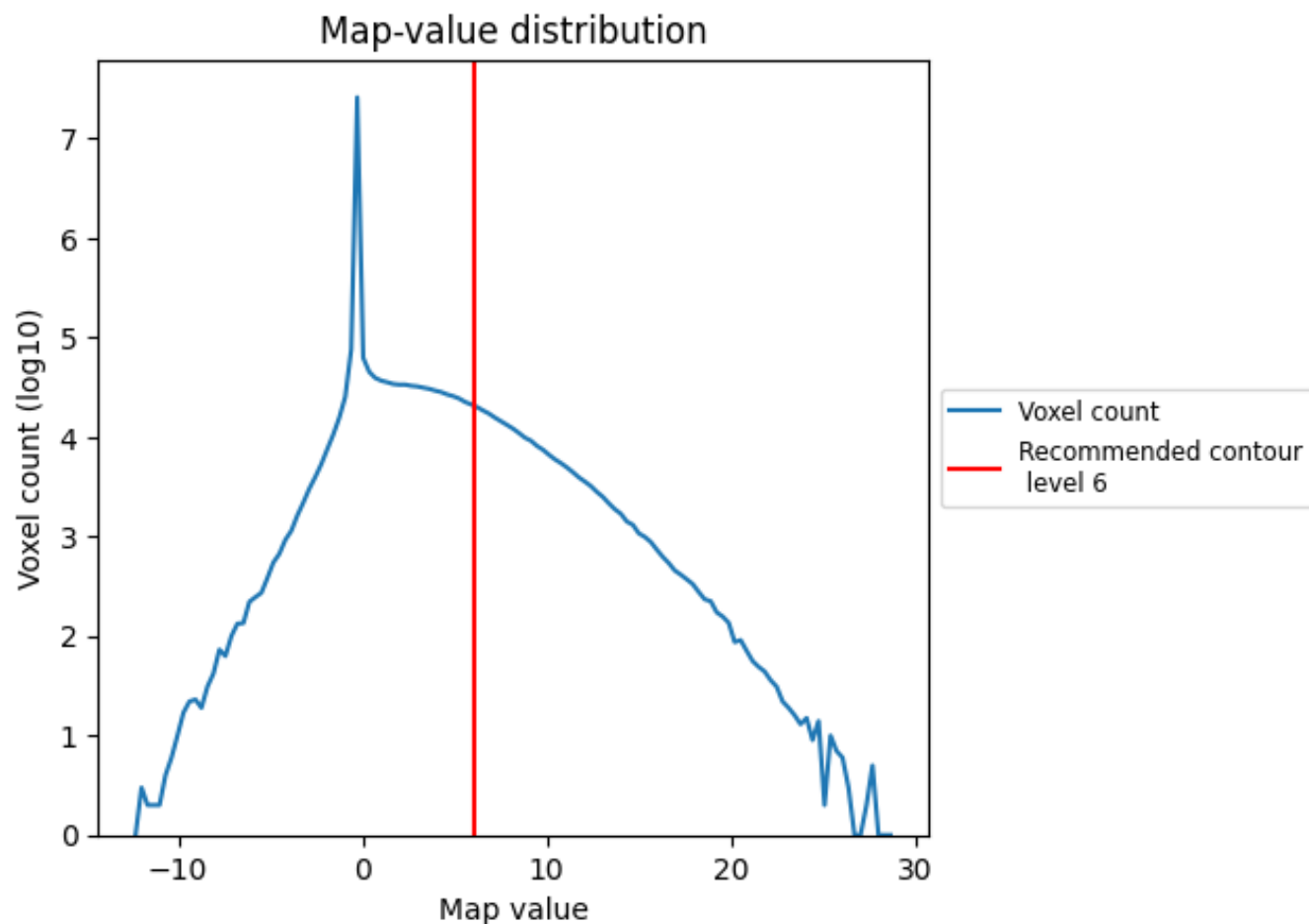
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

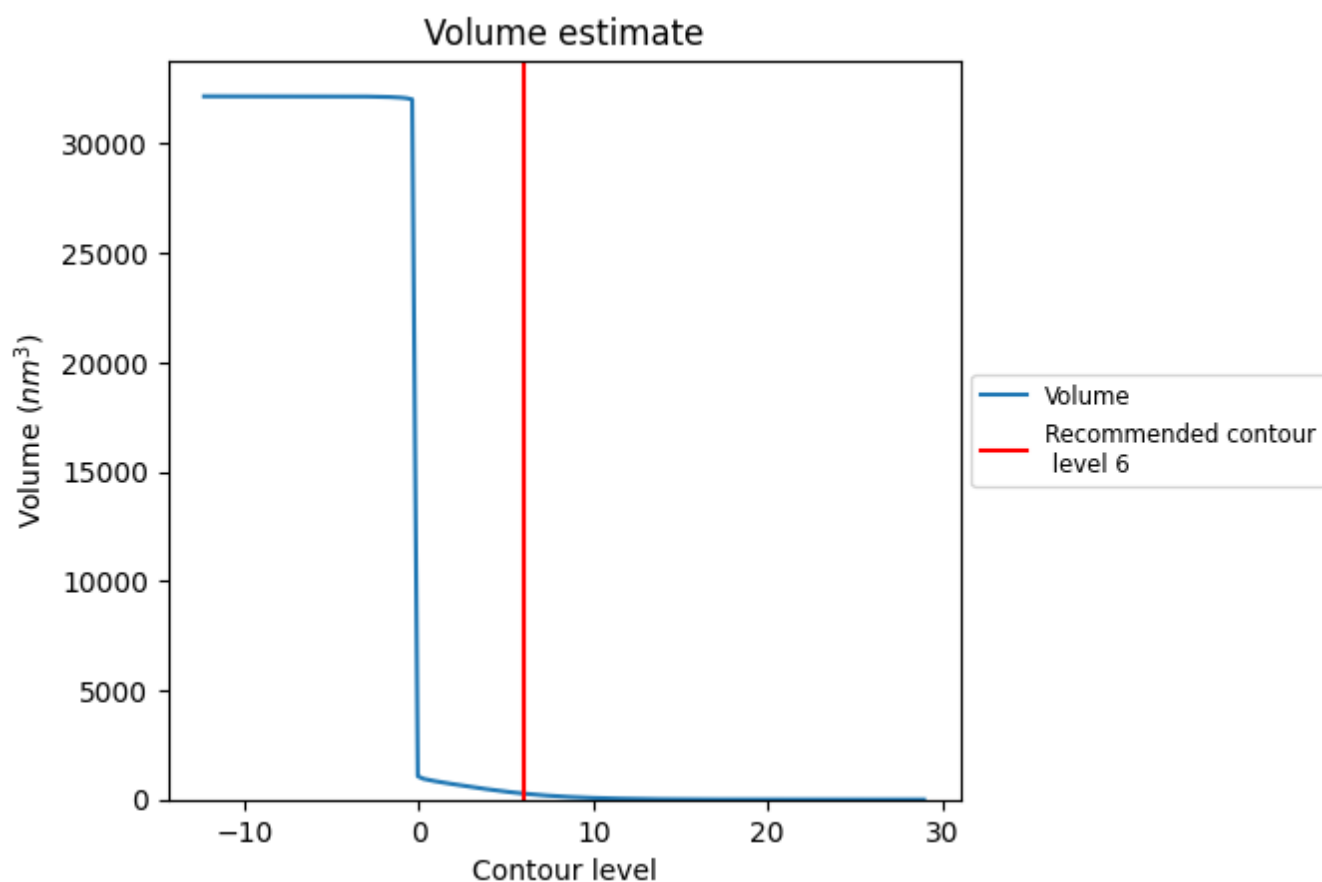
This section contains the results of statistical analysis of the map.

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.

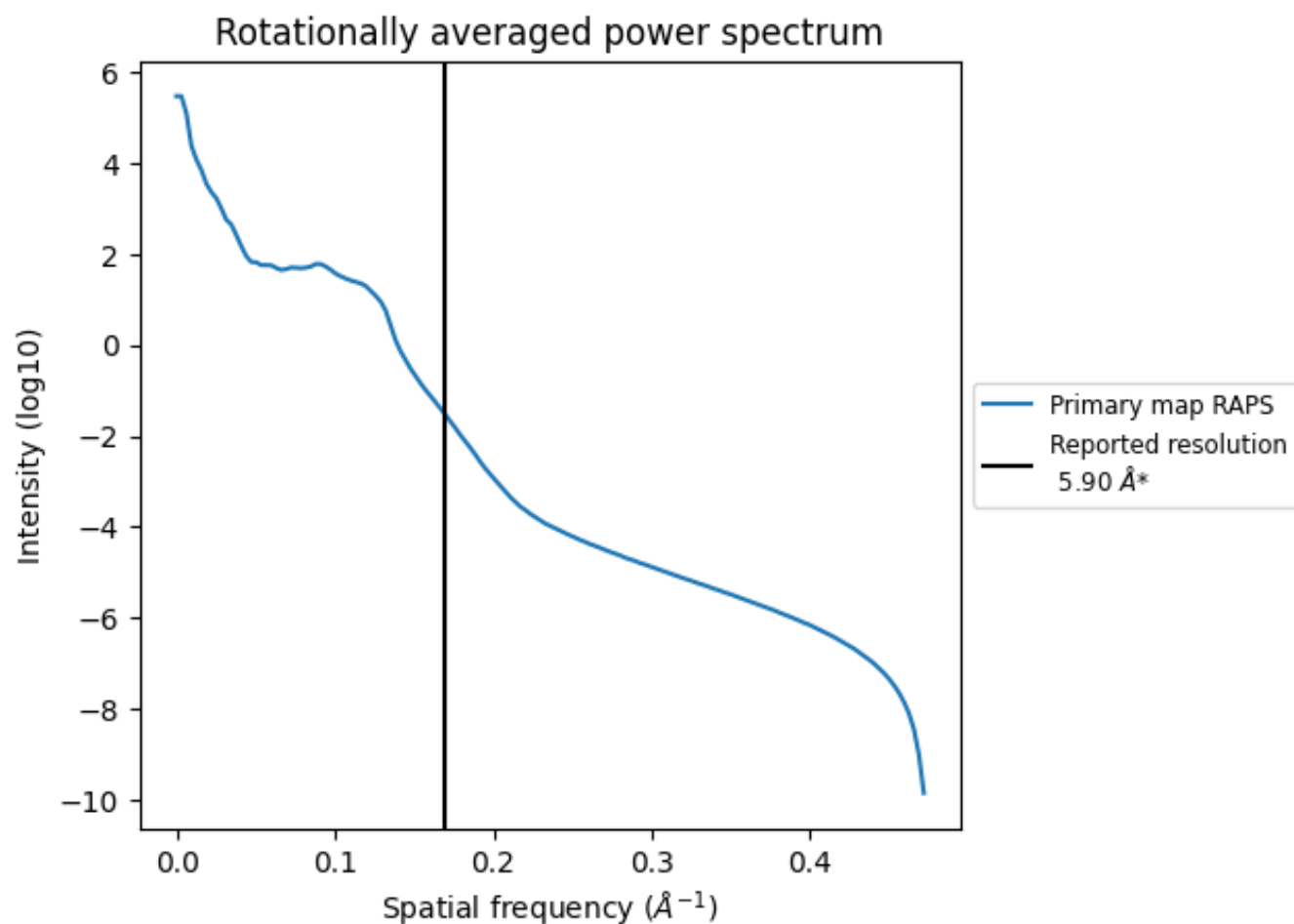
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 275 nm^3 ; this corresponds to an approximate mass of 248 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 0.169 Å⁻¹

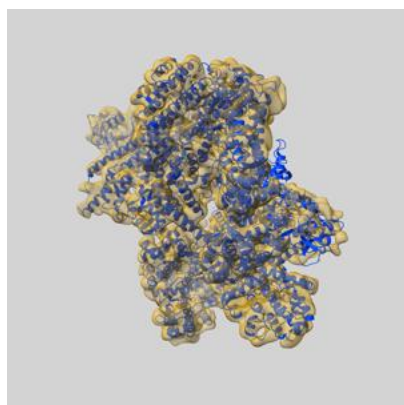
8 Fourier-Shell correlation

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

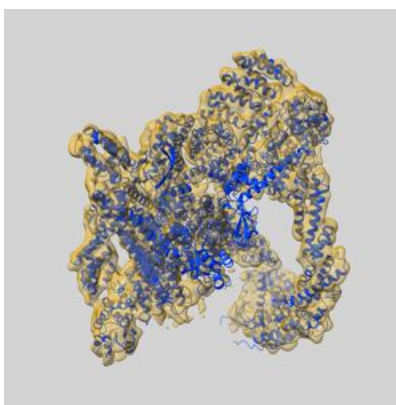
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4742 and PDB model 6R7I. Per-residue inclusion information can be found in section 3 on page 8.

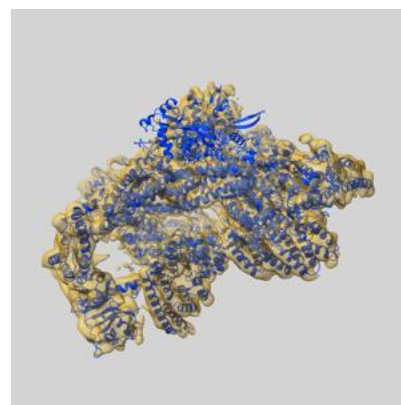
9.1 Map-model overlay [i](#)



X



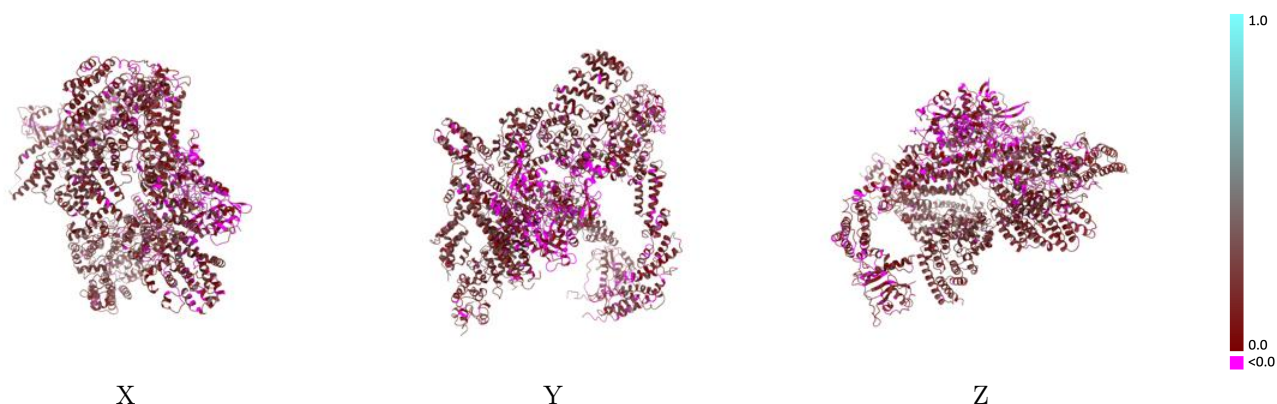
Y



Z

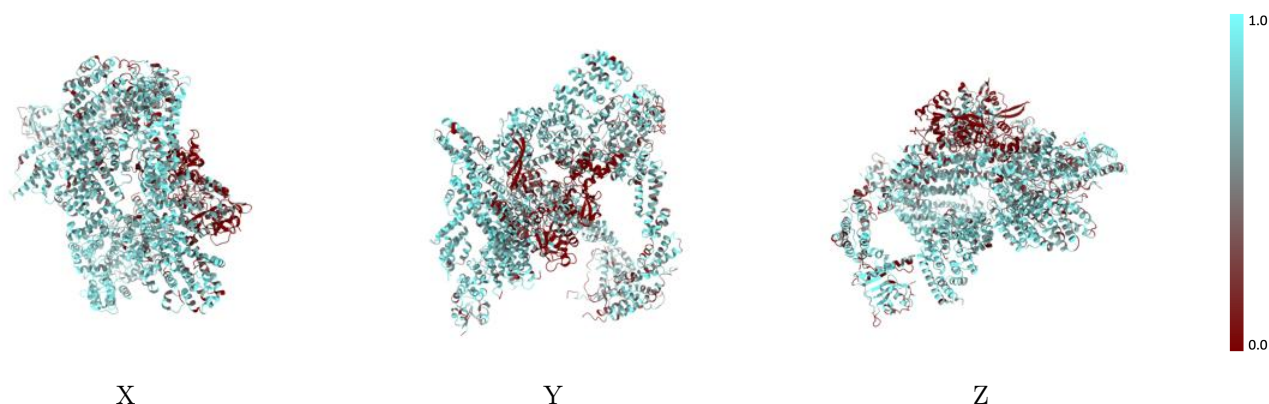
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



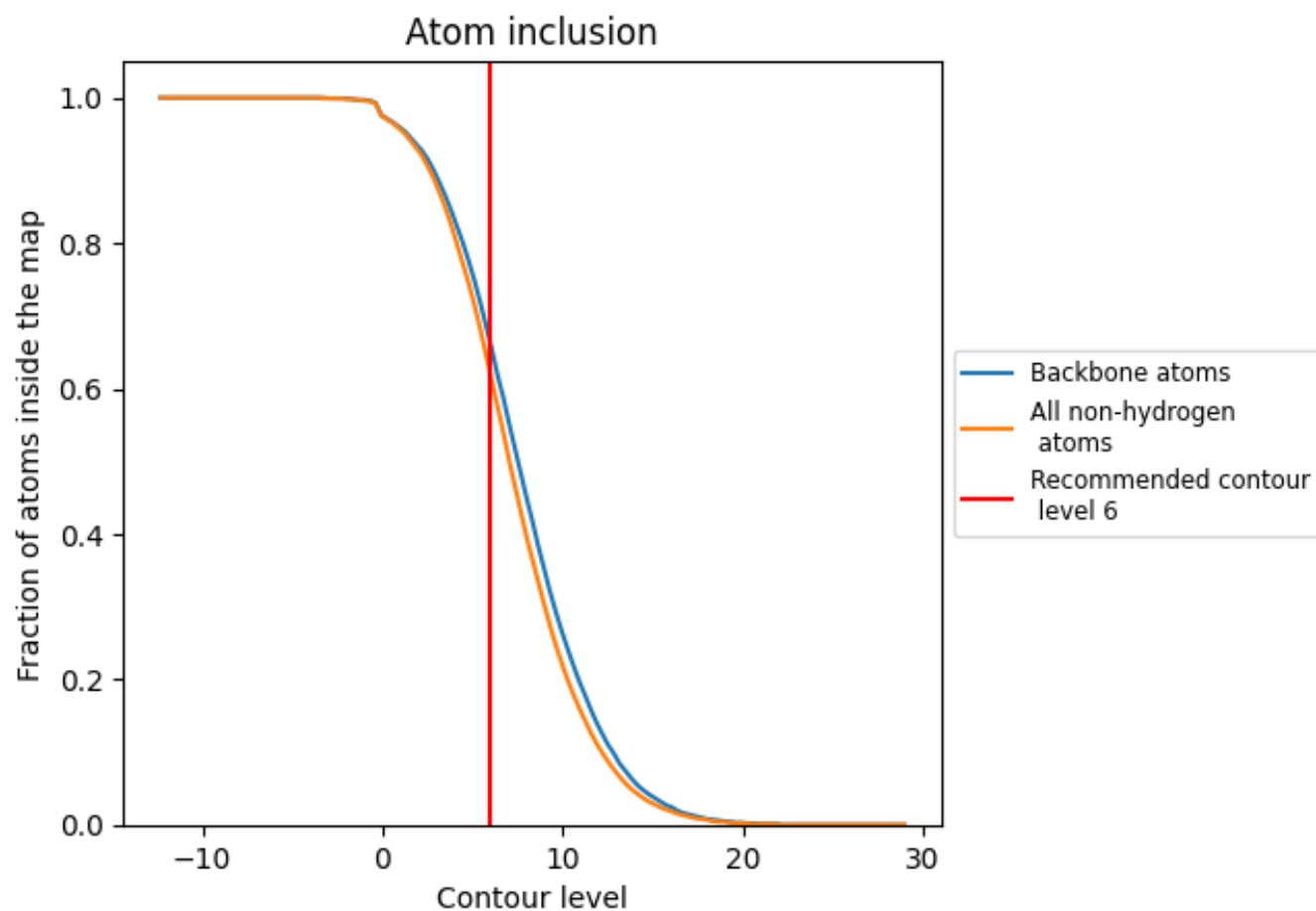
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 62% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6180	 0.1480
A	 0.7390	 0.2160
B	 0.6880	 0.1740
C	 0.7690	 0.2000
D	 0.7570	 0.2040
E	 0.2920	 0.0300
F	 0.4180	 0.0580
G	 0.6710	 0.1550
H	 0.8250	 0.2130
N	 0.0400	 0.0130
O	 0.5430	 0.1230
P	 0.6260	 0.1570
Q	 0.6560	 0.0980
R	 0.5270	 0.1260

