



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 09:49 PM EST

PDB ID : 3J45
EMDB ID : EMD-5692
Title : Structure of a non-translocating SecY protein channel with the 70S ribosome
Authors : Menetret, J.F.; Park, E.; Gumbart, J.C.; Ludtke, S.J.; Li, W.; Whynot, A.;
Rapoport, T.A.; Akey, C.W.
Deposited on : 2013-06-18
Resolution : 9.50 Å (reported)
Based on initial models : 2I2P, 3J01

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.31.3

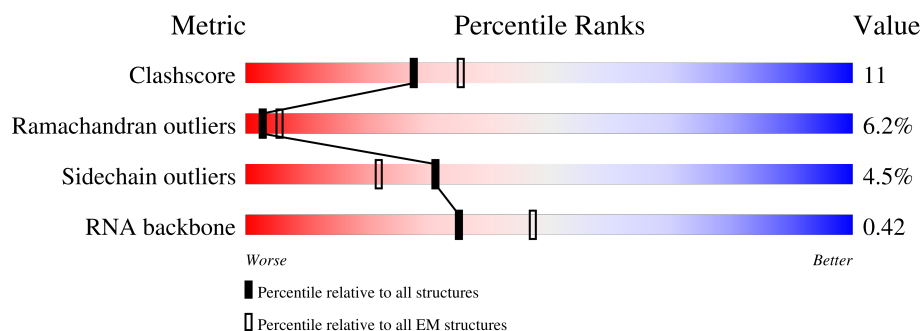
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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
RNA backbone	4643	859

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	y	437	<div> <div>16%</div> <div>74%</div> <div>21%</div> <div>.</div> </div>
2	E	56	<div> <div>18%</div> <div>64%</div> <div>32%</div> <div>.</div> </div>
3	G	65	<div> <div>25%</div> <div>51%</div> <div>34%</div> <div>12%</div> <div>.</div> </div>
4	T	100	<div> <div>5%</div> <div>67%</div> <div>26%</div> <div>7%</div> </div>
5	U	103	<div> <div>8%</div> <div>68%</div> <div>22%</div> <div>9%</div> <div>.</div> </div>
6	Y	63	<div> <div>71%</div> <div>25%</div> <div>.</div> </div>
7	1	63	<div> <div>46%</div> <div>38%</div> <div>16%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	2	36	 50% 36% 14%
9	3	18	 33% 50% 17%
10	4	61	 56% 43% .
11	5	108	 27% 55% 19%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12465 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 Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	y	437	Total	C	N	O	S	0	1
			3361	2220	554	570	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	5	ACE	-	ACETYLATION	UNP P0AGA2
y	441	NH2	-	AMIDATION	UNP P0AGA2

- Molecule 2 is a protein called Preprotein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	56	Total	C	N	O	S	0	1
			433	283	76	73	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	73	ACE	-	ACETYLATION	UNP P0AG96
E	128	NH2	-	AMIDATION	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	65	Total	C	N	O	S	0	0
			457	299	73	81	4		

- Molecule 4 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 5 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	U	103	Total	C	N	O	0	0
			789	498	148	143		

- Molecule 6 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	63	Total	C	N	O	P	0	0
			1350	603	245	439	63		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	36	Total	C	N	O	P	0	0
			775	345	142	252	36		

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	18	Total	C	N	O	P	0	0
			387	172	71	126	18		

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	61	Total	C	N	O	P	0	0
			1312	584	240	427	61		

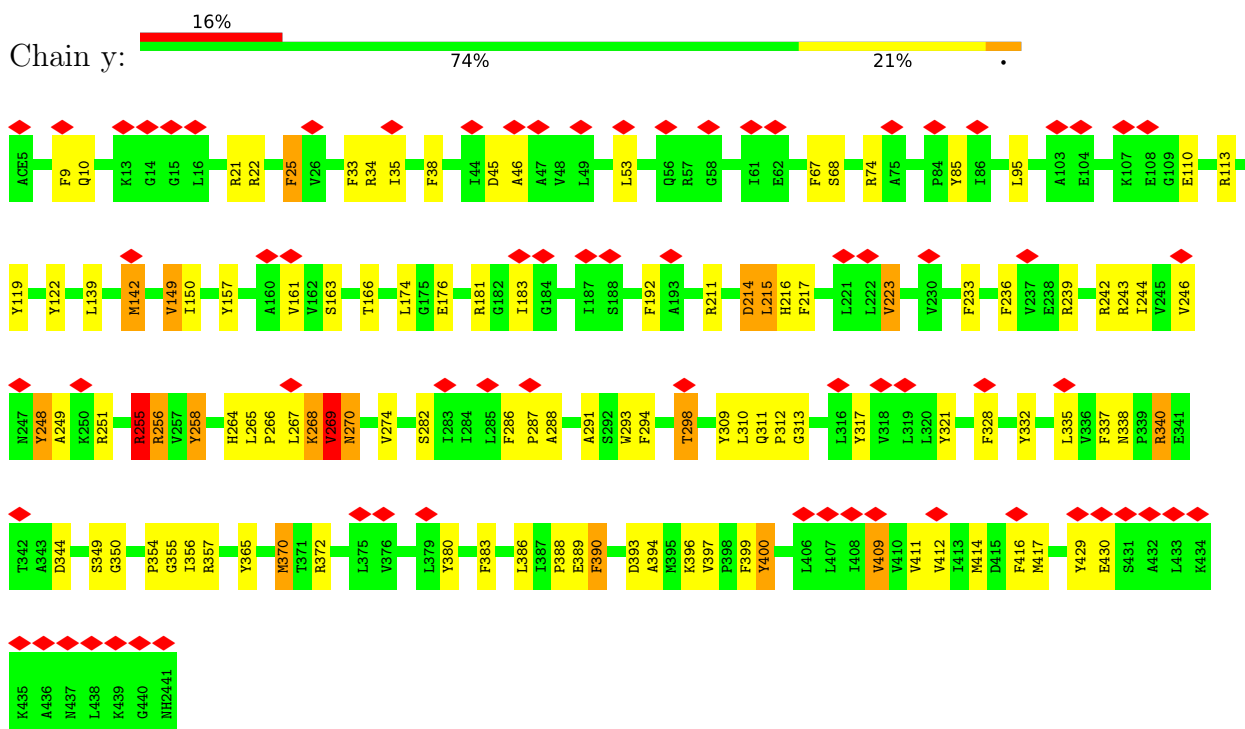
- Molecule 11 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	108	Total	C	N	O	P	0	0
			2305	1029	406	762	108		

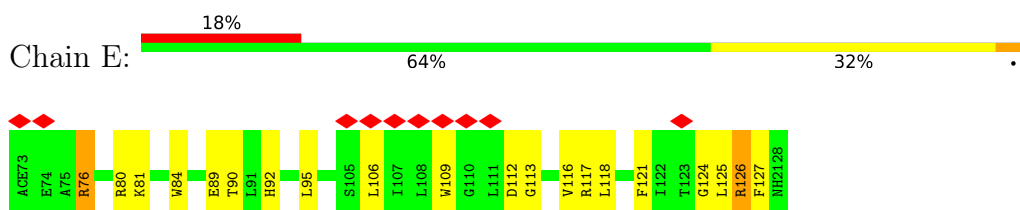
3 Residue-property plots

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.

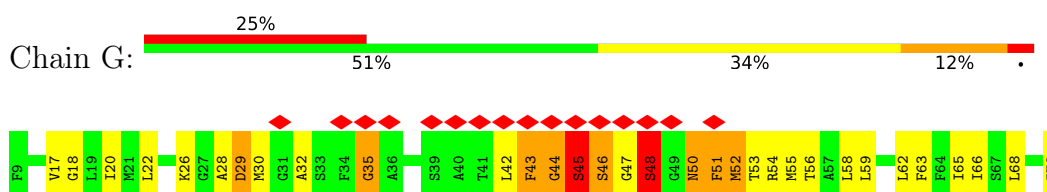
- Molecule 1: Protein translocase subunit SecY



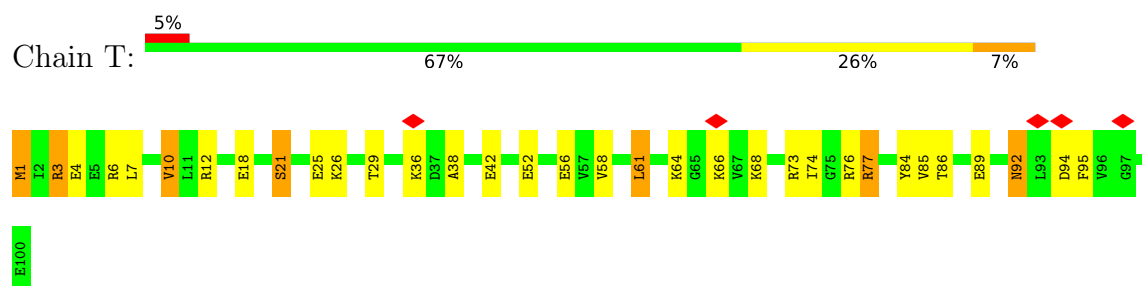
- Molecule 2: Preprotein translocase subunit SecE



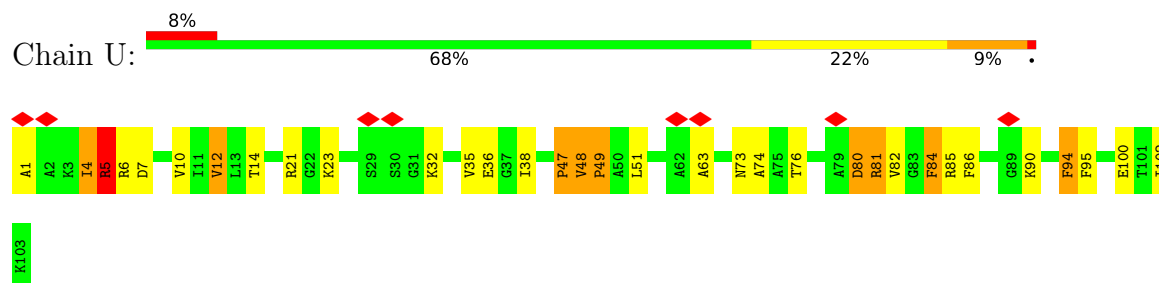
- Molecule 3: Protein-export membrane protein SecE



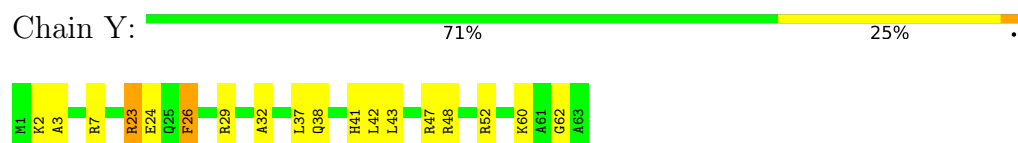
- Molecule 4: 50S ribosomal protein L23



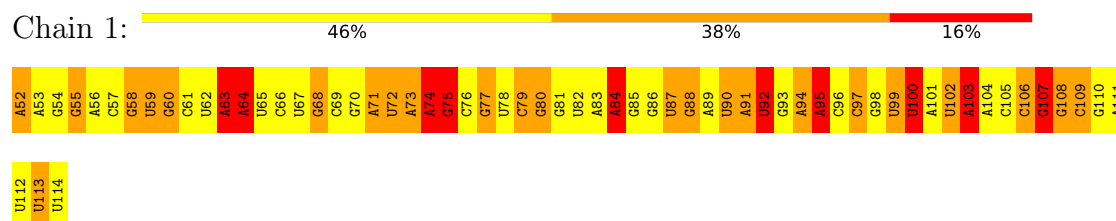
- Molecule 5: 50S ribosomal protein L24



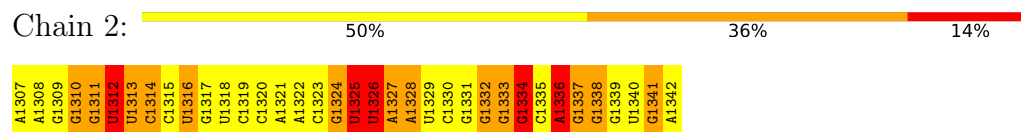
- Molecule 6: 50S ribosomal protein L29



- Molecule 7: 23S ribosomal RNA



- Molecule 8: 23S ribosomal RNA



- Molecule 9: 23S ribosomal RNA



Chain 5:

Epoch	Category
U2092	Yellow
G2093	Yellow
A2094	Yellow
A2095	Yellow
G2096	Yellow
A2097	Yellow
U2098	Yellow
U2099	Yellow
G2100	Yellow
A2101	Yellow
G2102	Yellow
G2103	Yellow
G2104	Yellow
U2105	Yellow
U2106	Yellow
G2107	Yellow
A2108	Yellow
U2109	Yellow
G2110	Yellow
U2111	Yellow
G2112	Yellow
U2113	Yellow
A2114	Yellow
G2115	Yellow
G2116	Yellow
A2117	Yellow
G2118	Yellow
A2119	Yellow
G2120	Yellow
G2121	Yellow
U2122	Yellow
G2123	Yellow
G2124	Yellow
G2125	Yellow
A2126	Yellow
G2127	Yellow
G2128	Yellow
G2129	Yellow
U2130	Yellow
U2131	Yellow
U2132	Yellow
G2133	Yellow
A2134	Yellow
A2135	Yellow
G2136	Yellow
U2137	Yellow
G2138	Yellow
U2139	Yellow
G2140	Yellow
G2141	Yellow
A2142	Yellow
G2143	Yellow
G2144	Yellow
G2145	Yellow
G2146	Yellow
A2147	Yellow
G2148	Yellow
U2149	Yellow
G2150	Yellow

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	51000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	11.232	Depositor
Minimum map value	-5.482	Depositor
Average map value	0.204	Depositor
Map value standard deviation	0.928	Depositor
Recommended contour level	1.8	Depositor
Map size (\AA)	393.12, 393.12, 393.12	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.73, 2.73, 2.73	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

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	y	1.70	23/3434 (0.7%)	2.02	104/4657 (2.2%)
2	E	1.79	5/437 (1.1%)	2.35	17/596 (2.9%)
3	G	0.27	0/462	1.57	12/620 (1.9%)
4	T	1.64	7/794 (0.9%)	1.92	16/1060 (1.5%)
5	U	1.71	7/797 (0.9%)	1.95	20/1062 (1.9%)
6	Y	1.80	5/510 (1.0%)	1.93	13/677 (1.9%)
7	1	3.51	207/1511 (13.7%)	3.45	299/2354 (12.7%)
8	2	3.40	117/867 (13.5%)	3.56	188/1351 (13.9%)
9	3	3.68	75/432 (17.4%)	3.86	100/672 (14.9%)
10	4	3.59	206/1468 (14.0%)	3.69	312/2289 (13.6%)
11	5	3.40	375/2577 (14.6%)	3.71	573/4015 (14.3%)
All	All	2.75	1027/13289 (7.7%)	3.01	1654/19353 (8.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	y	0	6
2	E	0	1
3	G	3	0
4	T	0	1
5	U	0	3
6	Y	0	1
7	1	0	30
8	2	0	15
9	3	0	10
10	4	0	20
11	5	0	54
All	All	3	141

The worst 5 of 1027 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1892	C	N1-C6	18.20	1.48	1.37
7	1	114	U	C2-N3	16.37	1.49	1.37
9	3	1532	A	N3-C4	-15.69	1.25	1.34
10	4	1854	A	N9-C4	-15.56	1.28	1.37
10	4	1850	G	N7-C5	-15.20	1.30	1.39

The worst 5 of 1654 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	3	1540	G	N1-C6-O6	26.41	135.75	119.90
11	5	2198	A	N1-C6-N6	26.09	134.26	118.60
10	4	1857	G	N1-C6-O6	24.56	134.64	119.90
10	4	1857	G	C5-C6-O6	-22.03	115.38	128.60
11	5	2171	A	N1-C6-N6	21.65	131.59	118.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	45	SER	CA
3	G	48	SER	CA
3	G	51	PHE	CA

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	y	216	HIS	Sidechain
1	y	248	TYR	Sidechain
1	y	25	PHE	Sidechain
1	y	309	TYR	Sidechain
1	y	390	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	y	3361	0	3514	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	433	0	466	24	0
3	G	457	0	481	63	0
4	T	787	0	846	5	0
5	U	789	0	847	4	0
6	Y	509	0	543	3	0
7	1	1350	0	676	1	0
8	2	775	0	385	0	0
9	3	387	0	196	0	0
10	4	1312	0	659	3	0
11	5	2305	0	1156	4	0
All	All	12465	0	9769	84	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 11.

The worst 5 of 84 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)
2:E:126:ARG:HE	3:G:68:LEU:CD2	1.54	1.20
2:E:126:ARG:CB	3:G:68:LEU:HD21	1.73	1.18
2:E:126:ARG:HE	3:G:68:LEU:HD22	1.02	1.08
2:E:126:ARG:NH2	3:G:65:ILE:HG12	1.68	1.08
2:E:126:ARG:HB3	3:G:68:LEU:CD2	1.87	1.04

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	y	435/437 (100%)	386 (89%)	27 (6%)	22 (5%)	2 19
2	E	54/56 (96%)	49 (91%)	3 (6%)	2 (4%)	3 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	63/65 (97%)	50 (79%)	7 (11%)	6 (10%)	0	10
4	T	98/100 (98%)	71 (72%)	18 (18%)	9 (9%)	1	11
5	U	101/103 (98%)	79 (78%)	13 (13%)	9 (9%)	1	11
6	Y	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	4	26
All	All	812/824 (98%)	683 (84%)	79 (10%)	50 (6%)	3	17

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	y	142	MET
1	y	258	TYR
1	y	266	PRO
1	y	338	ASN
1	y	340	ARG

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	y	353/353 (100%)	336 (95%)	17 (5%)	25	51
2	E	47/47 (100%)	45 (96%)	2 (4%)	29	53
3	G	46/46 (100%)	43 (94%)	3 (6%)	17	42
4	T	84/84 (100%)	80 (95%)	4 (5%)	25	51
5	U	84/84 (100%)	81 (96%)	3 (4%)	35	59
6	Y	55/55 (100%)	54 (98%)	1 (2%)	59	77
All	All	669/669 (100%)	639 (96%)	30 (4%)	31	52

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	370	MET
5	U	23	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	76	ARG
6	Y	41	HIS
4	T	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
6	Y	41	HIS
6	Y	38	GLN
4	T	70	HIS
4	T	59	ASN
4	T	92	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	4	60/61 (98%)	2 (3%)	0
11	5	107/108 (99%)	37 (34%)	8 (7%)
7	1	62/63 (98%)	12 (19%)	0
8	2	35/36 (97%)	7 (20%)	2 (5%)
9	3	17/18 (94%)	5 (29%)	0
All	All	281/286 (98%)	63 (22%)	10 (3%)

5 of 63 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	1	63	A
7	1	64	A
7	1	71	A
7	1	74	A
7	1	75	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	5	2152	G
11	5	2164	C
11	5	2172	U
11	5	2120	G
11	5	2126	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

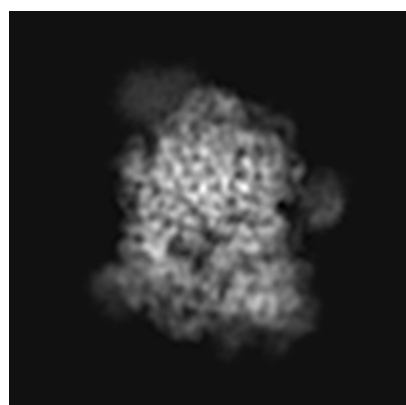
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5692. These allow visual inspection of the internal detail of the map and identification of artifacts.

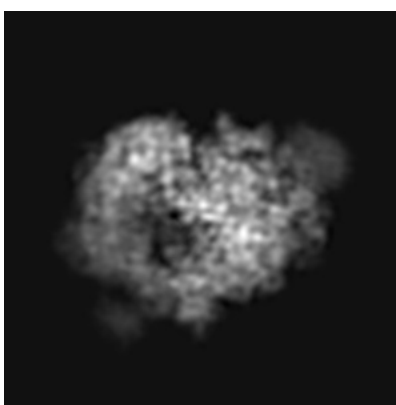
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

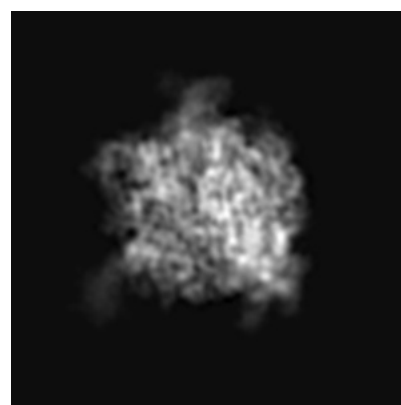
6.1.1 Primary map



X



Y

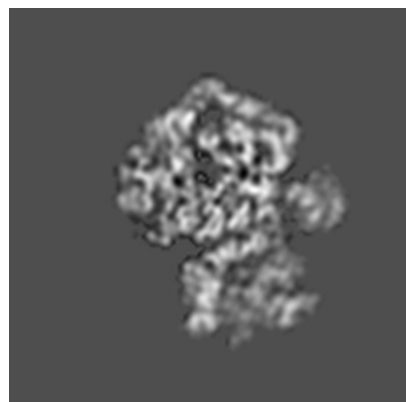


Z

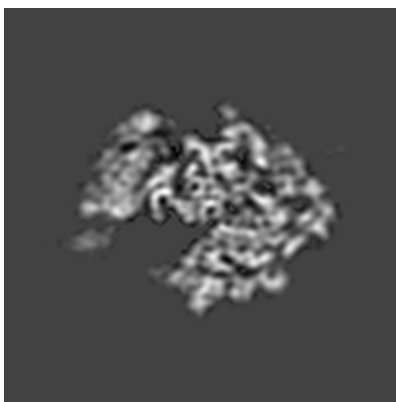
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

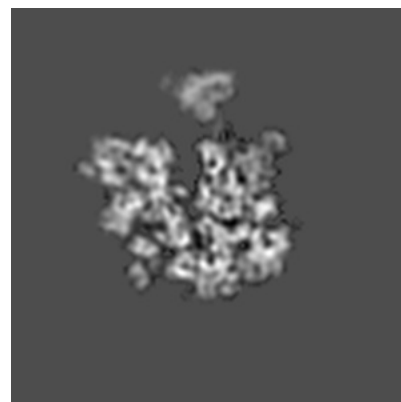
6.2.1 Primary map



X Index: 72



Y Index: 72

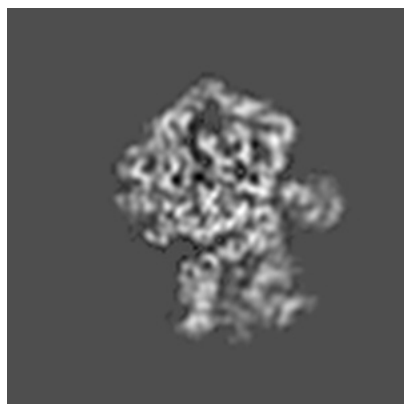


Z Index: 72

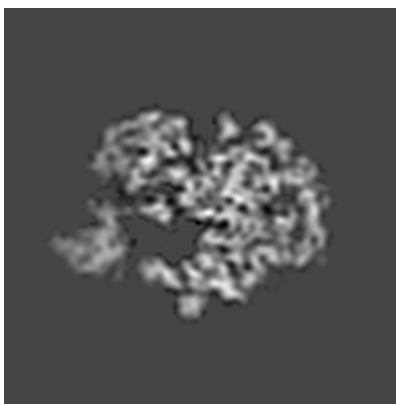
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

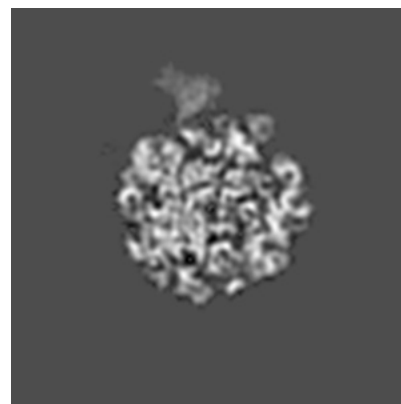
6.3.1 Primary map



X Index: 73



Y Index: 77

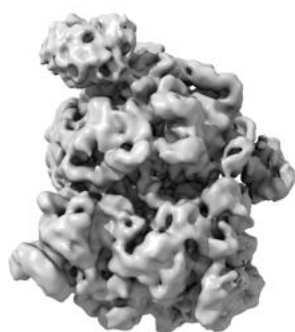


Z Index: 81

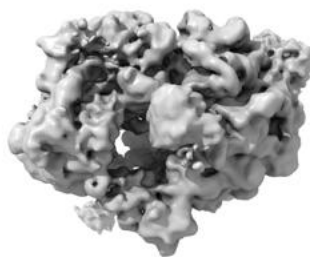
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

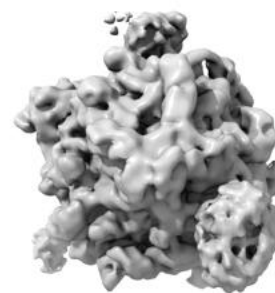
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

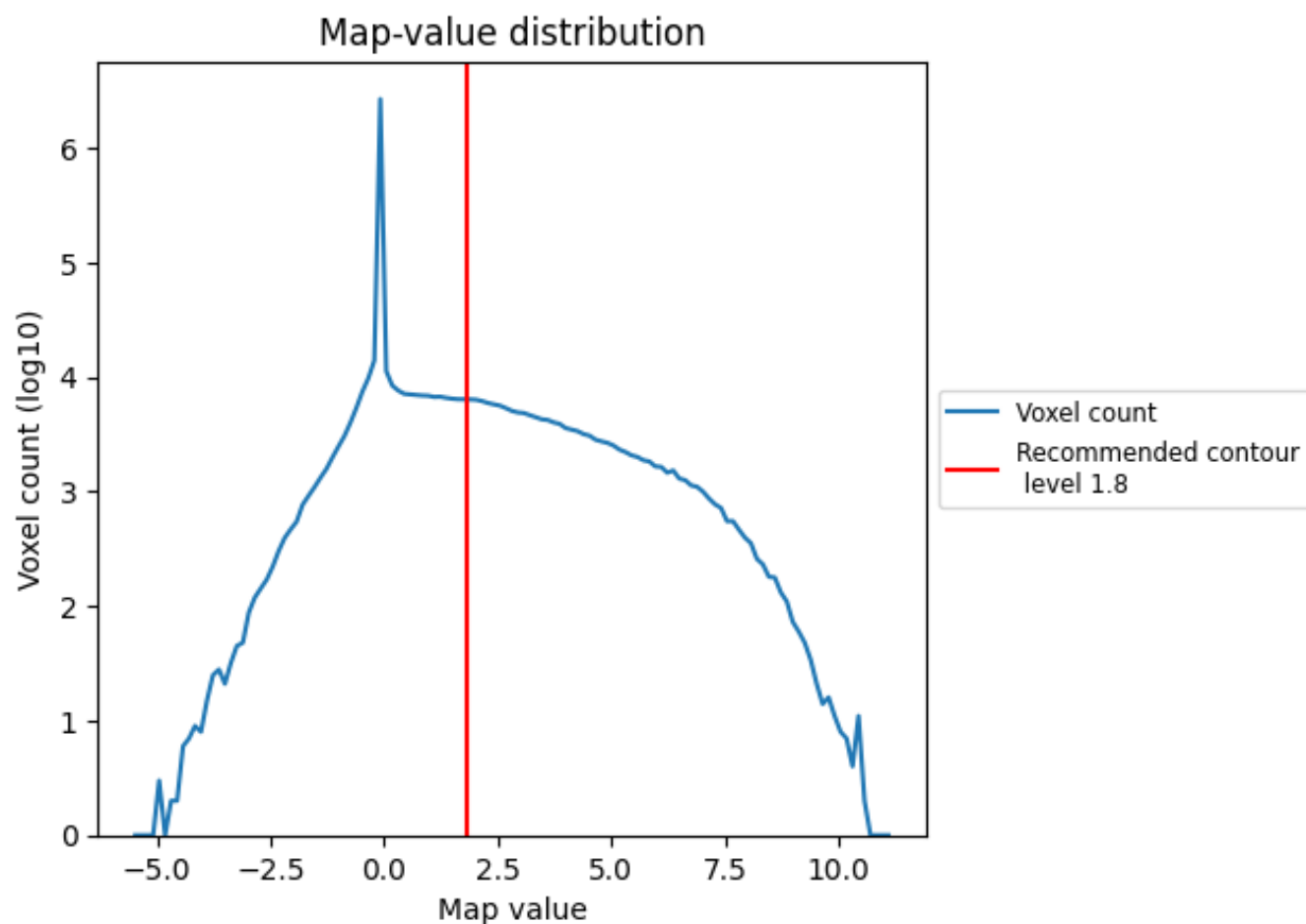
6.5 Mask visualisation

This section was not generated.

7 Map analysis [i](#)

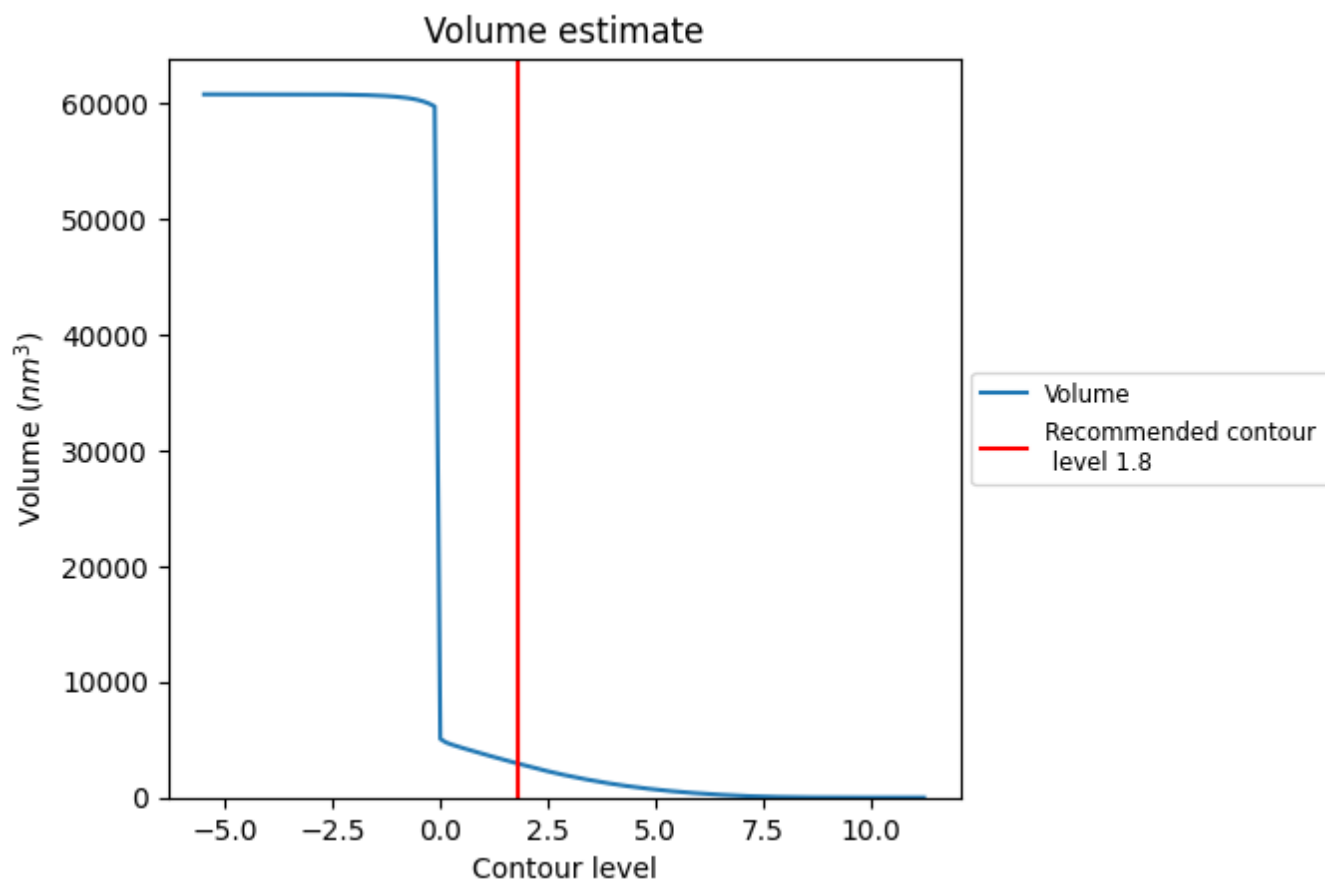
This section contains the results of statistical analysis of the map.

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.

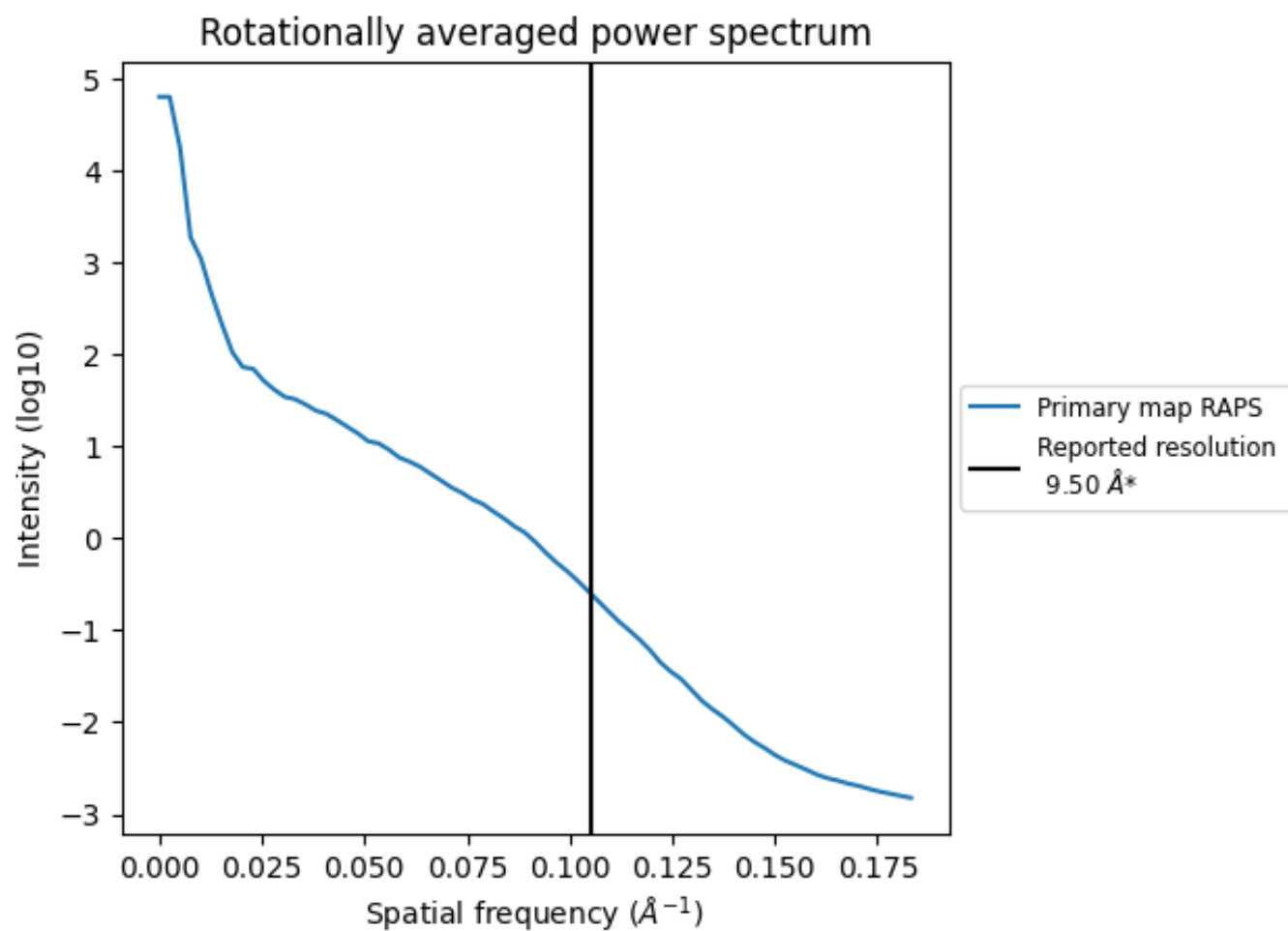
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2943 nm³; this corresponds to an approximate mass of 2659 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 0.105 Å⁻¹

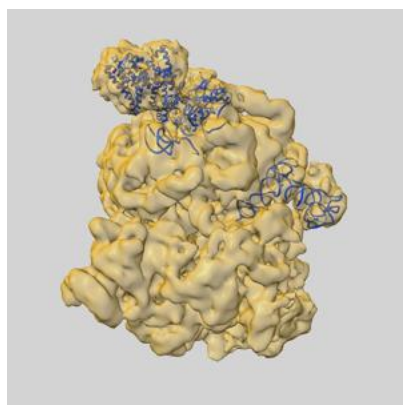
8 Fourier-Shell correlation

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

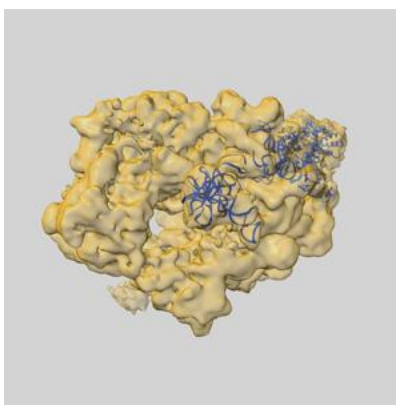
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5692 and PDB model 3J45. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

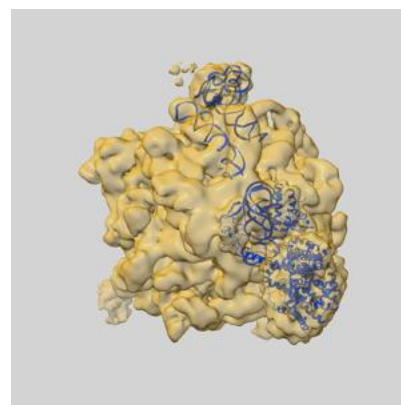
9.1 Map-model overlay [i](#)



X



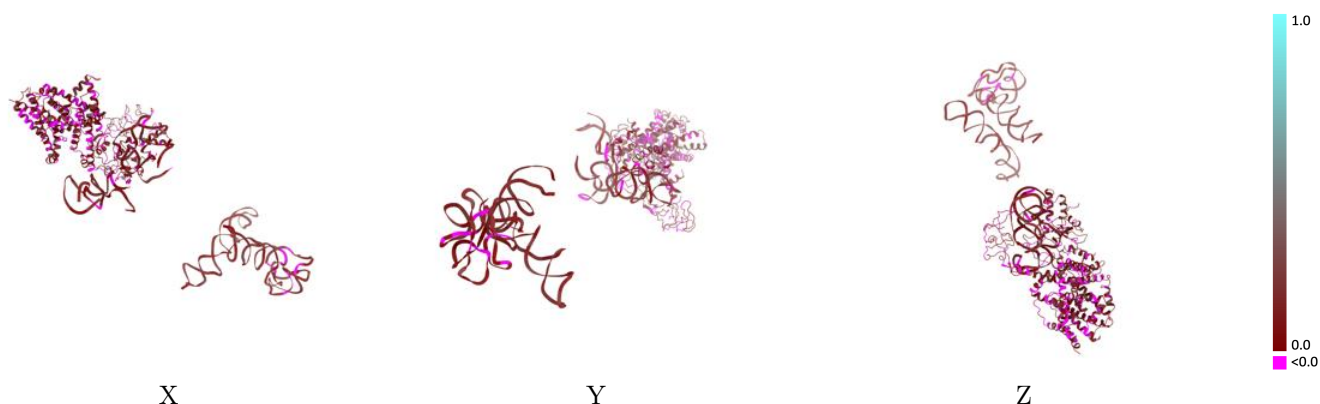
Y



Z

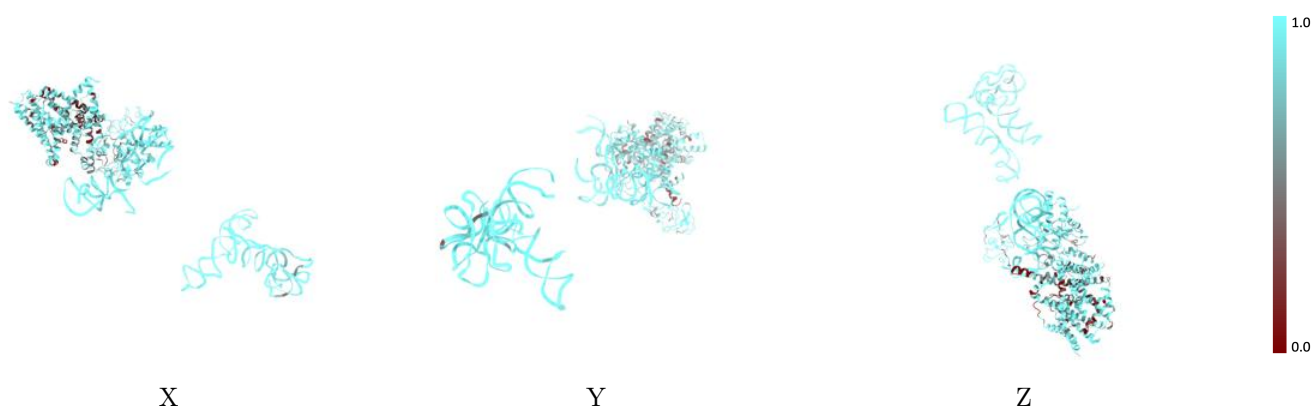
The images above show the 3D surface view of the map at the recommended contour level 1.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



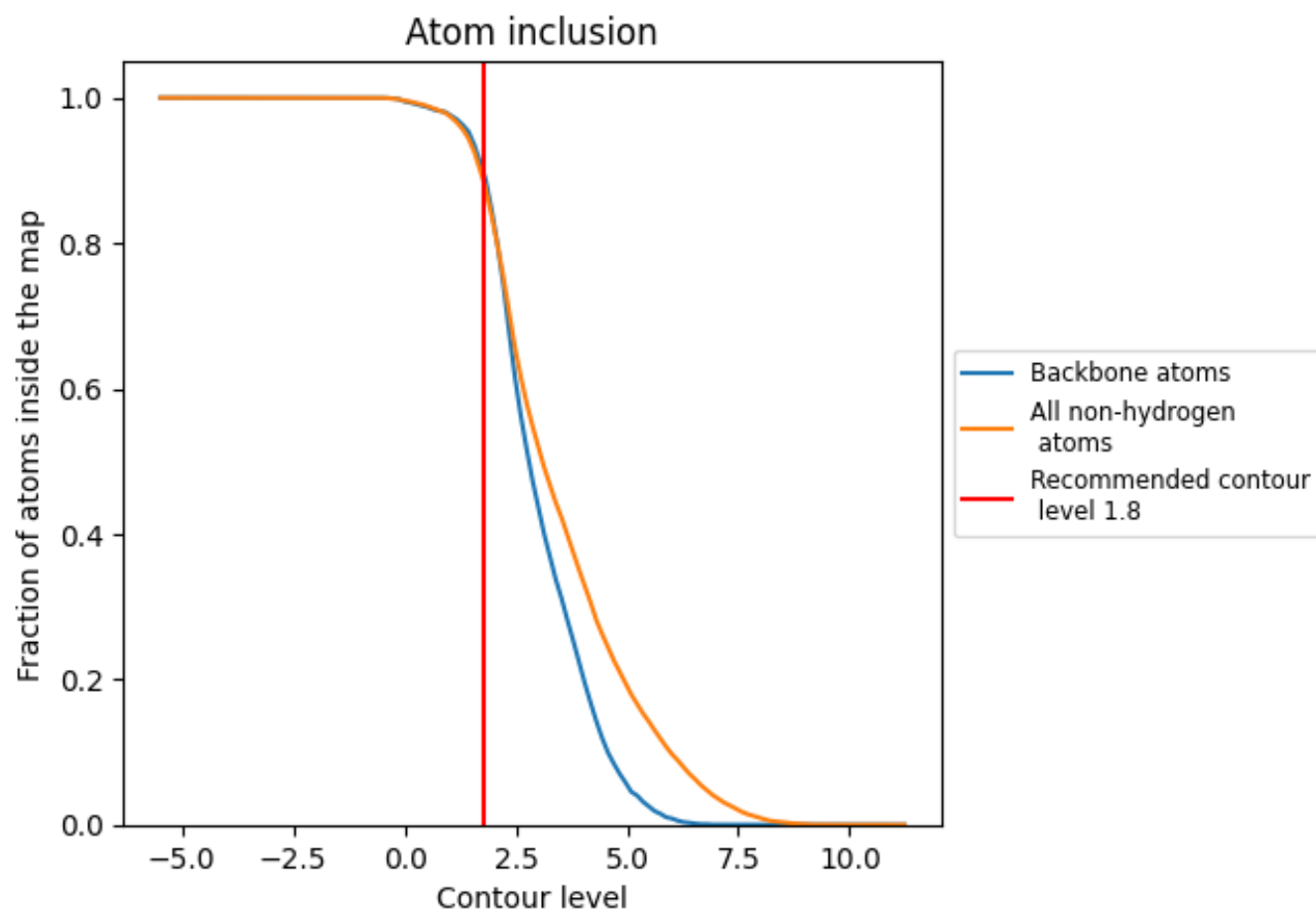
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8804	<div></div> 0.1030
1	<div></div> 0.9837	<div></div> 0.1370
2	<div></div> 0.9832	<div></div> 0.1250
3	<div></div> 0.9483	<div></div> 0.1510
4	<div></div> 0.9779	<div></div> 0.1660
5	<div></div> 0.9557	<div></div> 0.1170
E	<div></div> 0.7571	<div></div> 0.0690
G	<div></div> 0.7143	<div></div> 0.0290
T	<div></div> 0.8366	<div></div> 0.0830
U	<div></div> 0.8855	<div></div> 0.0870
Y	<div></div> 0.9276	<div></div> 0.1180
y	<div></div> 0.7553	<div></div> 0.0660

1.0

0.0

<0.0