W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Jun 26, 2025 – 12:11 AM JST

PDB ID	:	7E2C / pdb_00007e2c
EMDB ID	:	EMD-30954
Title	:	Monomer of TRAPPII (open)
Authors	:	Sui, S.F.; Sun, S.; Mi, C.C.
Deposited on	:	2021-02-05
Resolution	:	4.18 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:

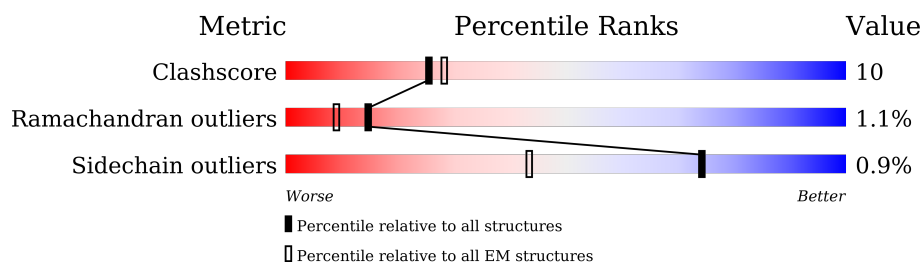|		
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 4.18 Å.

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

Metric	Percentile Ranks	Value
Clashscore		10
Ramachandran outliers		1.1%
Sidechain outliers		0.9%

Worse   *Better*

∎ Percentile relative to all structures
⬚ Percentile relative to all EM structures

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 <=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	152	10% / 70% / 25% / · ·
2	B	268	· / 53% / 19% / · / 27%
3	C	193	· / 76% / 19% / · / 5%
3	F	193	· / 78% / 16% / 6%
4	D	159	75% / 19% / · 5%
5	E	219	58% / 15% / 26%
6	G	283	59% / 13% / 28%
7	H	175	· / 62% / 18% / · / 17%

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Mol	Chain	Length	Quality of chain
8	I	1102	66% 6% 27%
9	J	1289	56% 11% 32%
10	K	559	39% 6% 55%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 23020 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 TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	150	Total 1206	C 781	N 188	O 233	S 4	0	0

- Molecule 2 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	195	Total 1458	C 939	N 247	O 264	S 8	0	0

- Molecule 3 is a protein called Trafficking protein particle complex subunit BET3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	184	Total 1482	C 947	N 244	O 280	S 11	0	0
3	F	182	Total 1470	C 939	N 242	O 278	S 11	0	0

- Molecule 4 is a protein called Trafficking protein particle complex subunit BET5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	151	Total 1234	C 792	N 209	O 227	S 6	0	0

- Molecule 5 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	161	Total 1295	C 838	N 206	O 242	S 9	0	0

- Molecule 6 is a protein called Trafficking protein particle complex subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	203	Total 1612	C 1029	N 282	O 292	S 9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	41	TYR	ILE	conflict	UNP Q03337
G	42	ILE	PRO	conflict	UNP Q03337

- Molecule 7 is a protein called Trafficking protein particle complex subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	146	Total 1172	C 758	N 194	O 215	S 5	0	0

- Molecule 8 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	799	Total 4258	C 2590	N 822	O 844	S 2	0	0

- Molecule 9 is a protein called Trafficking protein particle complex II-specific subunit 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	873	Total 6265	C 3988	N 1085	O 1173	S 19	0	0

- Molecule 10 is a protein called Trafficking protein particle complex II-specific subunit 65.

| Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	251	Total 1568	C 988	N 278	O 300	S 2	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TRAPP-associated protein TCA17
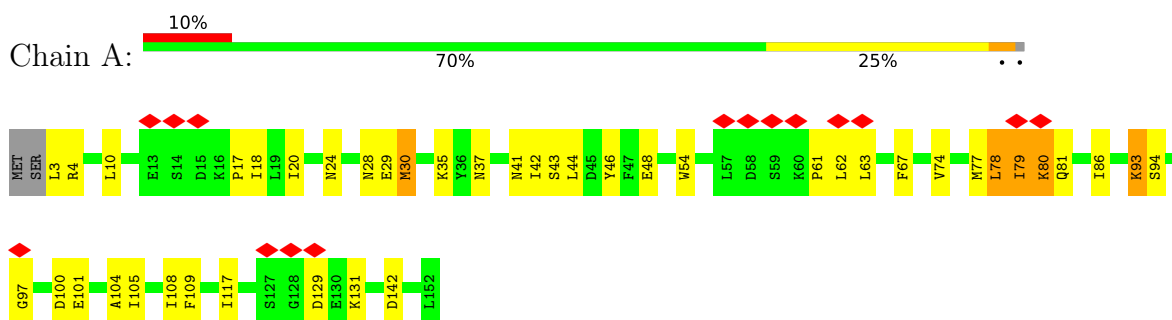
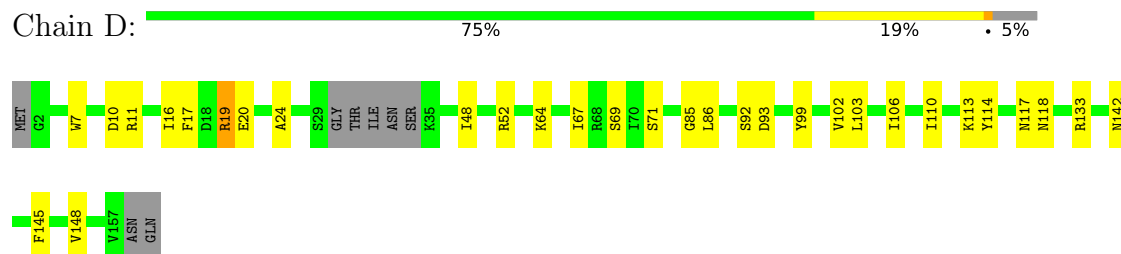• Molecule 2: Trafficking protein particle complex subunit 33
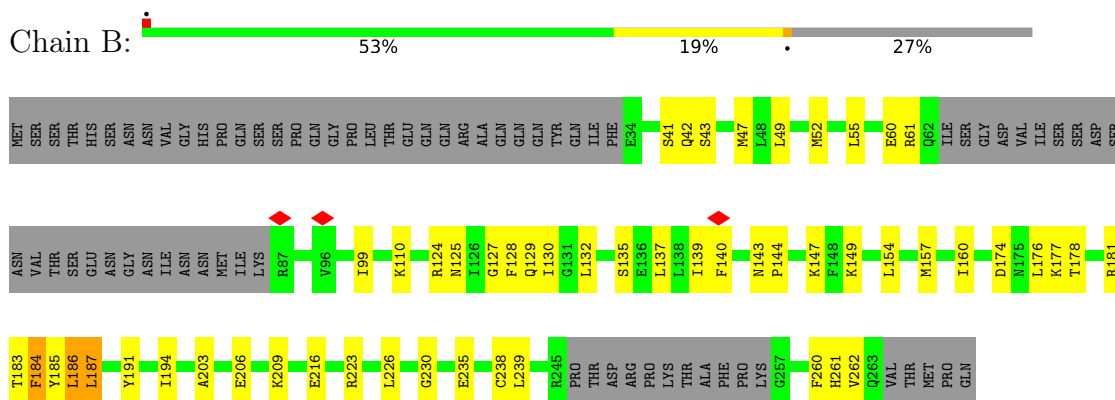
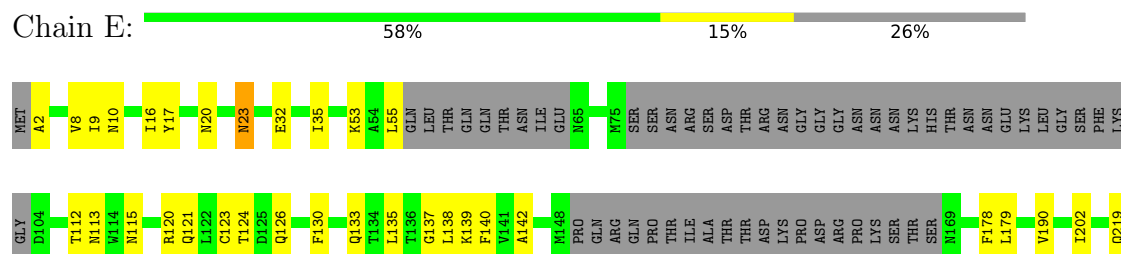• Molecule 3: Trafficking protein particle complex subunit BET3

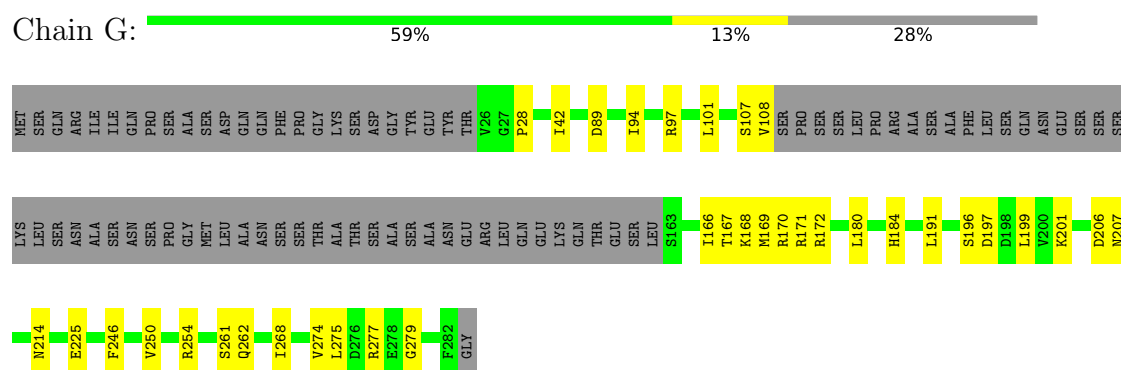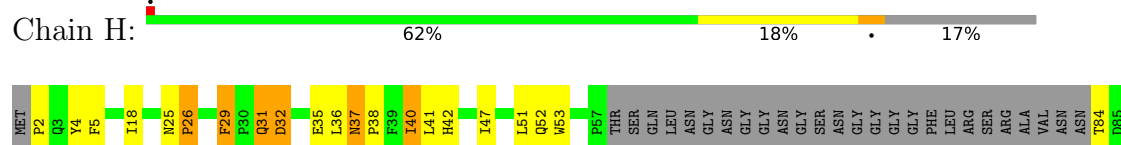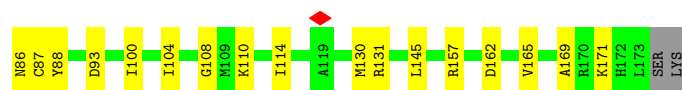• Molecule 3: Trafficking protein particle complex subunit BET3

Chain F:
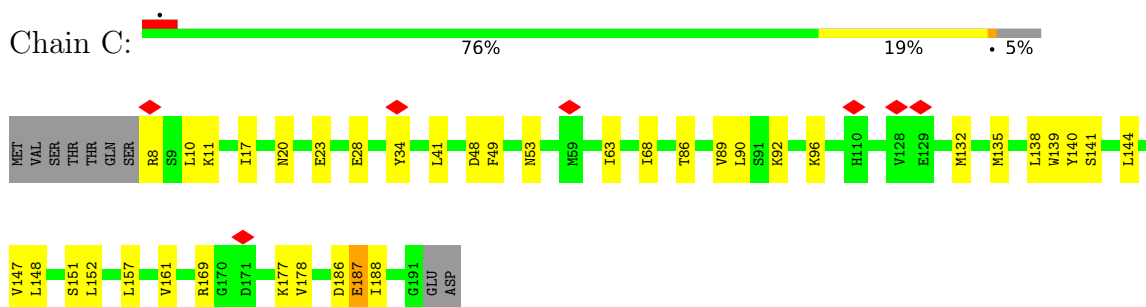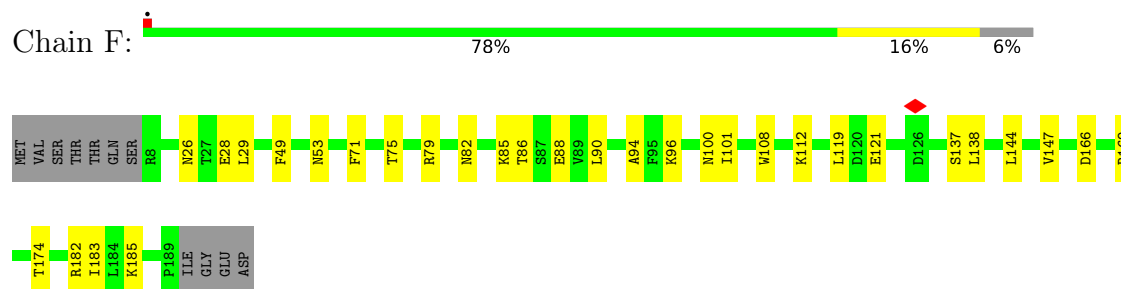
• Molecule 4: Trafficking protein particle complex subunit BET5

Chain D:

• Molecule 5: Trafficking protein particle complex subunit 23

Chain E:

• Molecule 6: Trafficking protein particle complex subunit 31

Chain G:
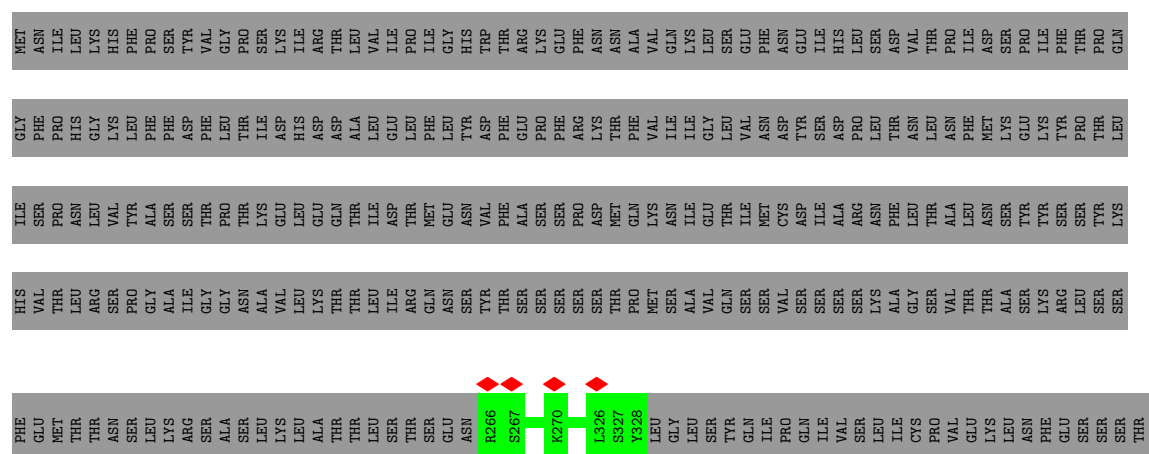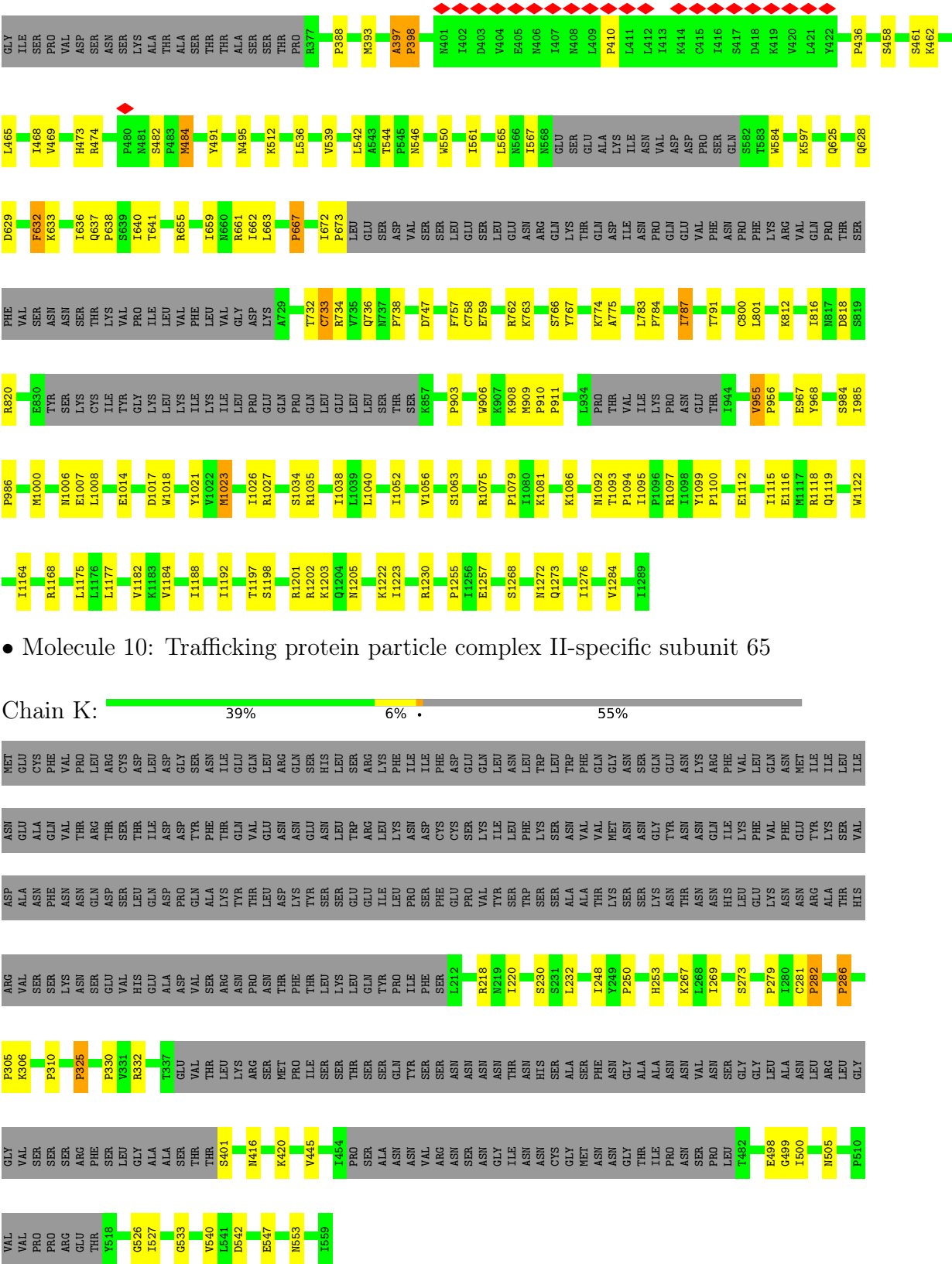

• Molecule 7: Trafficking protein particle complex subunit 20

Chain H:

• Molecule 8: Trafficking protein particle complex II-specific subunit 130

Chain I:　66%　6%　27%
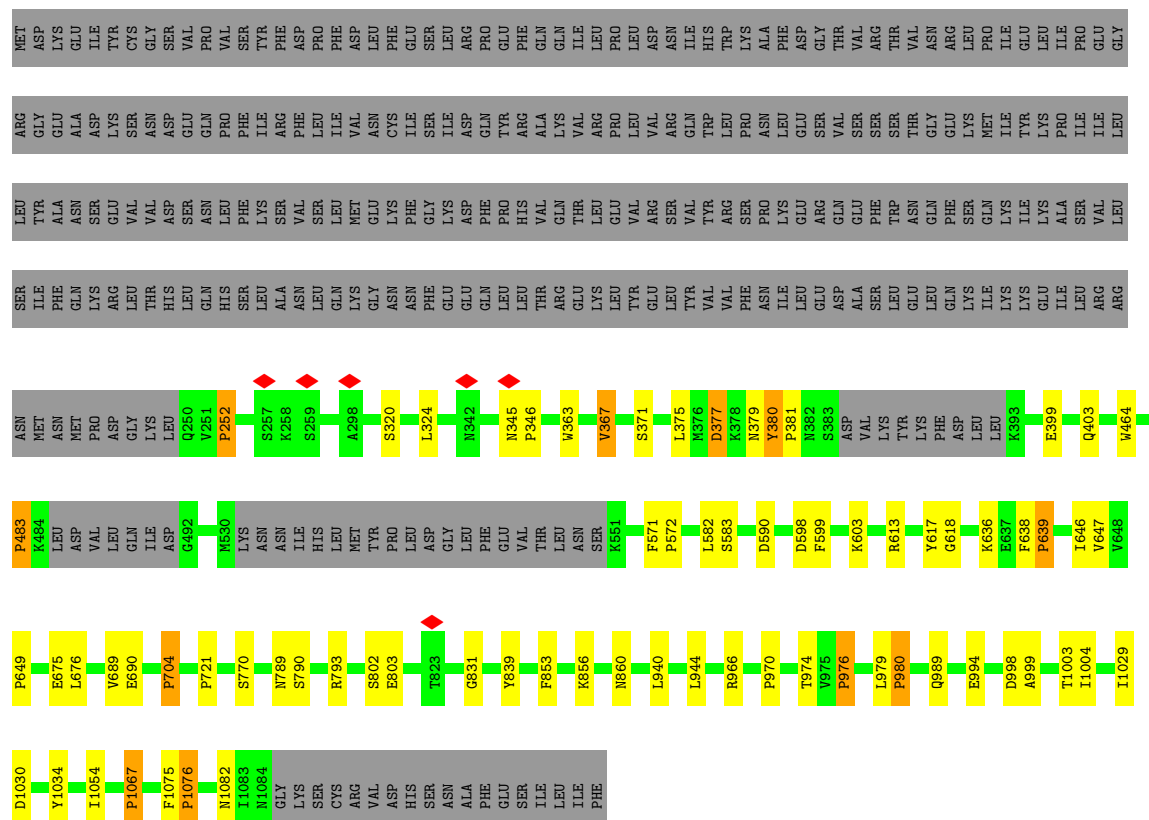
• Molecule 9: Trafficking protein particle complex II-specific subunit 120

Chain J:　56%　11%　32%

• Molecule 10: Trafficking protein particle complex II-specific subunit 65

Chain K:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	523.68, 523.68, 523.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.39	0/1226	0.92	4/1655 (0.2%)
2	B	0.42	0/1480	0.87	0/1998
3	C	0.36	0/1509	0.81	2/2040 (0.1%)
3	F	0.40	0/1497	0.85	1/2024 (0.0%)
4	D	0.42	0/1262	0.87	1/1702 (0.1%)
5	E	0.42	0/1319	0.77	2/1779 (0.1%)
6	G	0.43	0/1645	0.84	3/2217 (0.1%)
7	H	0.48	0/1202	0.92	3/1629 (0.2%)
8	I	0.40	0/4279	0.88	15/5936 (0.3%)
9	J	0.43	0/6368	0.96	24/8672 (0.3%)
10	K	0.46	0/1582	1.02	10/2169 (0.5%)
All	All	0.42	0/23369	0.90	65/31821 (0.2%)

There are no bond length outliers.

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	346	PRO	N-CA-CB	10.53	110.18	102.28
8	I	976	PRO	N-CA-CB	9.09	112.80	103.25
8	I	1076	PRO	N-CA-CB	8.38	112.05	103.25
7	H	26	PRO	N-CA-CB	8.24	111.90	103.25
10	K	325	PRO	N-CA-CB	8.14	111.80	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1206	0	1228	86	0
2	B	1458	0	1380	60	0
3	C	1482	0	1490	28	0
3	F	1470	0	1476	22	0
4	D	1234	0	1201	24	0
5	E	1295	0	1293	23	0
6	G	1612	0	1554	38	0
7	H	1172	0	1121	53	0
8	I	4258	0	2190	39	0
9	J	6265	0	5496	80	0
10	K	1568	0	1147	13	0
All	All	23020	0	19576	426	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 426 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)
1:A:35:LYS:HE2	8:I:377:ASP:CB	1.15	1.60
1:A:35:LYS:CE	8:I:377:ASP:CB	1.83	1.53
1:A:79:ILE:CG2	1:A:81:GLN:OE1	1.67	1.39
1:A:63:LEU:HD12	1:A:77:MET:CE	1.58	1.33
1:A:35:LYS:NZ	8:I:377:ASP:HA	1.45	1.30

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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	148/152 (97%)	128 (86%)	20 (14%)	0	100	100
2	B	189/268 (70%)	165 (87%)	23 (12%)	1 (0%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	182/193 (94%)	169 (93%)	13 (7%)	0	100	100
3	F	180/193 (93%)	164 (91%)	16 (9%)	0	100	100
4	D	147/159 (92%)	125 (85%)	22 (15%)	0	100	100
5	E	153/219 (70%)	139 (91%)	14 (9%)	0	100	100
6	G	199/283 (70%)	176 (88%)	23 (12%)	0	100	100
7	H	142/175 (81%)	124 (87%)	16 (11%)	2 (1%)	9	41
8	I	791/1102 (72%)	641 (81%)	129 (16%)	21 (3%)	4	28
9	J	861/1289 (67%)	691 (80%)	164 (19%)	6 (1%)	19	56
10	K	243/559 (44%)	183 (75%)	55 (23%)	5 (2%)	5	33
All	All	3235/4592 (70%)	2705 (84%)	495 (15%)	35 (1%)	15	46

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	26	PRO
7	H	37	ASN
8	I	252	PRO
8	I	380	TYR
8	I	381	PRO

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	140/142 (99%)	135 (96%)	5 (4%)	30	52
2	B	142/248 (57%)	139 (98%)	3 (2%)	48	66
3	C	169/178 (95%)	169 (100%)	0	100	100
3	F	168/178 (94%)	168 (100%)	0	100	100
4	D	135/145 (93%)	134 (99%)	1 (1%)	81	87
5	E	144/199 (72%)	144 (100%)	0	100	100
6	G	169/249 (68%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	126/152 (83%)	122 (97%)	4 (3%)	34	55
8	I	78/1023 (8%)	78 (100%)	0	100	100
9	J	551/1213 (45%)	546 (99%)	5 (1%)	75	83
10	K	93/517 (18%)	93 (100%)	0	100	100
All	All	1915/4244 (45%)	1897 (99%)	18 (1%)	74	83

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	484	MET
9	J	1007	GLU
9	J	955	VAL
4	D	19	ARG
9	J	482	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	72	GLN
9	J	471	ASN
9	J	1189	ASN
7	H	31	GLN
9	J	566	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-30954. 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 |
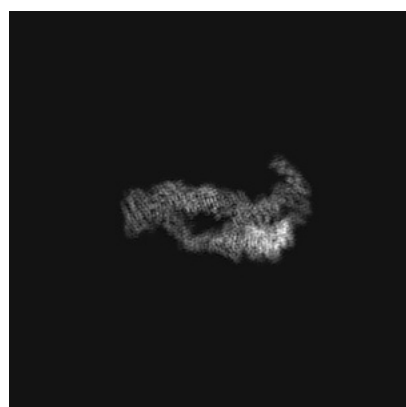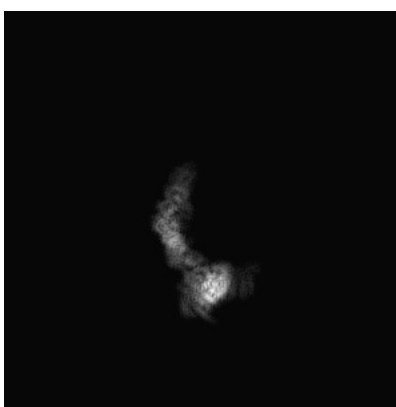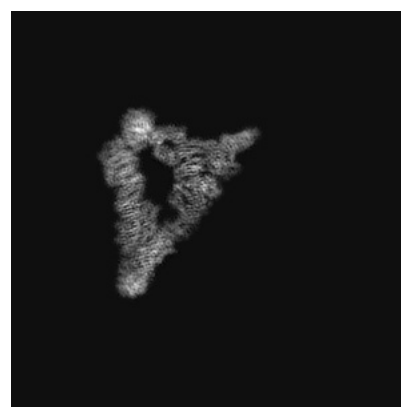
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
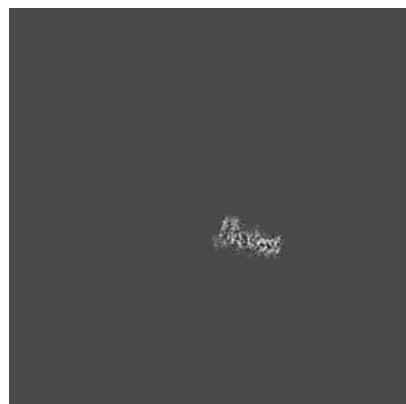
6.2.1 Primary map

| X Index: 240 | Y Index: 240 | Z Index: 240 |
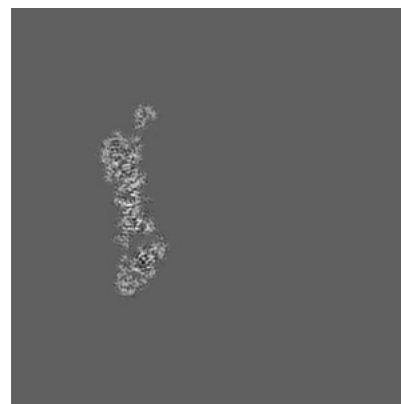
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ

6.3.1   Primary map

| X Index: 147 | Y Index: 322 | Z Index: 201 |

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

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

6.4.1   Primary map

| X | Y | Z |
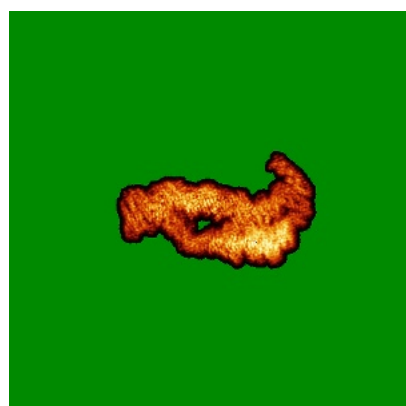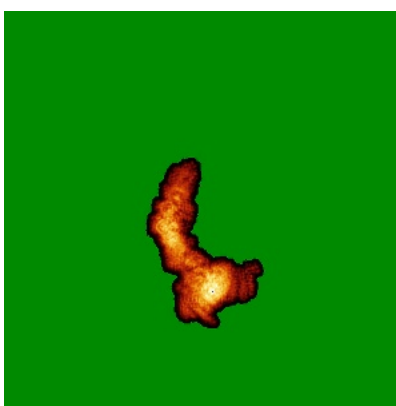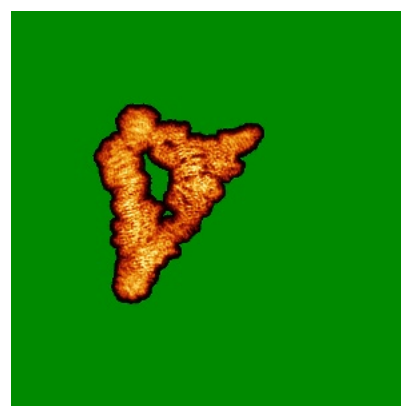
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views ⓘ

6.5.1   Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.
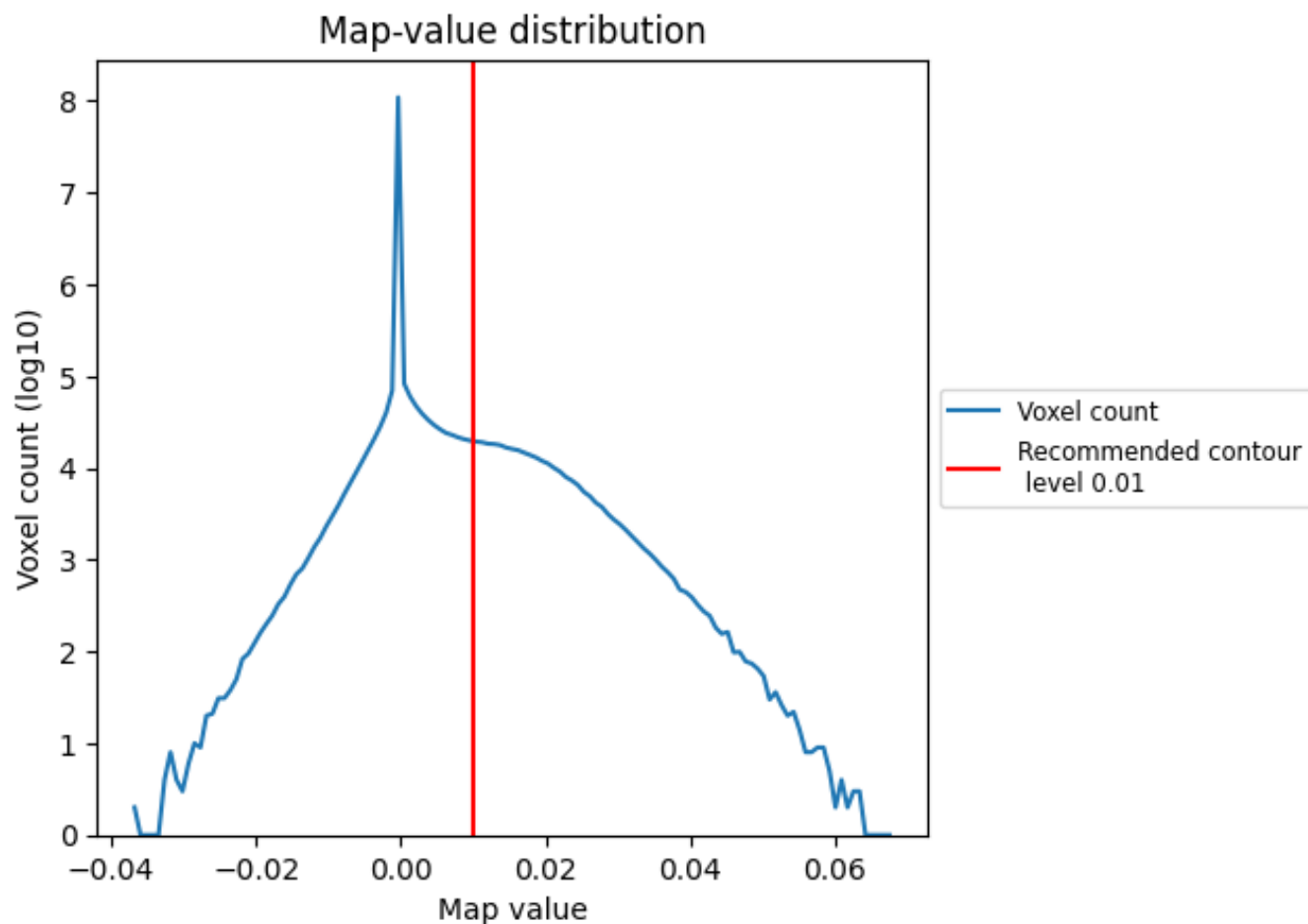
6.6   Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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

7.2   Volume estimate ⓘ
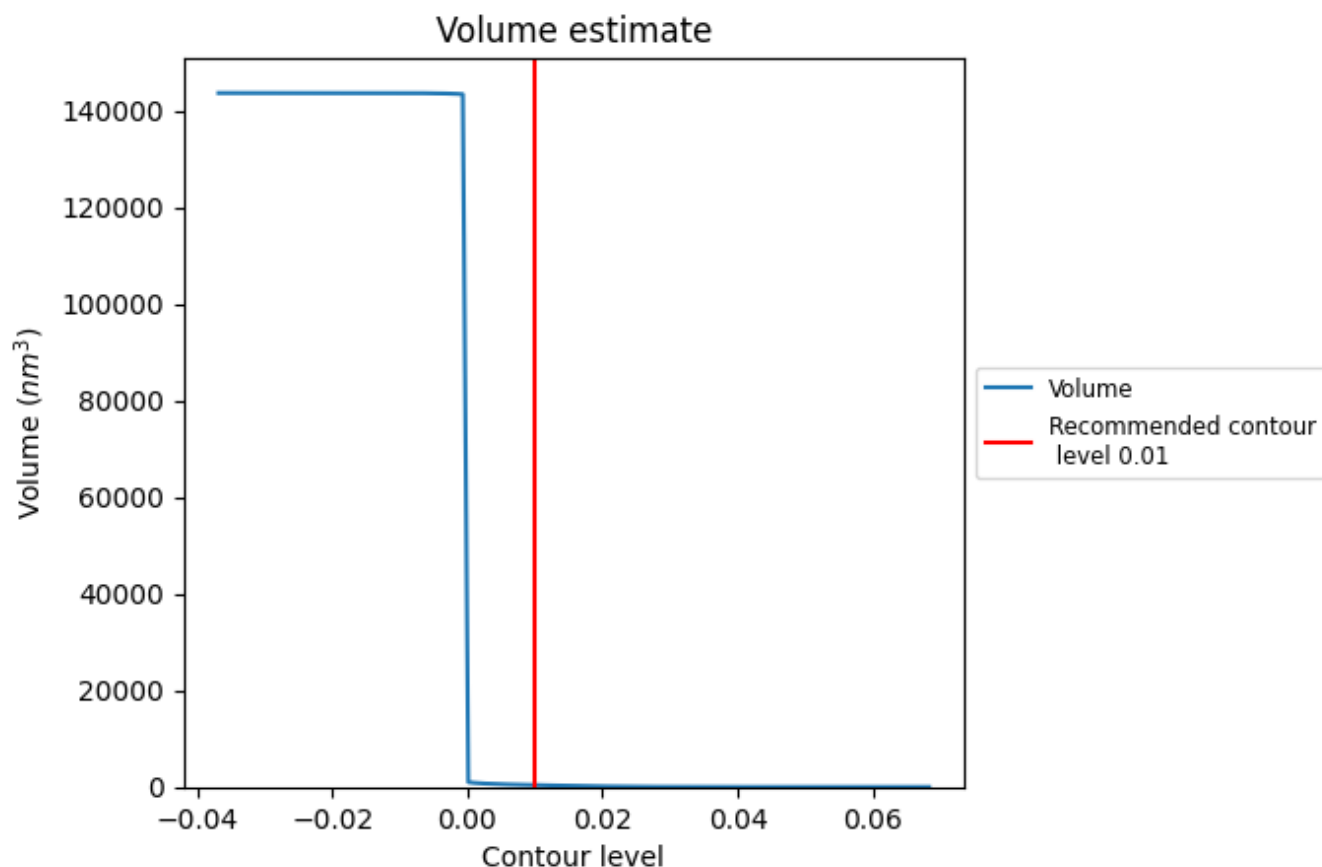
The volume at the recommended contour level is 386 nm^3; this corresponds to an approximate mass of 349 kDa.

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 ⓘ

Rotationally averaged power spectrum
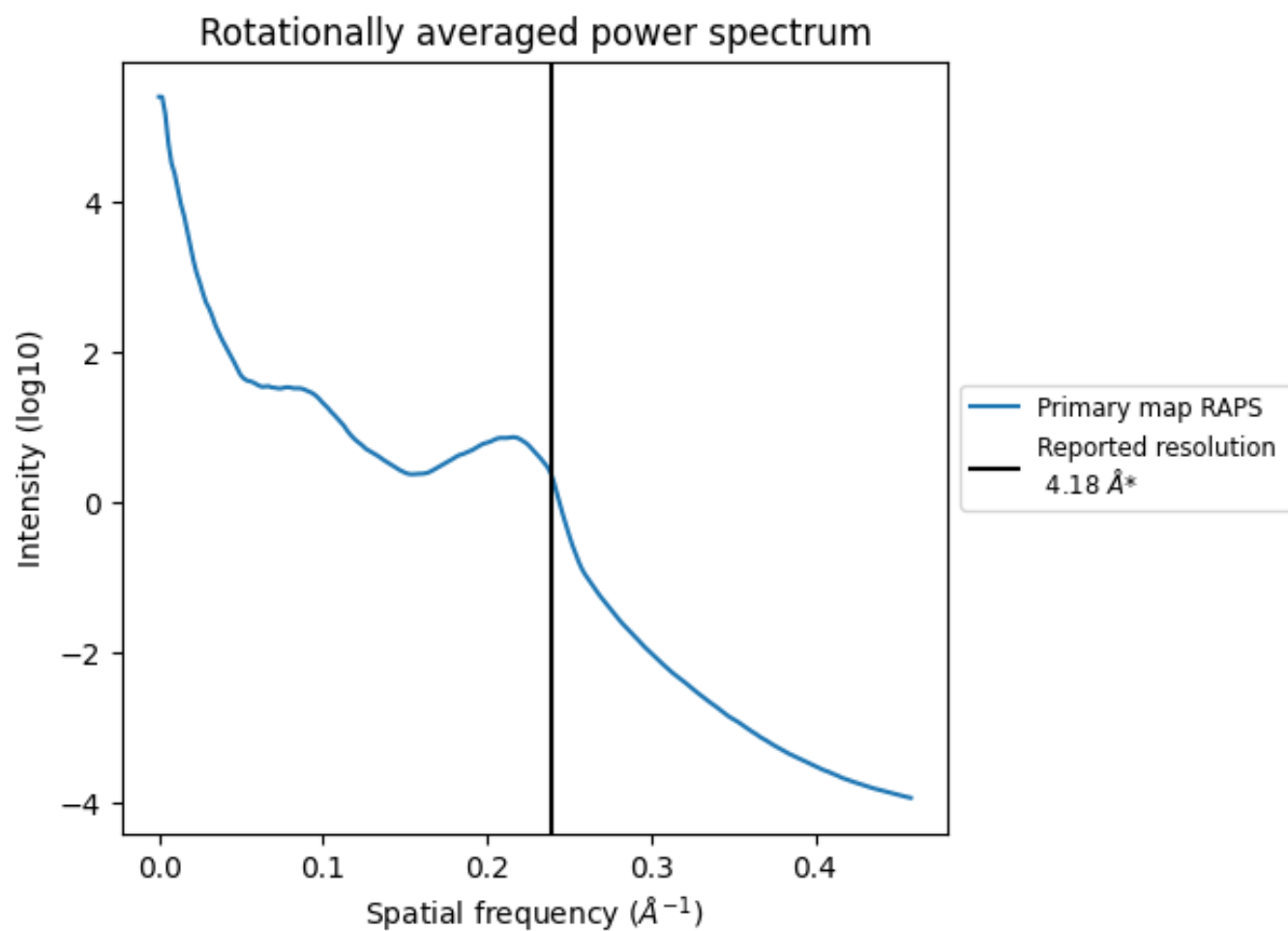
*Reported resolution corresponds to spatial frequency of 0.239 Å^{-1}

8 Fourier-Shell correlation ⓘ

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-30954 and PDB model 7E2C. Per-residue inclusion information can be found in section 3 on page 6.

9.1   Map-model overlay ⓘ

X	Y	Z
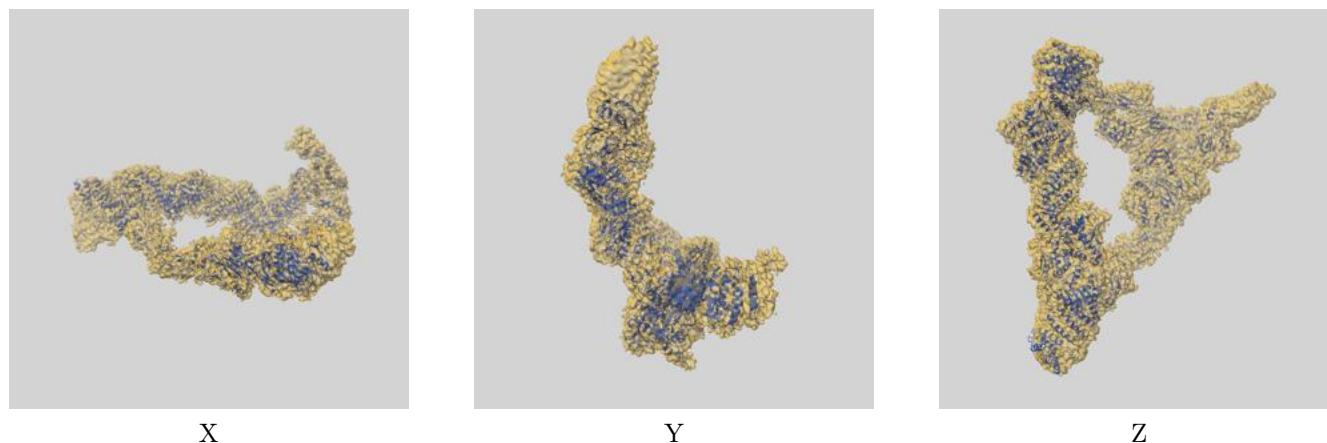
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X   Y   Z
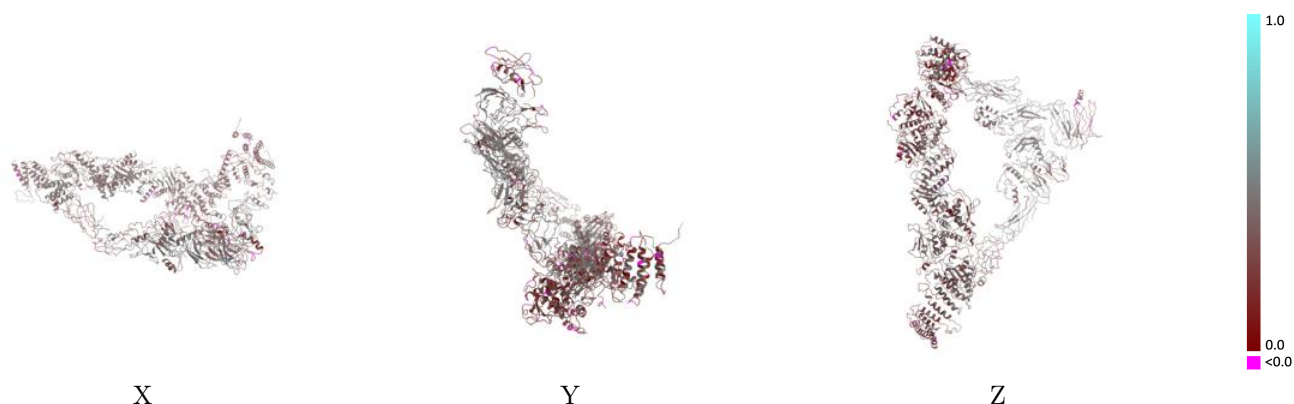
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ
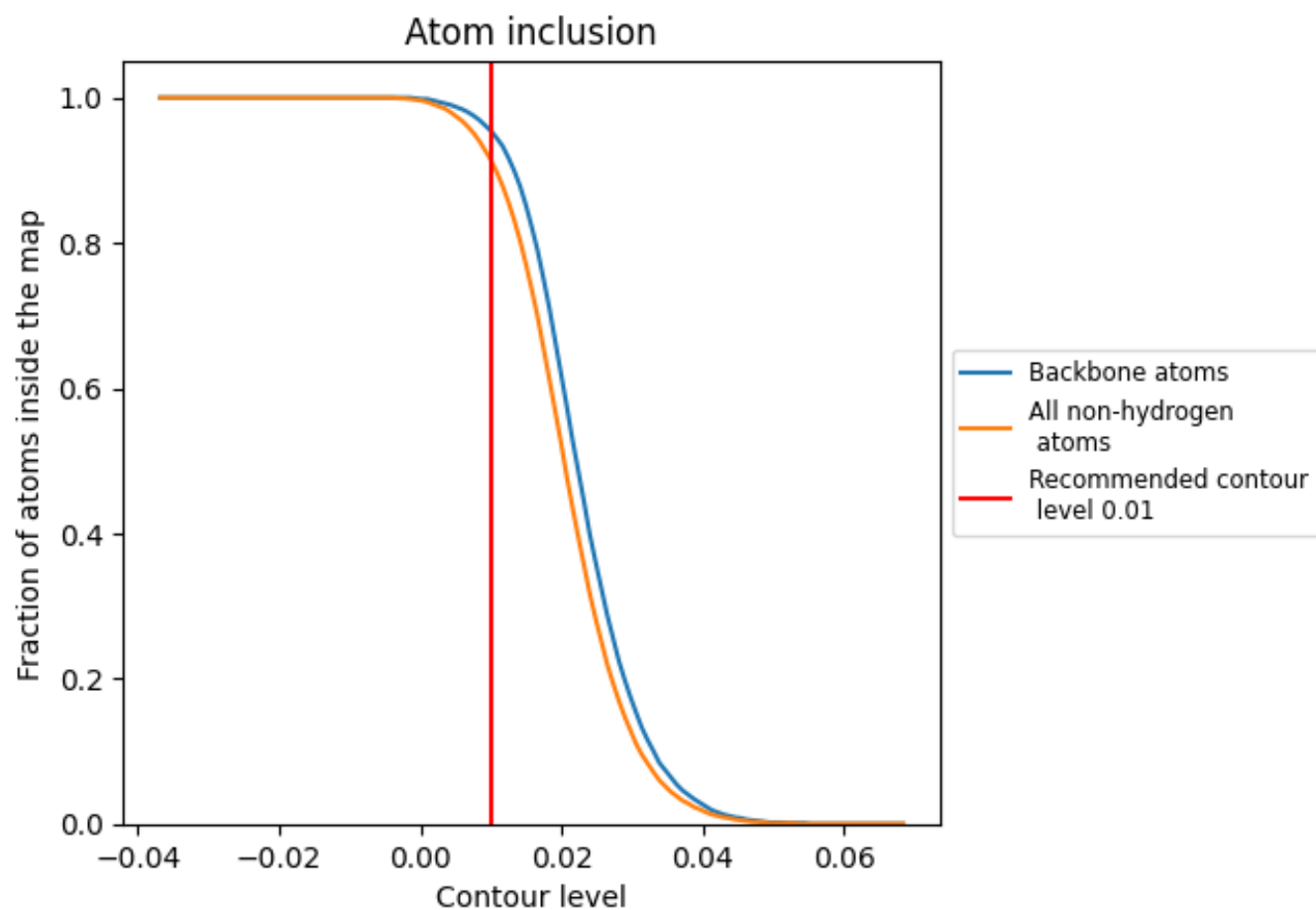
At the recommended contour level, 95% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.3570
A	0.7570	0.2690
B	0.8820	0.2850
C	0.8210	0.2630
D	0.9300	0.3600
E	0.9150	0.3770
F	0.9140	0.3540
G	0.9190	0.3750
H	0.9050	0.3620
I	0.9610	0.3870
J	0.9250	0.3850
K	0.9610	0.3490

1.0

0.0
<0.0