wwPDB EM Validation Summary Report

Nov 16, 2023 – 06:41 PM EST

PDB ID	:	8TAR
EMDB ID	:	EMD-41140
Title	:	APC/C-CDH1-UBE2C-Ubiquitin-CyclinB-NTD
Authors	:	Bodrug, T.; Welsh, K.A.; Bolhuis, D.L.; Paulakonis, E.; Martinez-Chacin, R.C.; Liu, B.; Pinkin, N.; Bonacci, T.; Cui, L.; Xu, P.; Roscow, O.; Amann, S.J.; Grishkovskaya, I.; Emanuele, M.J.; Harrison, J.S.; Steimel, J.P.; Hahn, K.M.; Zhang, W.; Zhong, E.; Haselbach, D.; Brown, N.G.
Deposited on	:	2023-06-27
Resolution	:	4.00 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:

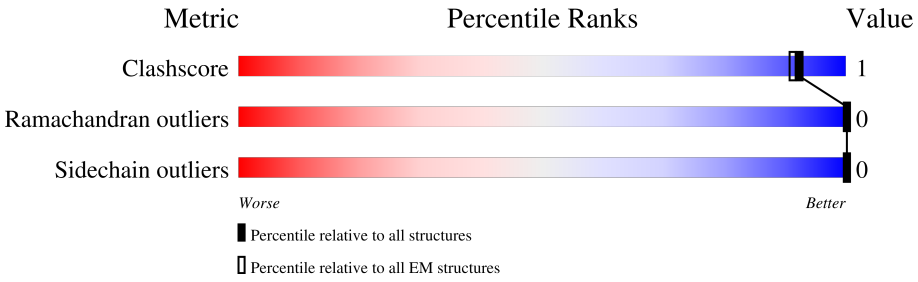
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.00 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	1944	83% · 15%
2	B	12	75% 100%
3	C	84	67% 98% ·
4	D	56	· 100%
5	G	85	32% 68%
5	W	85	31% 69%
6	H	58	· 97% ·
7	I	808	· 90% · 8%

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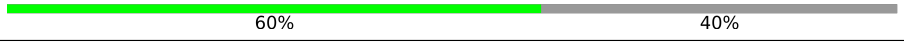
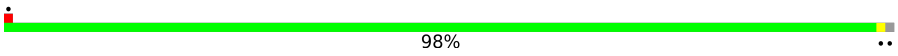
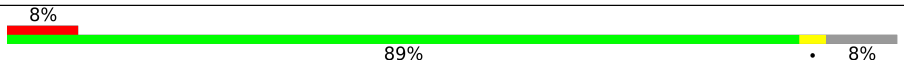
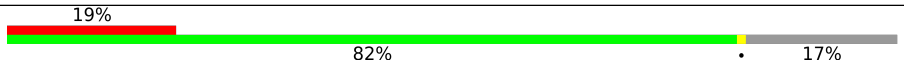
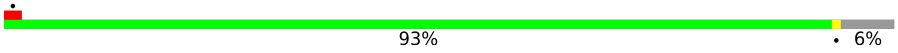
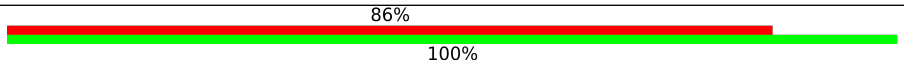
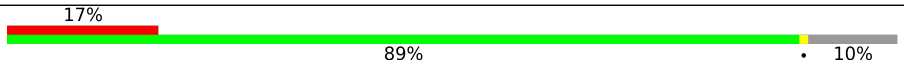
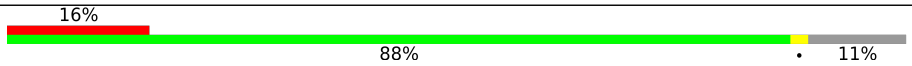
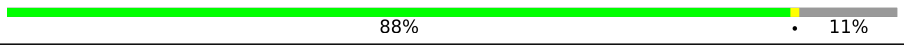
Mol	Chain	Length	Quality of chain
8	J	824	
8	P	824	
9	K	620	
9	S	620	
10	L	185	
11	M	74	
12	N	822	
13	O	755	
14	Q	145	
15	R	496	
16	U	597	
16	V	597	
17	Y	565	
17	Z	565	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 54010 atoms, of which 18053 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1648	Total	C	H	N	O	0	0
			9883	3296	3291	1648	1648		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLU	SER	engineered mutation	UNP Q9H1A4
A	286	GLU	SER	engineered mutation	UNP Q9H1A4
A	291	GLU	THR	engineered mutation	UNP Q9H1A4
A	313	GLU	SER	engineered mutation	UNP Q9H1A4
A	316	GLU	THR	engineered mutation	UNP Q9H1A4
A	317	GLU	SER	engineered mutation	UNP Q9H1A4
A	334	GLU	SER	engineered mutation	UNP Q9H1A4
A	341	GLU	SER	engineered mutation	UNP Q9H1A4
A	343	GLU	SER	engineered mutation	UNP Q9H1A4
A	355	GLU	SER	engineered mutation	UNP Q9H1A4
A	362	GLU	SER	engineered mutation	UNP Q9H1A4
A	372	GLU	SER	engineered mutation	UNP Q9H1A4
A	377	GLU	SER	engineered mutation	UNP Q9H1A4
A	537	GLU	THR	engineered mutation	UNP Q9H1A4
A	547	GLU	SER	engineered mutation	UNP Q9H1A4
A	555	GLU	SER	engineered mutation	UNP Q9H1A4
A	569	GLU	SER	engineered mutation	UNP Q9H1A4
A	688	GLU	SER	engineered mutation	UNP Q9H1A4
A	699	GLU	SER	engineered mutation	UNP Q9H1A4
A	916	GLU	SER	engineered mutation	UNP Q9H1A4
A	1347	GLU	SER	engineered mutation	UNP Q9H1A4

- Molecule 2 is a protein called G2/mitotic-specific cyclin-B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	12	Total	C	H	N	O	0	0
			76	24	27	12	13		

- Molecule 3 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	84	Total	C	H	N	O	0	0
			508	168	171	84	85		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	56	Total	C	H	N	O	0	0
			335	112	110	56	57		

- Molecule 5 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	27	Total	C	H	N	O	0	0
			163	54	55	27	27		
5	W	26	Total	C	H	N	O	0	0
			157	52	53	26	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	51	GLU	SER	engineered mutation	UNP Q8NHZ8
G	52	GLU	SER	engineered mutation	UNP Q8NHZ8
G	82	GLU	SER	engineered mutation	UNP Q8NHZ8
W	51	GLU	SER	engineered mutation	UNP Q8NHZ8
W	52	GLU	SER	engineered mutation	UNP Q8NHZ8
W	82	GLU	SER	engineered mutation	UNP Q8NHZ8

- Molecule 6 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	58	Total	C	H	N	O	0	0
			351	116	118	58	59		

- Molecule 7 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	742	Total	C	H	N	O	0	0
			4458	1484	1490	742	742		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	777	GLU	SER	engineered mutation	UNP Q9UJX5
I	779	GLU	SER	engineered mutation	UNP Q9UJX5

- Molecule 8 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	510	Total	C	H	N	O	0	0
			3067	1020	1027	510	510		
8	P	496	Total	C	H	N	O	0	0
			2982	992	998	496	496		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	200	GLU	THR	engineered mutation	UNP P30260
J	205	GLU	THR	engineered mutation	UNP P30260
J	220	GLU	SER	engineered mutation	UNP P30260
J	241	GLU	SER	engineered mutation	UNP P30260
J	276	GLU	SER	engineered mutation	UNP P30260
J	320	GLU	SER	engineered mutation	UNP P30260
J	336	GLU	SER	engineered mutation	UNP P30260
J	339	GLU	SER	engineered mutation	UNP P30260
J	386	GLU	SER	engineered mutation	UNP P30260
J	387	GLU	SER	engineered mutation	UNP P30260
J	393	GLU	SER	engineered mutation	UNP P30260
J	426	GLU	SER	engineered mutation	UNP P30260
J	435	GLU	SER	engineered mutation	UNP P30260
J	446	GLU	THR	engineered mutation	UNP P30260
P	200	GLU	THR	engineered mutation	UNP P30260
P	205	GLU	THR	engineered mutation	UNP P30260
P	220	GLU	SER	engineered mutation	UNP P30260
P	241	GLU	SER	engineered mutation	UNP P30260
P	276	GLU	SER	engineered mutation	UNP P30260
P	320	GLU	SER	engineered mutation	UNP P30260
P	336	GLU	SER	engineered mutation	UNP P30260
P	339	GLU	SER	engineered mutation	UNP P30260
P	386	GLU	SER	engineered mutation	UNP P30260
P	387	GLU	SER	engineered mutation	UNP P30260
P	393	GLU	SER	engineered mutation	UNP P30260
P	426	GLU	SER	engineered mutation	UNP P30260
P	435	GLU	SER	engineered mutation	UNP P30260
P	446	GLU	THR	engineered mutation	UNP P30260

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	531	Total	C	H	N	O	0	0
			3195	1065	1066	531	533		
9	S	506	Total	C	H	N	O	0	0
			3043	1012	1019	506	506		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	112	GLU	SER	engineered mutation	UNP Q13042
K	560	GLU	SER	engineered mutation	UNP Q13042
K	581	GLU	THR	engineered mutation	UNP Q13042
K	585	GLU	THR	engineered mutation	UNP Q13042
K	586	GLU	SER	engineered mutation	UNP Q13042
S	112	GLU	SER	engineered mutation	UNP Q13042
S	560	GLU	SER	engineered mutation	UNP Q13042
S	581	GLU	THR	engineered mutation	UNP Q13042
S	585	GLU	THR	engineered mutation	UNP Q13042
S	586	GLU	SER	engineered mutation	UNP Q13042

- Molecule 10 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	183	Total	C	H	N	O	0	0
			1097	366	364	183	184		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLU	THR	engineered mutation	UNP Q9UM13

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	68	Total	C	H	N	O	0	0
			409	136	137	68	68		

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	682	Total	C	H	N	O	0	0
			4091	1364	1363	682	682		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	218	GLU	SER	engineered mutation	UNP Q9UJX6
N	314	GLU	SER	engineered mutation	UNP Q9UJX6
N	470	GLU	SER	engineered mutation	UNP Q9UJX6
N	534	GLU	SER	engineered mutation	UNP Q9UJX6
N	811	GLU	SER	engineered mutation	UNP Q9UJX6

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	707	Total	C	H	N	O	0	0
			4254	1414	1425	707	708		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	178	GLU	THR	engineered mutation	UNP Q9UJX4
O	179	GLU	SER	engineered mutation	UNP Q9UJX4
O	195	GLU	SER	engineered mutation	UNP Q9UJX4
O	202	GLU	SER	engineered mutation	UNP Q9UJX4
O	221	GLU	SER	engineered mutation	UNP Q9UJX4
O	232	GLU	THR	engineered mutation	UNP Q9UJX4
O	364	GLU	SER	engineered mutation	UNP Q9UJX4

- Molecule 14 is a protein called Ubiquitin-conjugating enzyme E2 C.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	145	Total	C	H	N	O	0	0
			872	290	292	145	145		

- Molecule 15 is a protein called Fizzy-related protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	440	Total	C	H	N	O	0	0
			2658	880	897	440	441		

- Molecule 16 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	540	Total	C	H	N	O	0	0
			3244	1080	1084	540	540		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	534	Total	C	H	N	O	0	0
			3216	1071	1075	534	536		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	542	GLU	THR	engineered mutation	UNP Q9UJX2
U	562	GLU	THR	engineered mutation	UNP Q9UJX2
U	582	GLU	THR	engineered mutation	UNP Q9UJX2
U	588	GLU	SER	engineered mutation	UNP Q9UJX2
U	596	GLU	THR	engineered mutation	UNP Q9UJX2
V	542	GLU	THR	engineered mutation	UNP Q9UJX2
V	562	GLU	THR	engineered mutation	UNP Q9UJX2
V	582	GLU	THR	engineered mutation	UNP Q9UJX2
V	588	GLU	SER	engineered mutation	UNP Q9UJX2
V	596	GLU	THR	engineered mutation	UNP Q9UJX2

- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	501	Total	C	H	N	O	0	0
			3012	1002	1008	501	501		
17	Z	488	Total	C	H	N	O	0	0
			2935	976	983	488	488		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

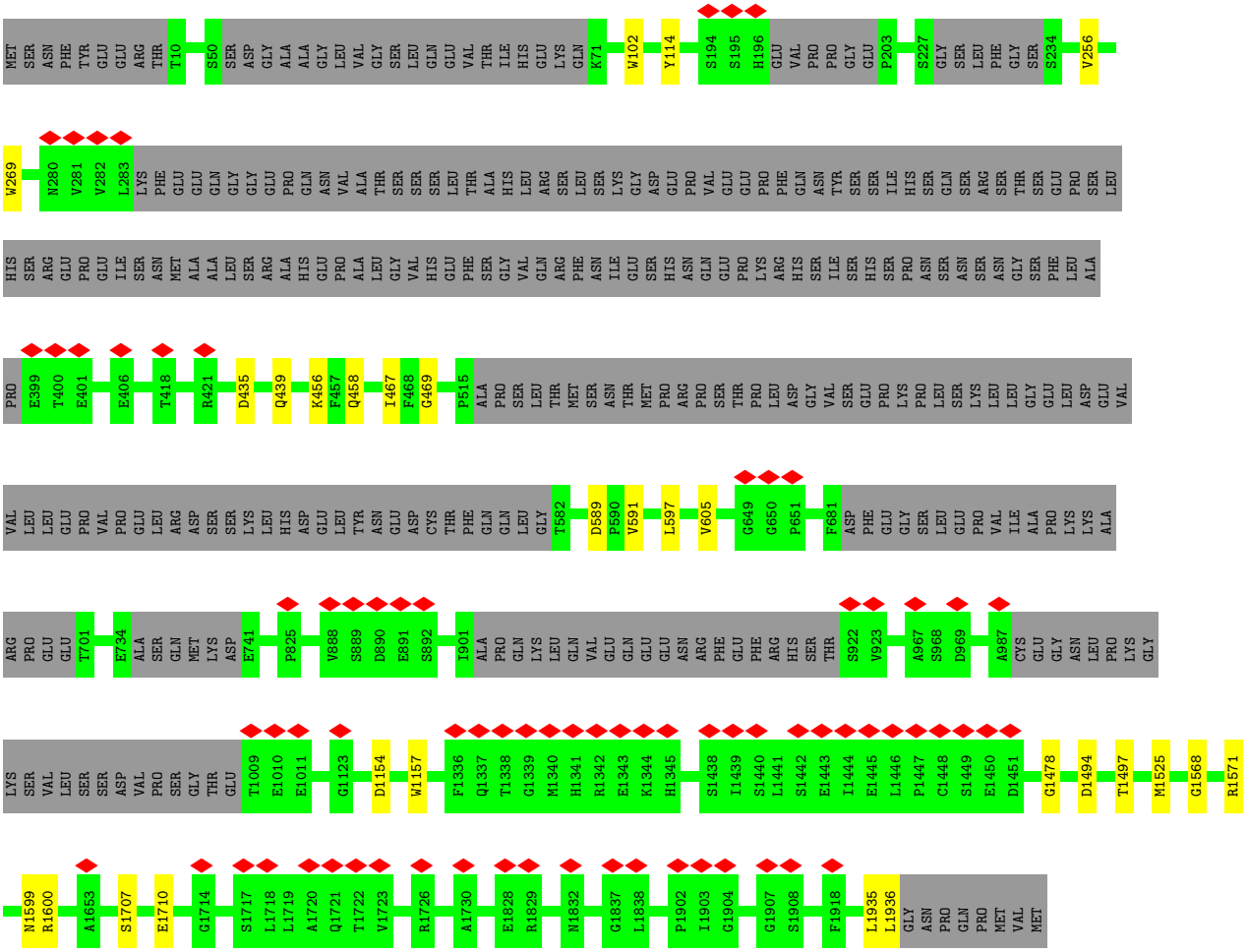
Mol	Chain	Residues	Atoms		AltConf
18	C	3	Total	Zn	0
			3	3	
18	N	1	Total	Zn	0
			1	1	

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.

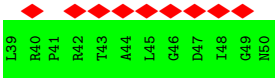
• Molecule 1: Anaphase-promoting complex subunit 1

Chain A:



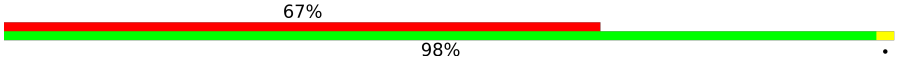
• Molecule 2: G2/mitotic-specific cyclin-B1

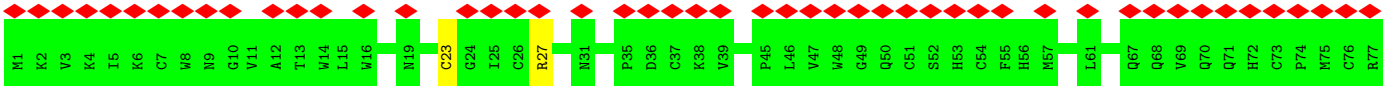
Chain B:

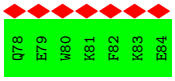


• Molecule 3: Anaphase-promoting complex subunit 11

Chain C:

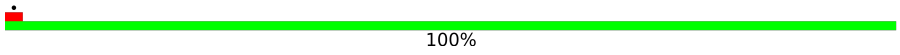






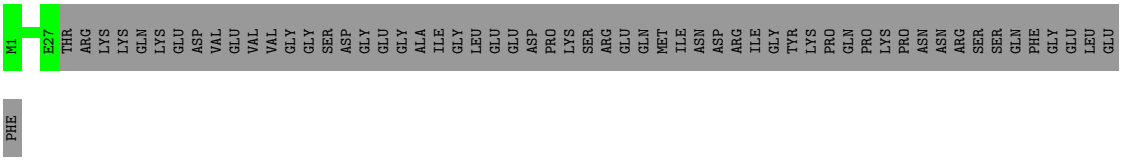
• Molecule 4: Anaphase-promoting complex subunit 15

Chain D:



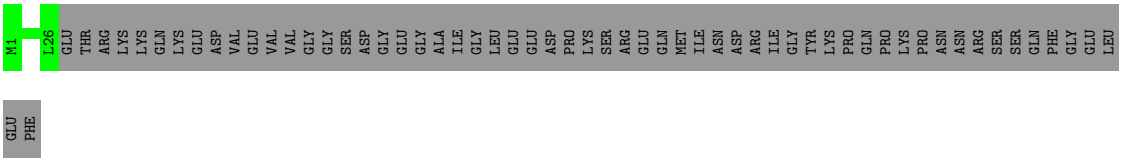
• Molecule 5: Anaphase-promoting complex subunit CDC26

Chain G:



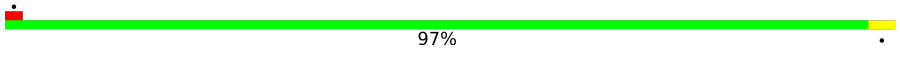
• Molecule 5: Anaphase-promoting complex subunit CDC26

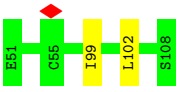
Chain W:



• Molecule 6: Anaphase-promoting complex subunit 16

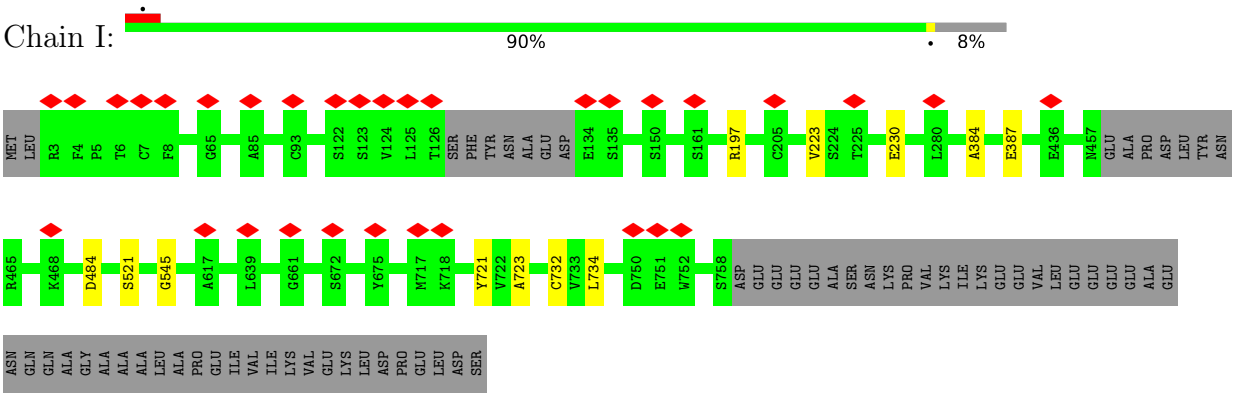
Chain H:





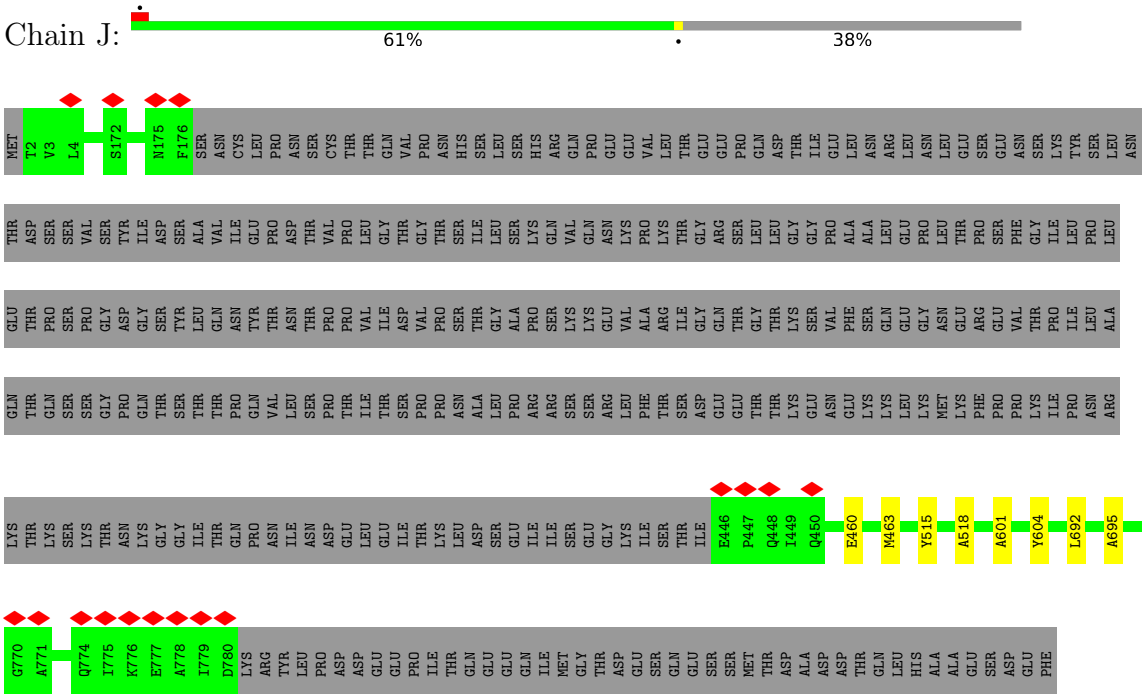
• Molecule 7: Anaphase-promoting complex subunit 4

Chain I:



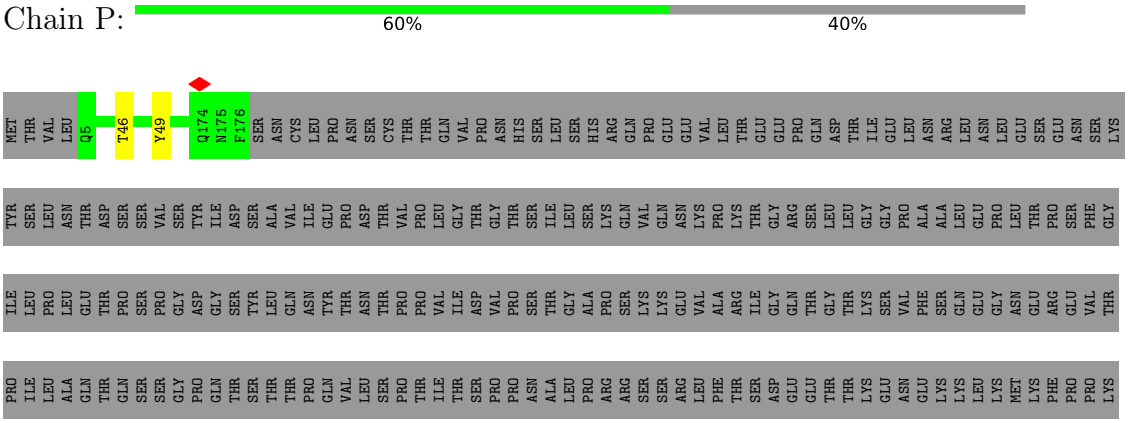
• Molecule 8: Cell division cycle protein 27 homolog

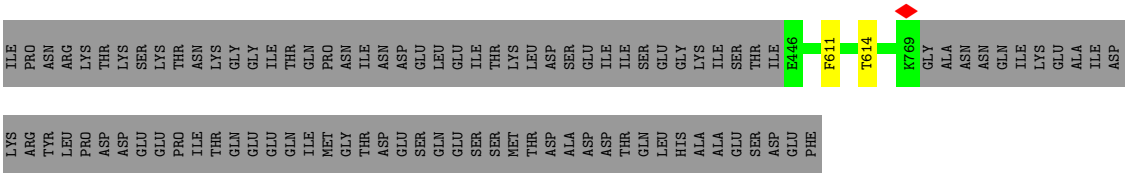
Chain J:



• Molecule 8: Cell division cycle protein 27 homolog

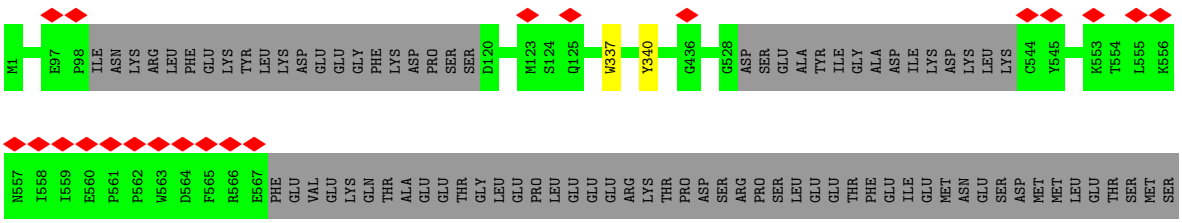
Chain P:





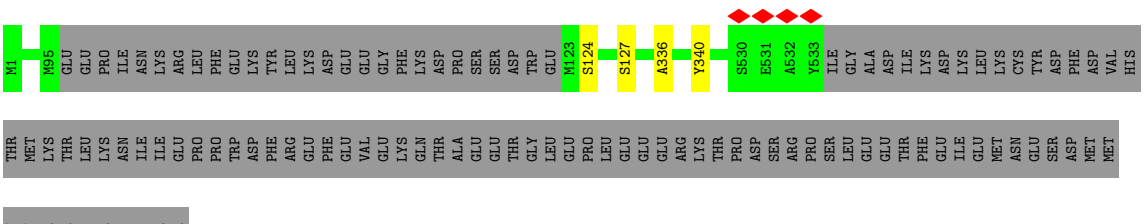
• Molecule 9: Cell division cycle protein 16 homolog

Chain K:



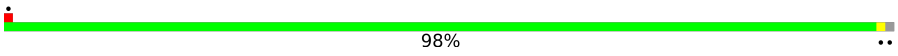
• Molecule 9: Cell division cycle protein 16 homolog

Chain S:



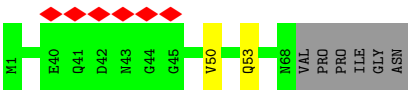
• Molecule 10: Anaphase-promoting complex subunit 10

Chain L:



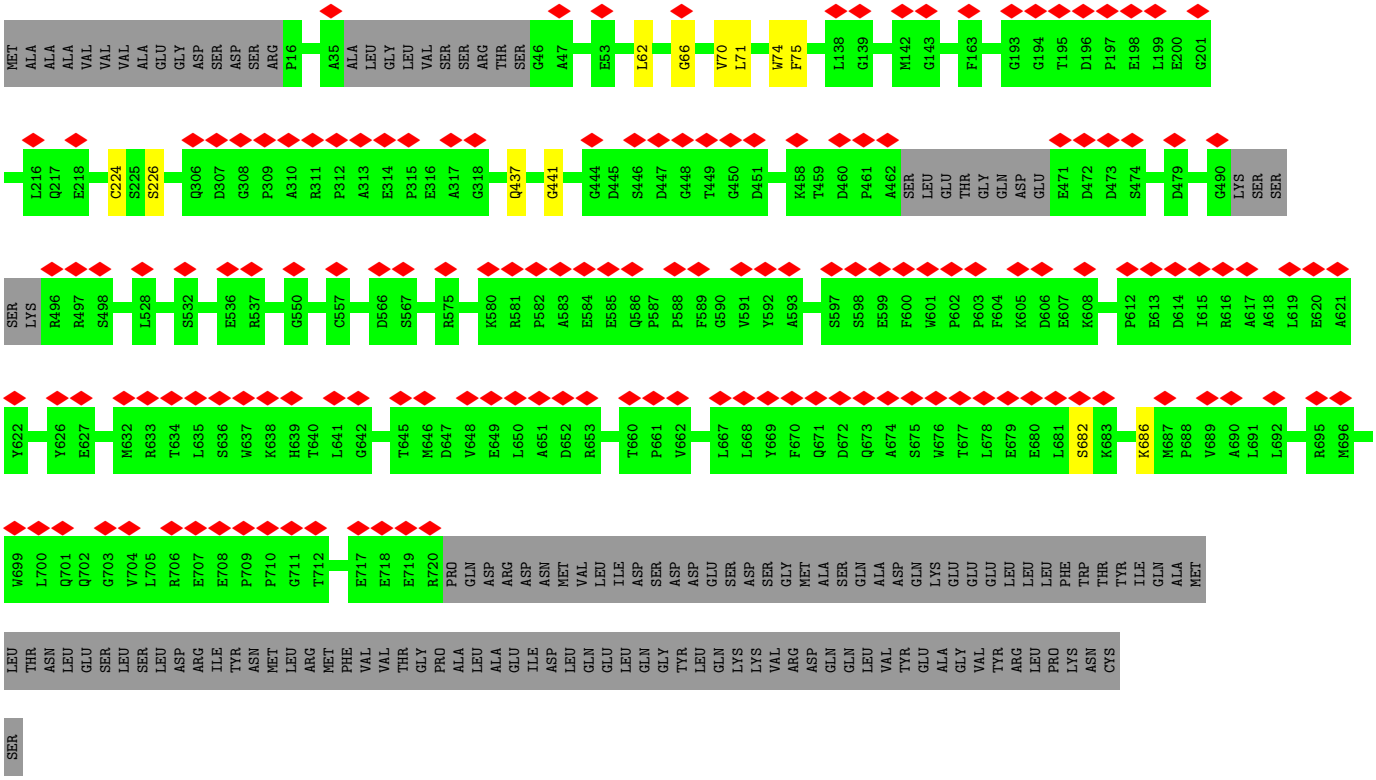
• Molecule 11: Anaphase-promoting complex subunit 13

Chain M:



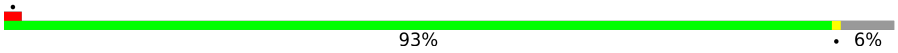
• Molecule 12: Anaphase-promoting complex subunit 2

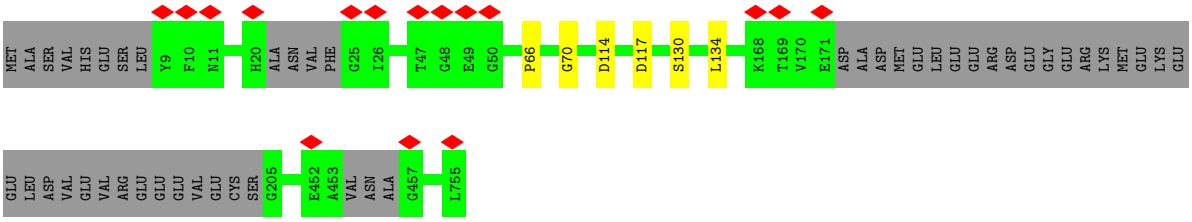
Chain N:



• Molecule 13: Anaphase-promoting complex subunit 5

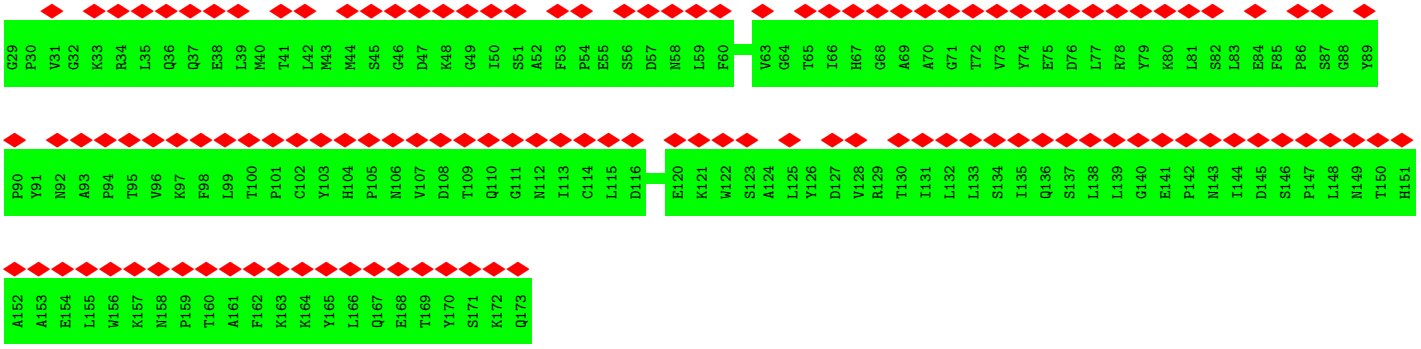
Chain O:





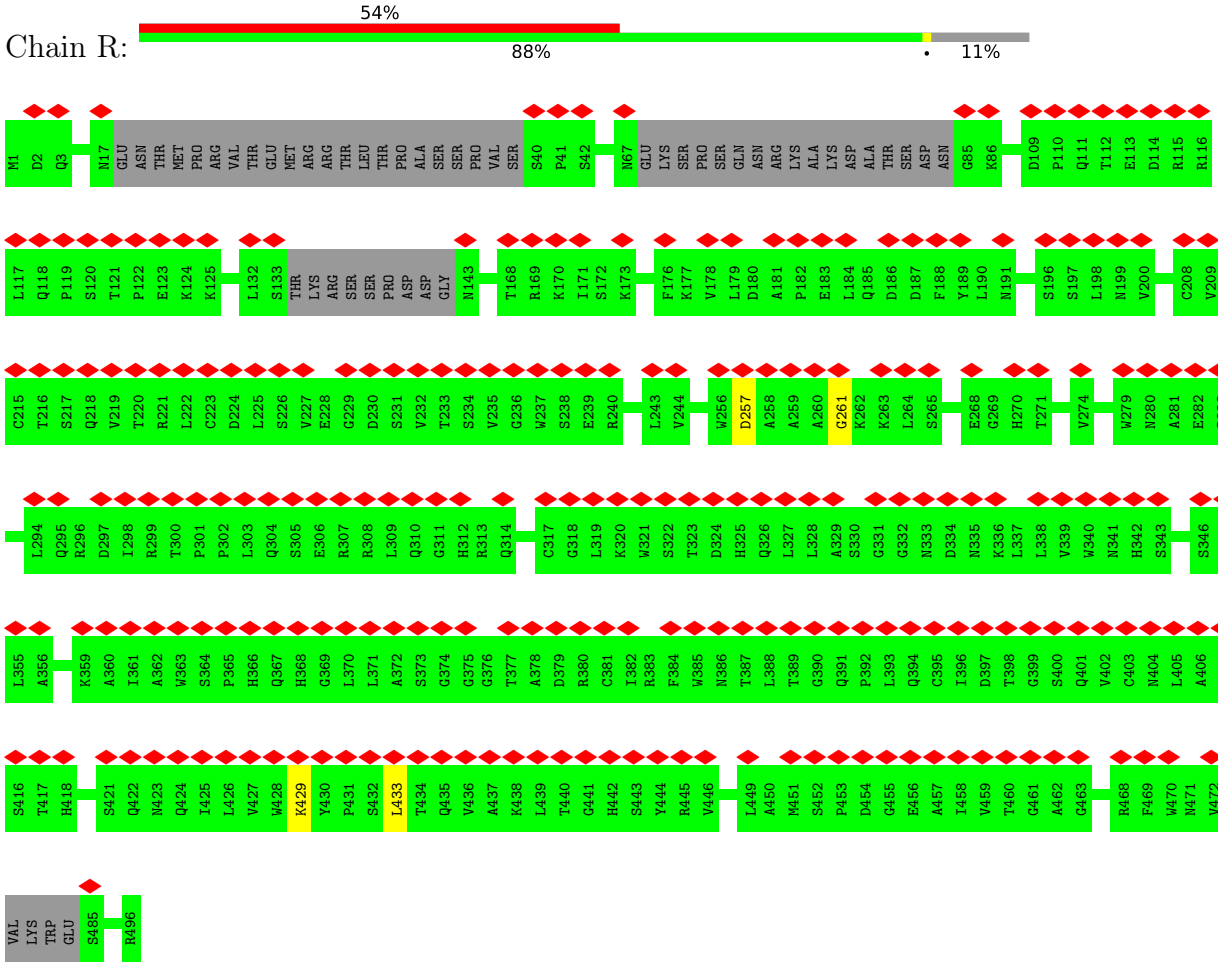
• Molecule 14: Ubiquitin-conjugating enzyme E2 C

Chain Q:



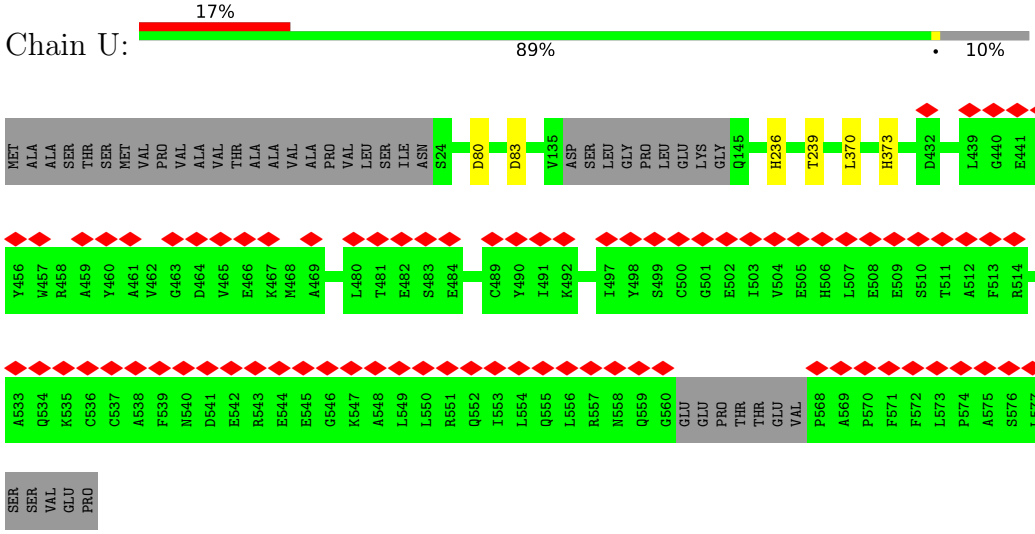
• Molecule 15: Fizzy-related protein homolog

Chain R:



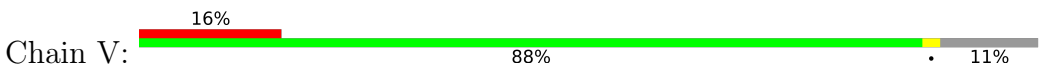
• Molecule 16: Cell division cycle protein 23 homolog

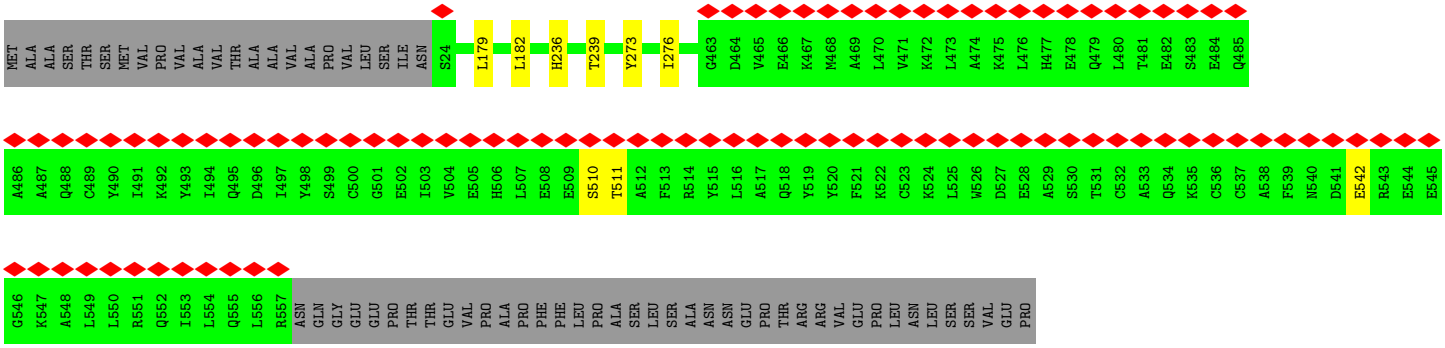
Chain U:



• Molecule 16: Cell division cycle protein 23 homolog

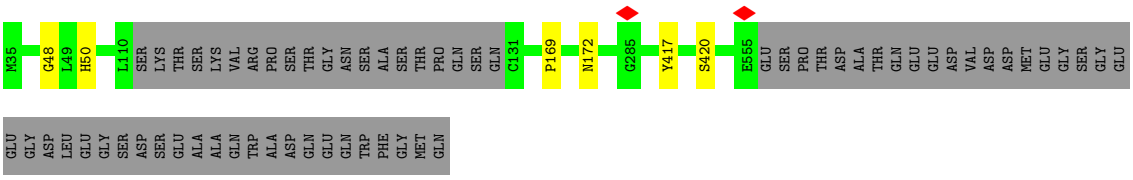
Chain V:





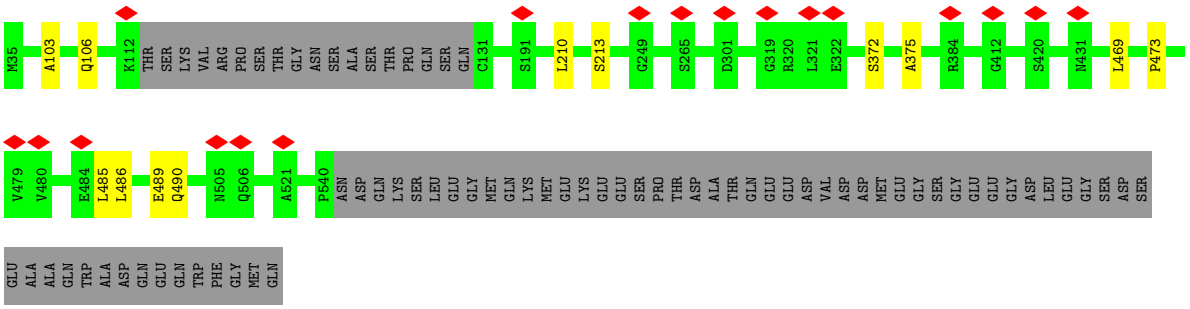
• Molecule 17: Anaphase-promoting complex subunit 7

Chain Y:



• Molecule 17: Anaphase-promoting complex subunit 7

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	661289	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.977	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	452.0, 452.0, 452.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.13, 1.13, 1.13	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	0/6582	0.57	0/8210
2	B	0.21	0/48	0.61	0/57
3	C	0.24	0/336	0.53	0/417
4	D	0.30	0/224	0.57	0/277
5	G	0.32	0/107	0.42	0/132
5	W	0.28	0/103	0.47	0/127
6	H	0.28	0/232	0.49	0/287
7	I	0.28	0/2965	0.56	0/3701
8	J	0.37	0/2038	0.57	0/2544
8	P	0.37	0/1982	0.57	0/2474
9	K	0.34	0/2126	0.59	0/2653
9	S	0.37	0/2022	0.56	0/2524
10	L	0.29	0/732	0.61	0/912
11	M	0.33	0/271	0.52	0/337
12	N	0.26	0/2724	0.51	0/3398
13	O	0.35	0/2825	0.58	0/3523
14	Q	0.25	0/579	0.50	0/722
15	R	0.24	0/1756	0.55	0/2185
16	U	0.33	0/2157	0.54	0/2691
16	V	0.34	0/2140	0.57	0/2674
17	Y	0.33	0/2002	0.54	0/2499
17	Z	0.30	0/1950	0.52	0/2434
All	All	0.32	0/35901	0.56	0/44778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6592	3291	1722	15	0
2	B	49	27	14	0	0
3	C	337	171	92	1	0
4	D	225	110	52	0	0
5	G	108	55	28	0	0
5	W	104	53	27	0	0
6	H	233	118	59	1	0
7	I	2968	1490	776	6	0
8	J	2040	1027	538	4	0
8	P	1984	998	522	2	0
9	K	2129	1066	557	1	0
9	S	2024	1019	531	2	0
10	L	733	364	190	1	0
11	M	272	137	72	1	0
12	N	2728	1363	713	6	0
13	O	2829	1425	744	3	0
14	Q	580	292	154	0	0
15	R	1761	897	486	2	0
16	U	2160	1084	561	3	0
16	V	2141	1075	565	6	0
17	Y	2004	1008	526	3	0
17	Z	1952	983	511	6	0
18	C	3	0	0	0	0
18	N	1	0	0	0	0
All	All	35957	18053	9440	63	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 1.

The worst 5 of 63 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)
16:V:511:THR:CA	16:V:542:GLU:OE2	2.33	0.77
1:A:1478:GLY:N	1:A:1525:MET:O	2.24	0.70
12:N:682:SER:O	12:N:686:LYS:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1494:ASP:O	1:A:1497:THR:N	2.27	0.67
15:R:429:LYS:O	15:R:433:LEU:N	2.26	0.66

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	1628/1944 (84%)	1595 (98%)	33 (2%)	0	100	100
2	B	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
3	C	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
4	D	54/56 (96%)	54 (100%)	0	0	100	100
5	G	25/85 (29%)	24 (96%)	1 (4%)	0	100	100
5	W	24/85 (28%)	24 (100%)	0	0	100	100
6	H	56/58 (97%)	56 (100%)	0	0	100	100
7	I	736/808 (91%)	715 (97%)	21 (3%)	0	100	100
8	J	506/824 (61%)	499 (99%)	7 (1%)	0	100	100
8	P	492/824 (60%)	480 (98%)	12 (2%)	0	100	100
9	K	525/620 (85%)	520 (99%)	5 (1%)	0	100	100
9	S	502/620 (81%)	493 (98%)	9 (2%)	0	100	100
10	L	181/185 (98%)	177 (98%)	4 (2%)	0	100	100
11	M	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
12	N	674/822 (82%)	663 (98%)	11 (2%)	0	100	100
13	O	699/755 (93%)	692 (99%)	7 (1%)	0	100	100
14	Q	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
15	R	430/496 (87%)	421 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	U	534/597 (89%)	525 (98%)	9 (2%)	0	100	100
16	V	532/597 (89%)	524 (98%)	8 (2%)	0	100	100
17	Y	497/565 (88%)	491 (99%)	6 (1%)	0	100	100
17	Z	484/565 (86%)	470 (97%)	14 (3%)	0	100	100
All	All	8880/10821 (82%)	8719 (98%)	161 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
9	K	1/548 (0%)	1 (100%)	0	100	100
16	V	1/520 (0%)	1 (100%)	0	100	100
All	All	2/1068 (0%)	2 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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)

There are no chain breaks in this entry.

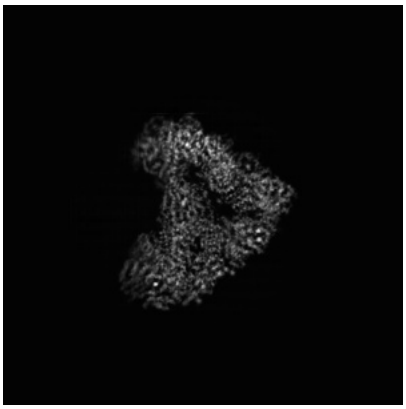
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41140. These allow visual inspection of the internal detail of the map and identification of artifacts.

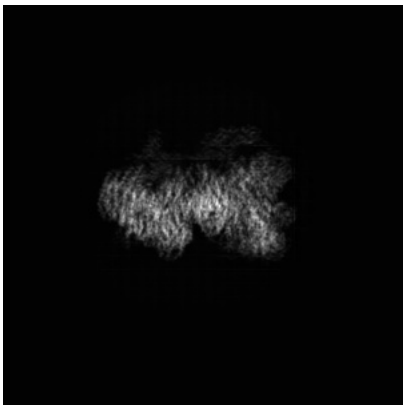
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



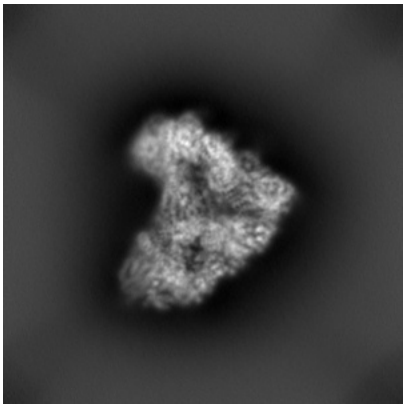
X



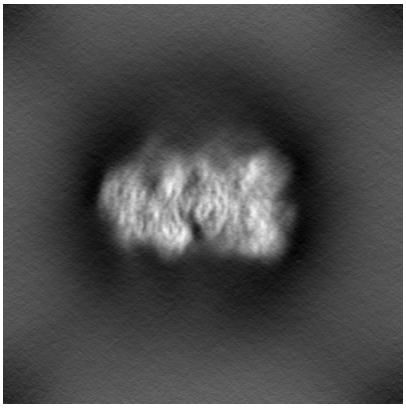
Y

Z

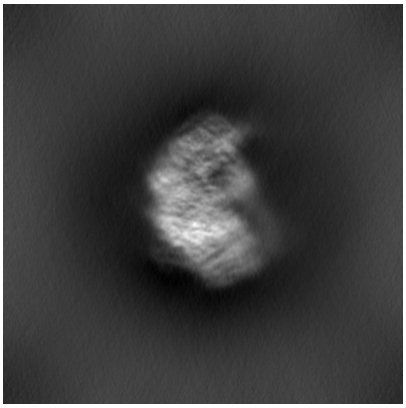
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

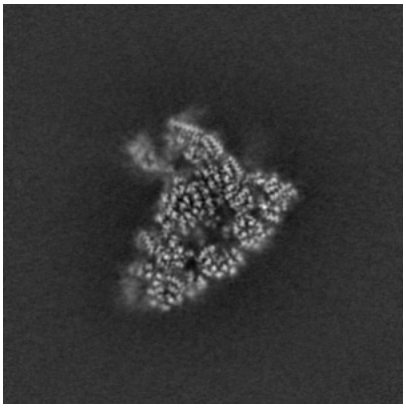
6.2.1 Primary map

X Index: 200

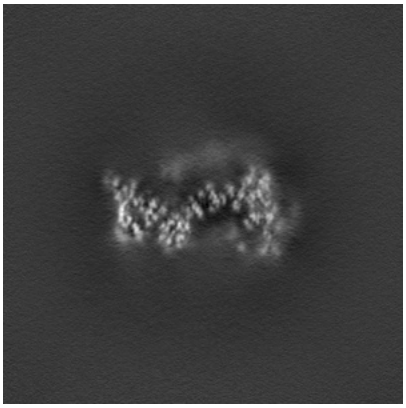
Y Index: 200

Z Index: 200

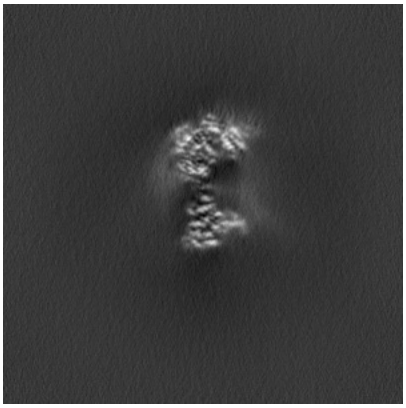
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

6.3 Largest variance slices (i)

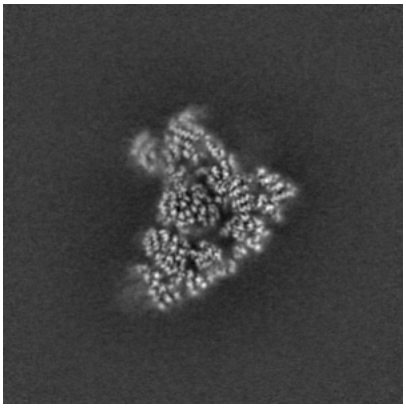
6.3.1 Primary map

X Index: 194

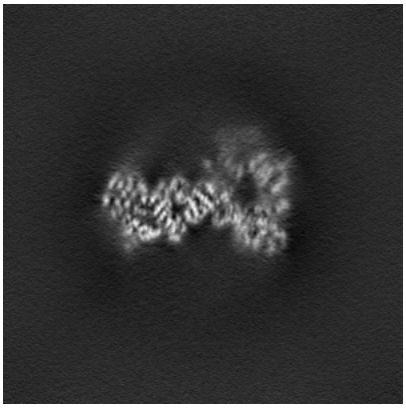
Y Index: 170

Z Index: 215

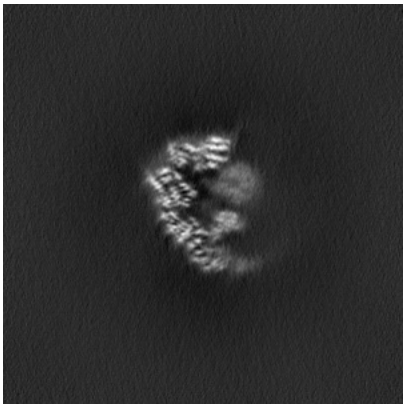
6.3.2 Raw map



X Index: 195



Y Index: 170



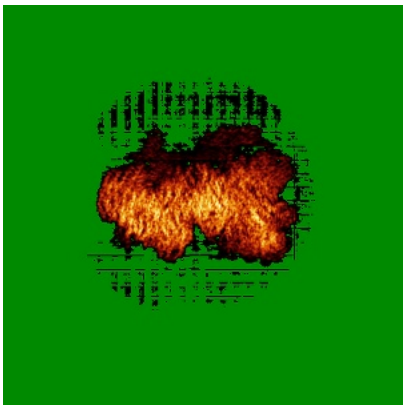
Z Index: 165

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

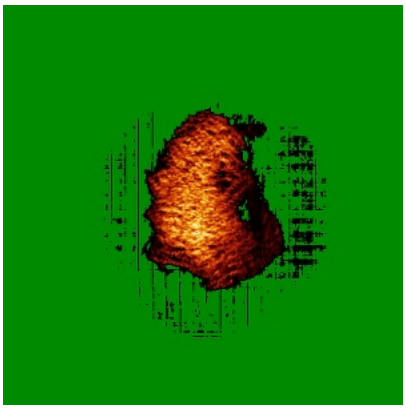
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

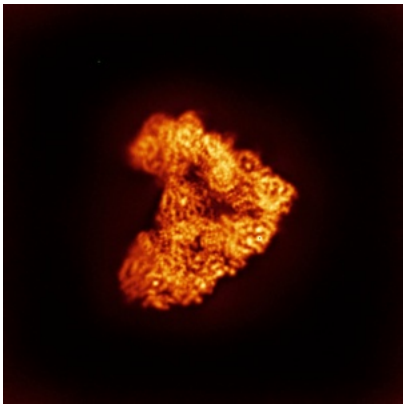


Y

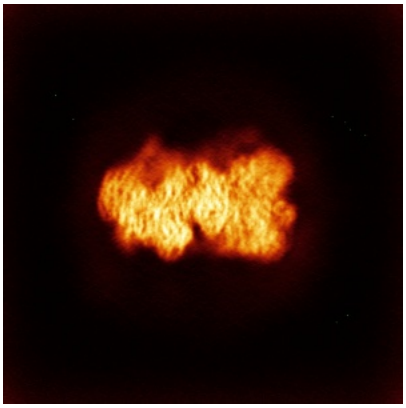


Z

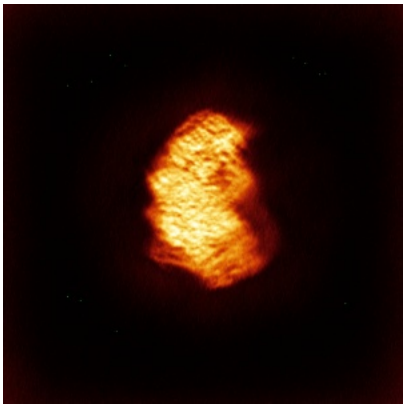
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

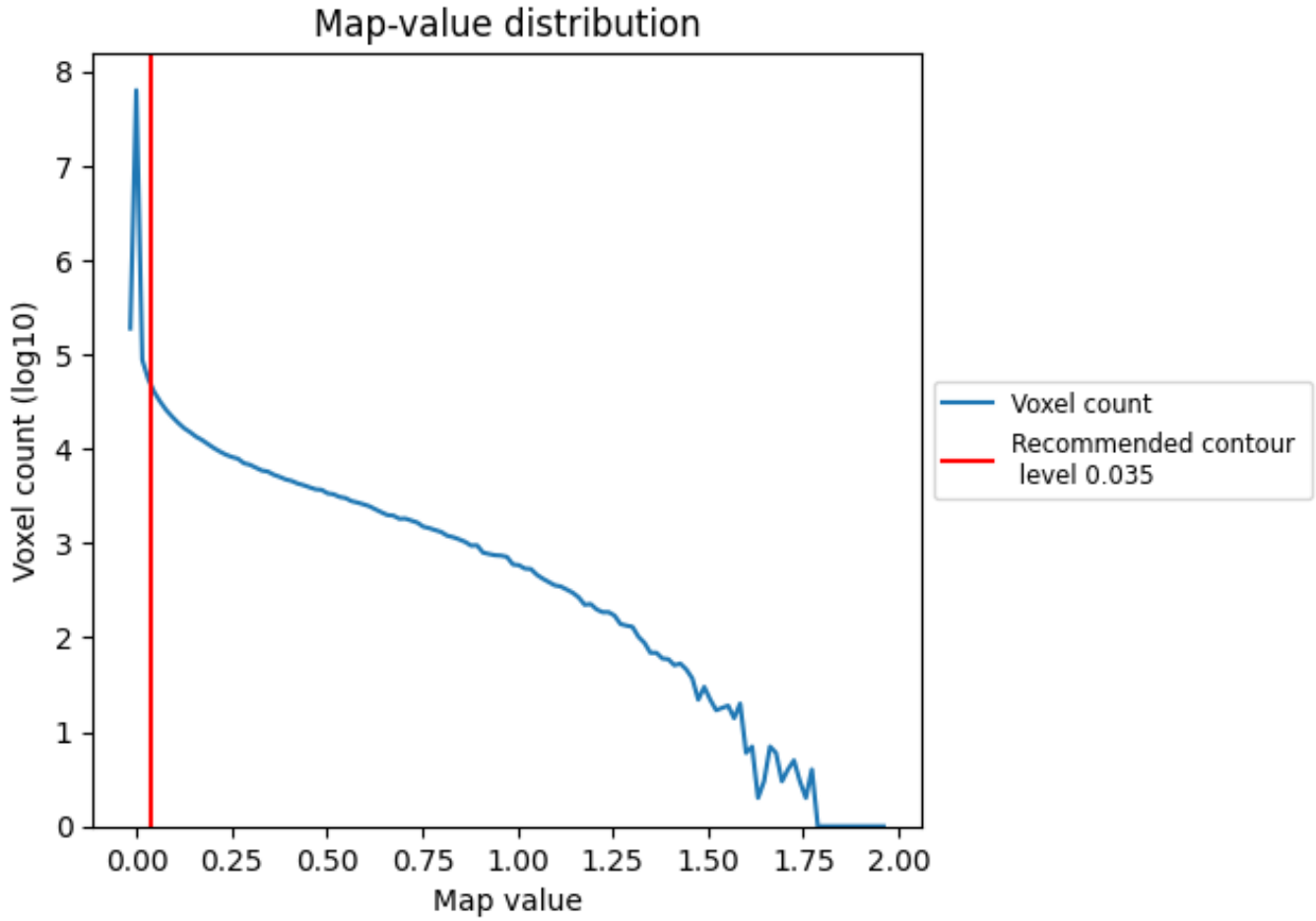
6.6 Mask visualisation (i)

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

7 Map analysis

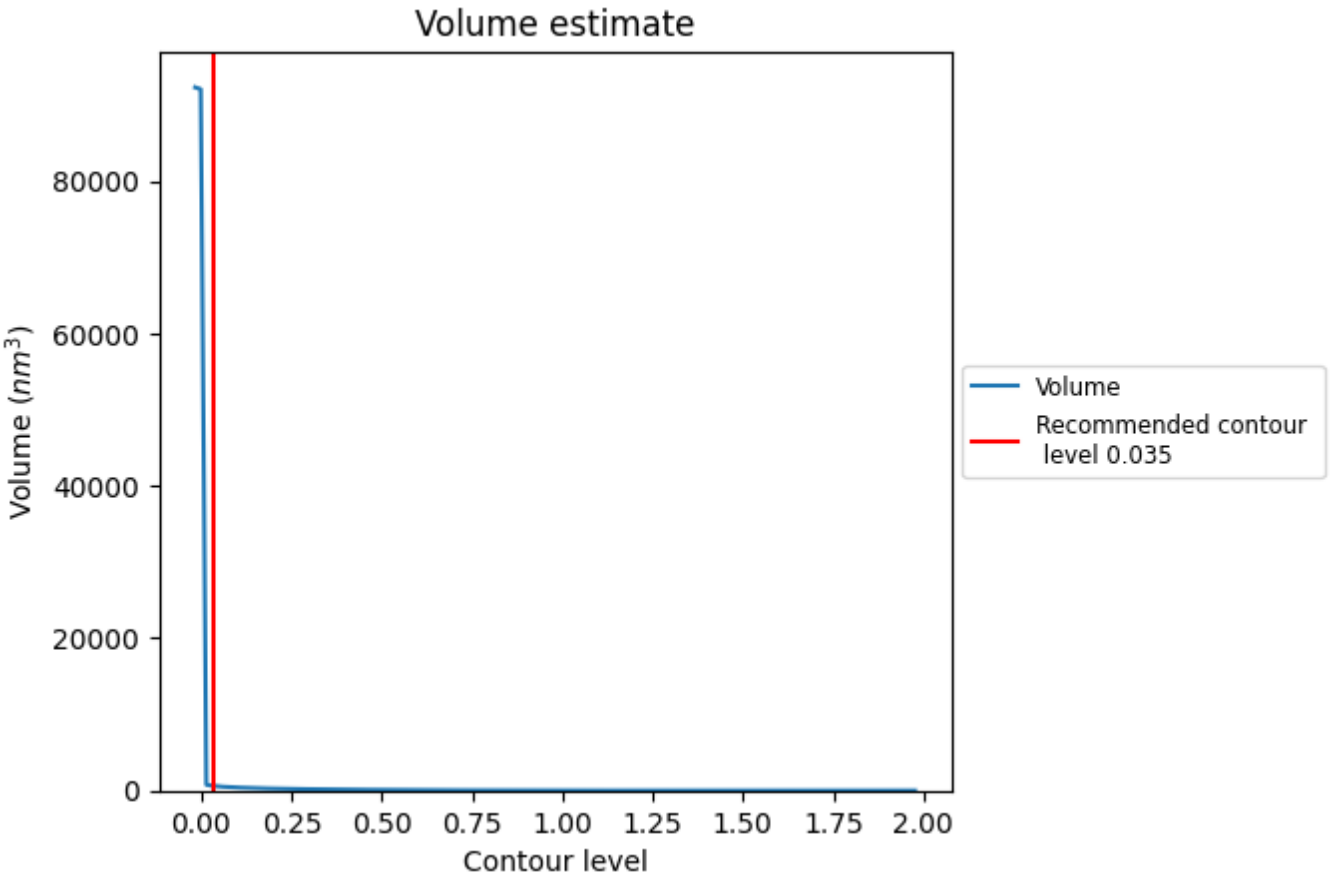
This section contains the results of statistical analysis of the map.

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.

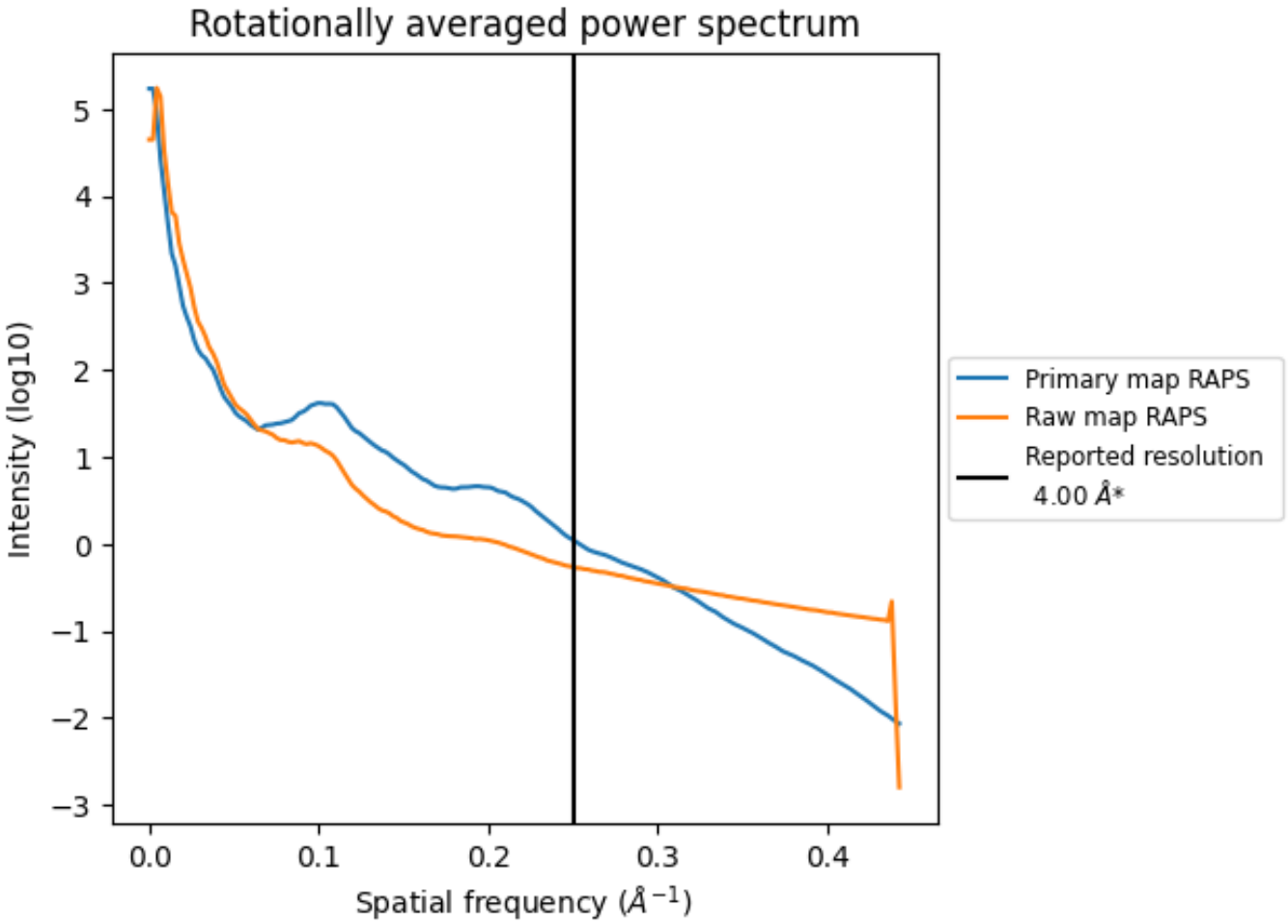
7.2 Volume estimate (i)



The volume at the recommended contour level is 611 nm^3; this corresponds to an approximate mass of 552 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)

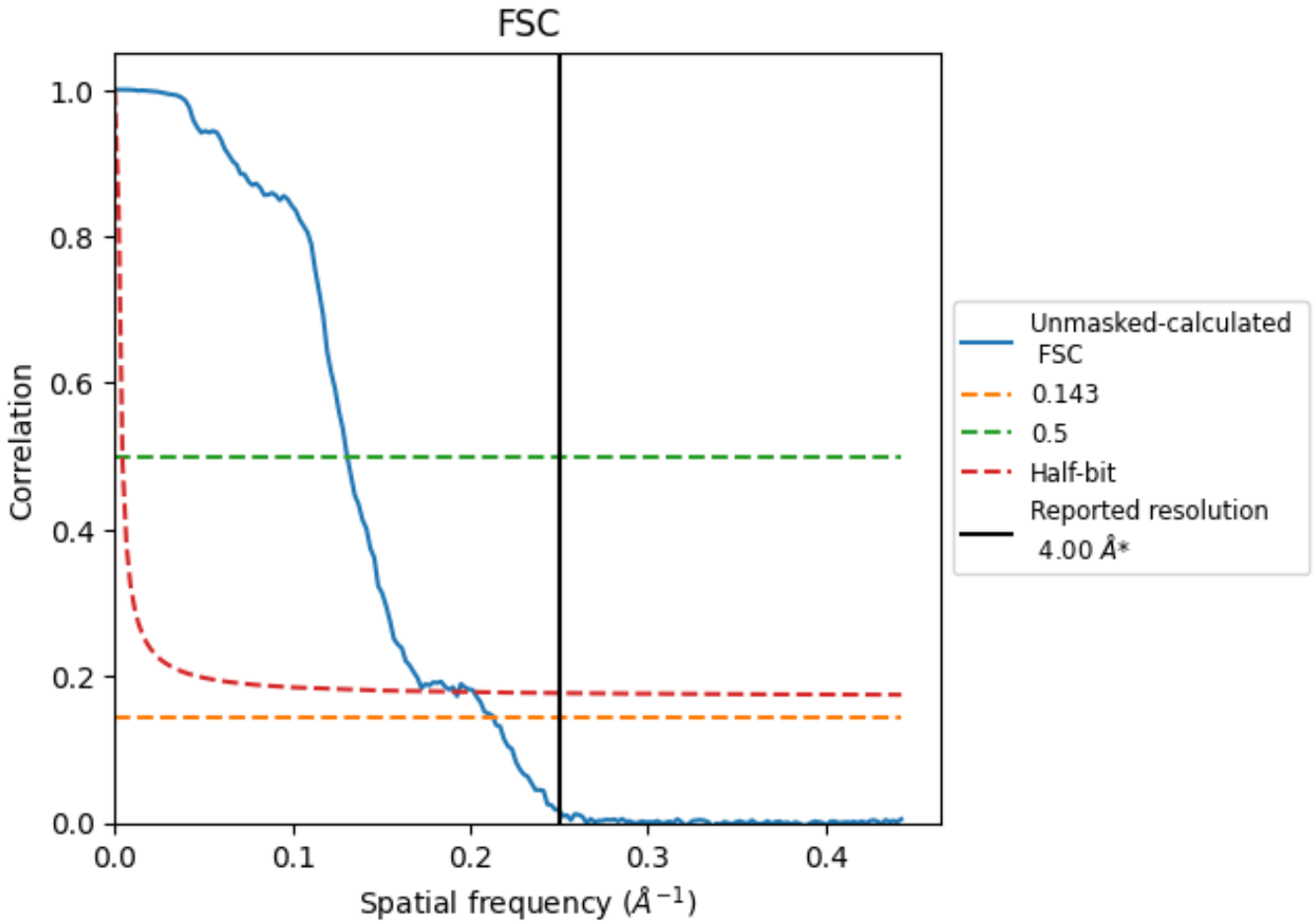


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

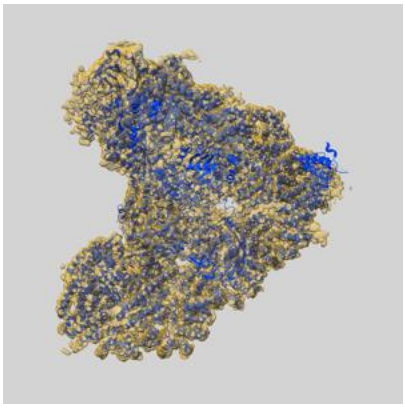
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.70	7.65	5.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.70 differs from the reported value 4.0 by more than 10 %

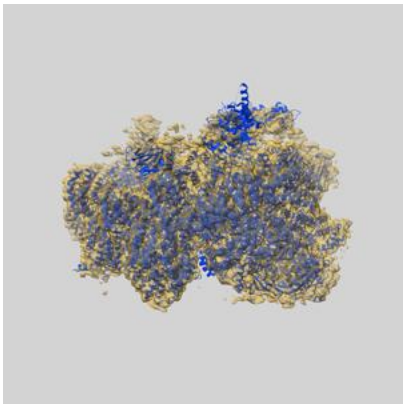
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41140 and PDB model 8TAR. Per-residue inclusion information can be found in section 3 on page 10.

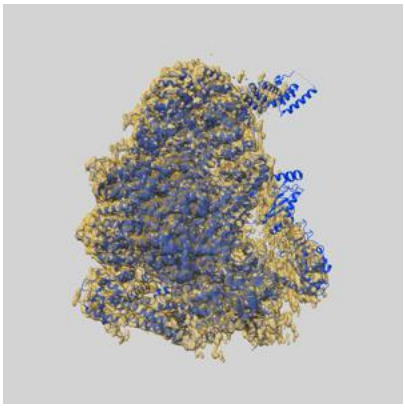
9.1 Map-model overlay



X



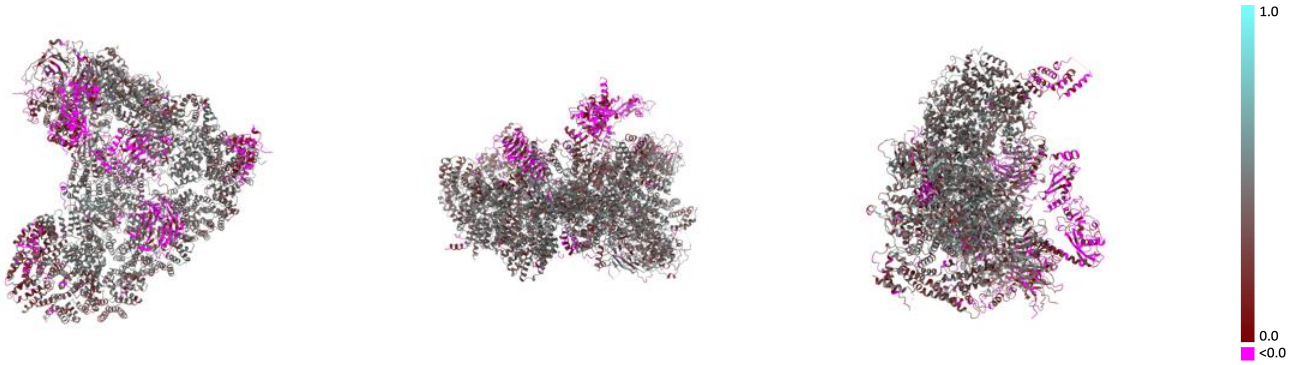
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

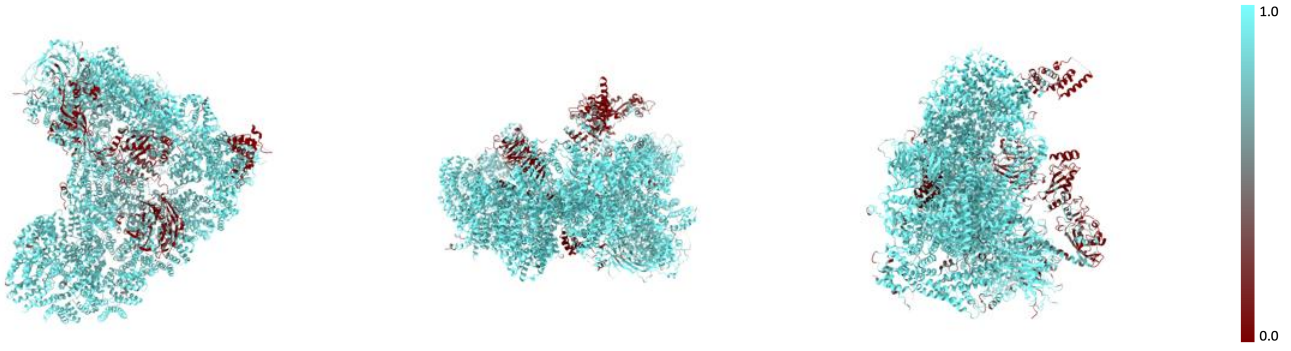
9.2 Q-score mapped to coordinate model



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.

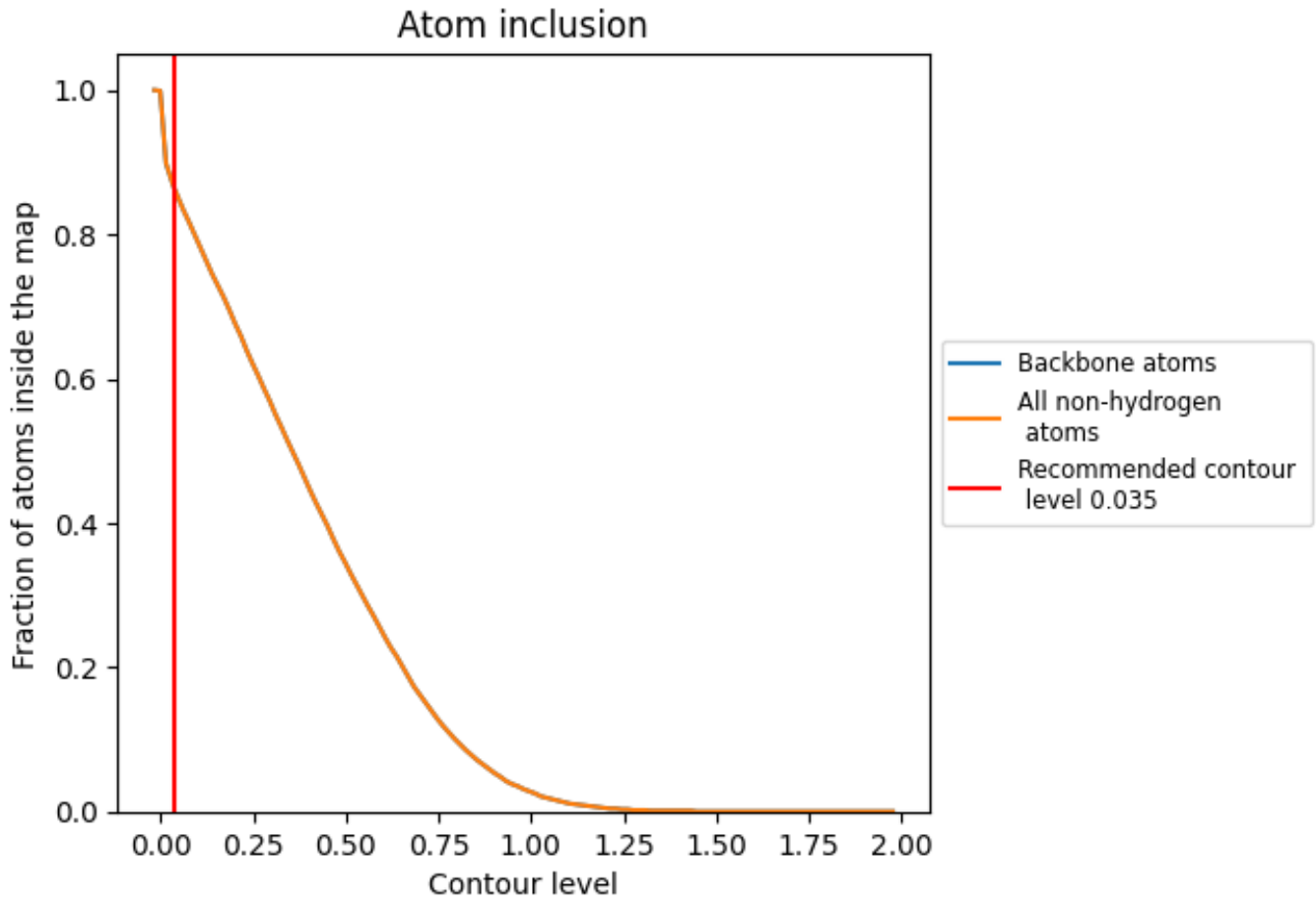
9.3 Atom inclusion mapped to coordinate model



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8660	0.3480
A	0.9330	0.4040
B	0.1840	0.0420
C	0.3030	-0.0160
D	0.9640	0.4490
G	0.9910	0.4970
H	0.9570	0.4220
I	0.9120	0.3470
J	0.9560	0.4160
K	0.9510	0.4180
L	0.9710	0.4470
M	0.8750	0.4300
N	0.7270	0.1930
O	0.9690	0.4300
P	0.9810	0.4260
Q	0.1260	-0.0190
R	0.3550	0.1040
S	0.9890	0.4140
U	0.7930	0.3180
V	0.8140	0.3660
W	0.9710	0.4720
Y	0.9810	0.3600
Z	0.9200	0.2780