



wwPDB EM Validation Summary Report ⓘ

Sep 2, 2026 – 07:30 PM EDT

PDB ID : 36QV / pdb_000036qv
EMDB ID : EMD-77787
Title : Arabidopsis thaliana V-type ATPase, State 2, Backbone model
Authors : Khamina, M.; Rubinstein, J.L.
Deposited on : 2026-06-26
Resolution : 3.00 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.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

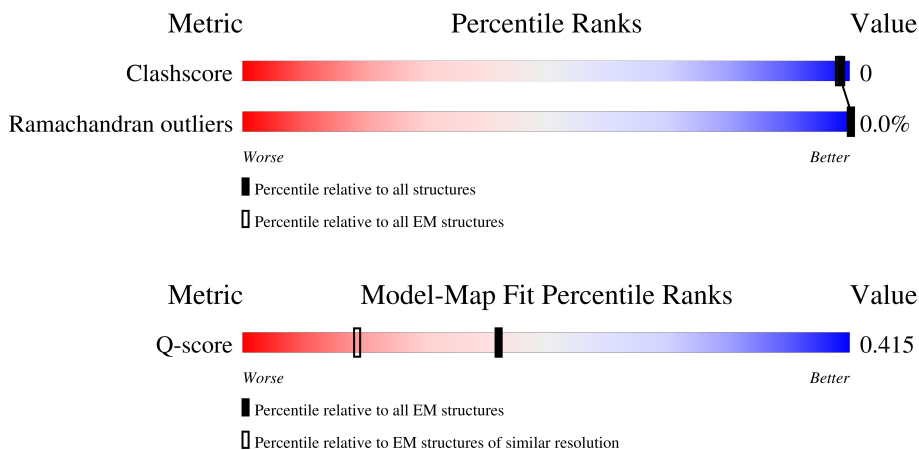
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



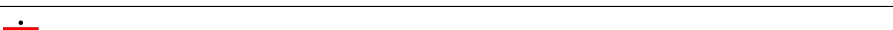
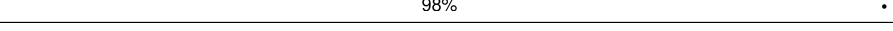
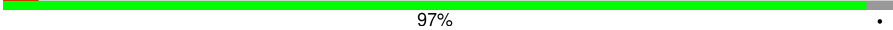
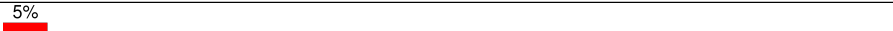
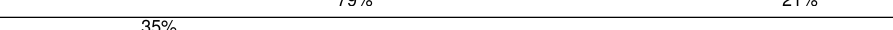
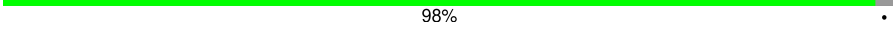
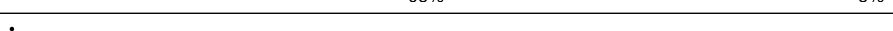
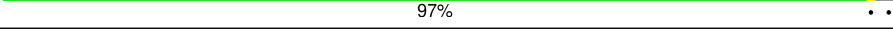
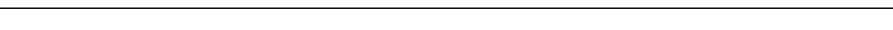
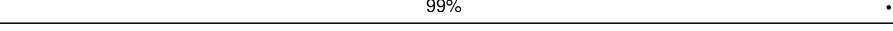
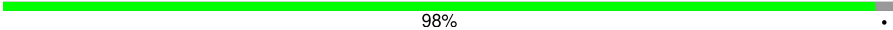
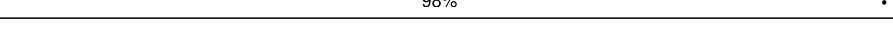
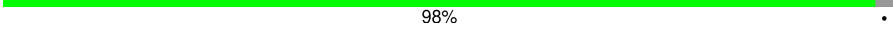
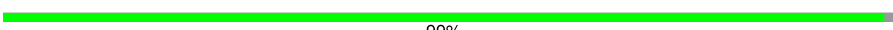
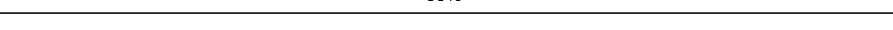
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	B	486	93% 6%
1	D	486	95% 5%
1	F	486	94% 6%
2	G	230	89% 11%
2	I	230	93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	230	
3	H	110	
3	J	110	
3	L	110	
4	M	261	
5	N	128	
6	P	441	
7	b	321	
8	c	180	
9	d	351	
10	e	70	
11	g	164	
11	h	164	
11	i	164	
11	j	164	
11	k	164	
11	l	164	
11	m	164	
11	n	164	
11	o	164	
12	r	364	
13	A	623	
13	C	623	
13	E	623	
14	O	375	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	a	821	 89% 11%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32258 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 V-type proton ATPase subunit B1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	456	Total	C	N	O	0	0
			1824	912	456	456		
1	D	462	Total	C	N	O	0	0
			1848	924	462	462		
1	B	458	Total	C	N	O	0	0
			1832	916	458	458		

- Molecule 2 is a protein called V-type proton ATPase subunit E1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	205	Total	C	N	O	0	0
			820	410	205	205		
2	I	214	Total	C	N	O	0	0
			856	428	214	214		
2	K	216	Total	C	N	O	0	0
			864	432	216	216		

- Molecule 3 is a protein called V-type proton ATPase subunit G1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	105	Total	C	N	O	0	0
			420	210	105	105		
3	J	110	Total	C	N	O	0	0
			441	220	110	111		
3	L	107	Total	C	N	O	0	0
			429	215	107	107		

- Molecule 4 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	191	Total	C	N	O	0	0
			764	382	191	191		

- Molecule 5 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	101	Total	C	N	O	0	0
			404	202	101	101		

- Molecule 6 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	433	Total	C	N	O	0	0
			1732	866	433	433		

- Molecule 7 is a protein called V-type proton ATPase subunit AP1 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	b	44	Total	C	N	O	0	0
			176	88	44	44		

- Molecule 8 is a protein called V-type proton ATPase subunit c"1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	c	171	Total	C	N	O	0	0
			685	342	171	172		

- Molecule 9 is a protein called V-type proton ATPase subunit d1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	d	342	Total	C	N	O	0	0
			1369	684	342	343		

- Molecule 10 is a protein called V-type proton ATPase subunit e2.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	66	Total	C	N	O	0	0
			264	132	66	66		

- Molecule 11 is a protein called V-type proton ATPase subunit c1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	g	162	Total	C	N	O	0	0
			648	324	162	162		
11	h	162	Total	C	N	O	0	0
			648	324	162	162		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
11	i	161	Total 644	C 322	N 161	O 161	0	0
11	j	161	Total 644	C 322	N 161	O 161	0	0
11	k	161	Total 644	C 322	N 161	O 161	0	0
11	l	161	Total 644	C 322	N 161	O 161	0	0
11	m	162	Total 648	C 324	N 162	O 162	0	0
11	n	162	Total 648	C 324	N 162	O 162	0	0
11	o	159	Total 636	C 318	N 159	O 159	0	0

- Molecule 12 is a protein called V-type proton ATPase subunit AP2 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	r	48	Total 192	C 96	N 48	O 48	0	0

- Molecule 13 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	C	607	Total 2428	C 1214	N 607	O 607	0	0
13	E	616	Total 2465	C 1232	N 616	O 617	0	0
13	A	577	Total 2308	C 1154	N 577	O 577	0	0

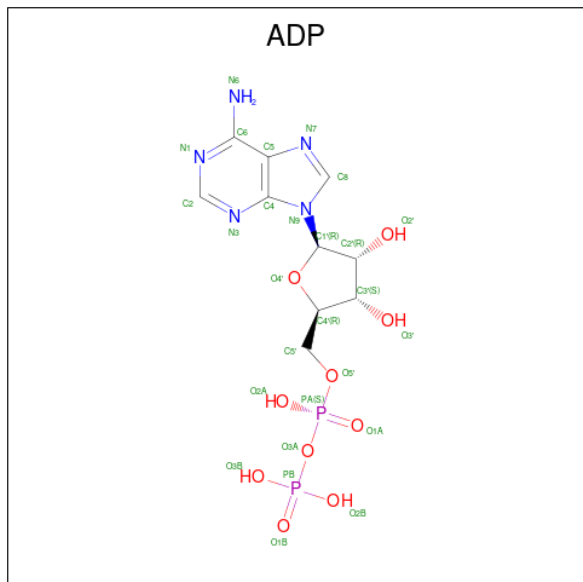
- Molecule 14 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	342	Total 1369	C 685	N 342	O 342	0	0

- Molecule 15 is a protein called V-type proton ATPase subunit a3.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	a	734	Total 2936	C 1468	N 734	O 734	0	0

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

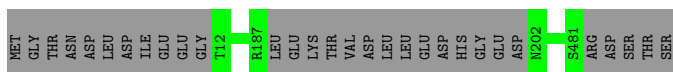
Mol	Chain	Residues	Atoms		AltConf
17	E	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

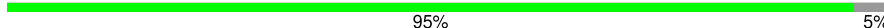
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

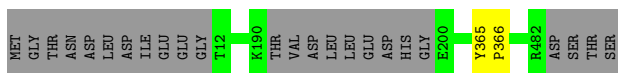
- Molecule 1: V-type proton ATPase subunit B1

Chain F: 

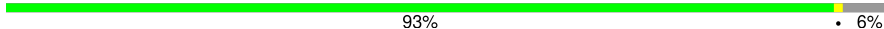


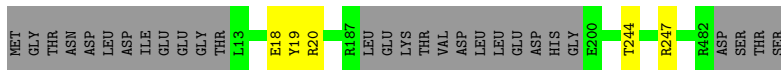
- Molecule 1: V-type proton ATPase subunit B1

Chain D: 



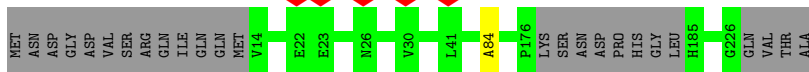
- Molecule 1: V-type proton ATPase subunit B1

Chain B: 

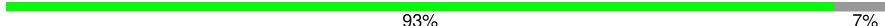


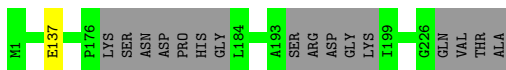
- Molecule 2: V-type proton ATPase subunit E1

Chain G: 



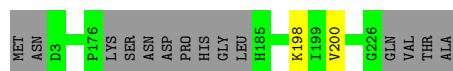
- Molecule 2: V-type proton ATPase subunit E1

Chain I: 

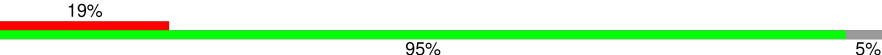


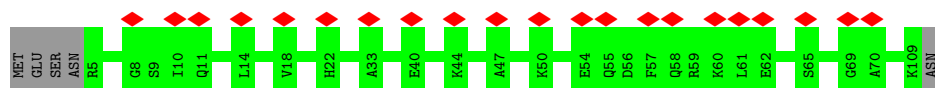
- Molecule 2: V-type proton ATPase subunit E1

Chain K:  93% • 6%

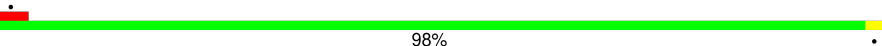


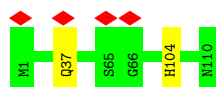
- Molecule 3: V-type proton ATPase subunit G1

Chain H:  19% 95% 5%

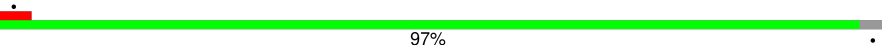


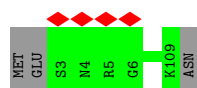
- Molecule 3: V-type proton ATPase subunit G1

Chain J:  98% •



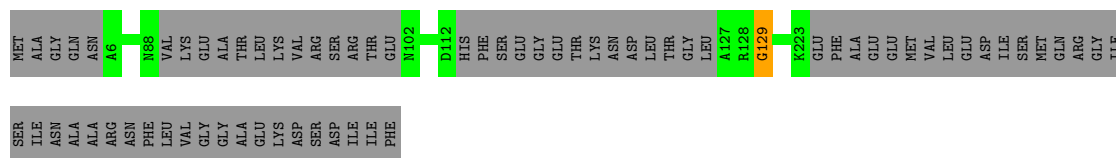
- Molecule 3: V-type proton ATPase subunit G1

Chain L:  97% •



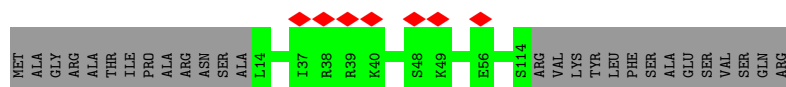
- Molecule 4: V-type proton ATPase subunit D

Chain M:  73% 27%

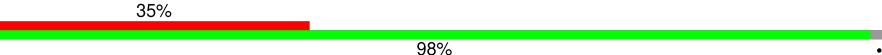


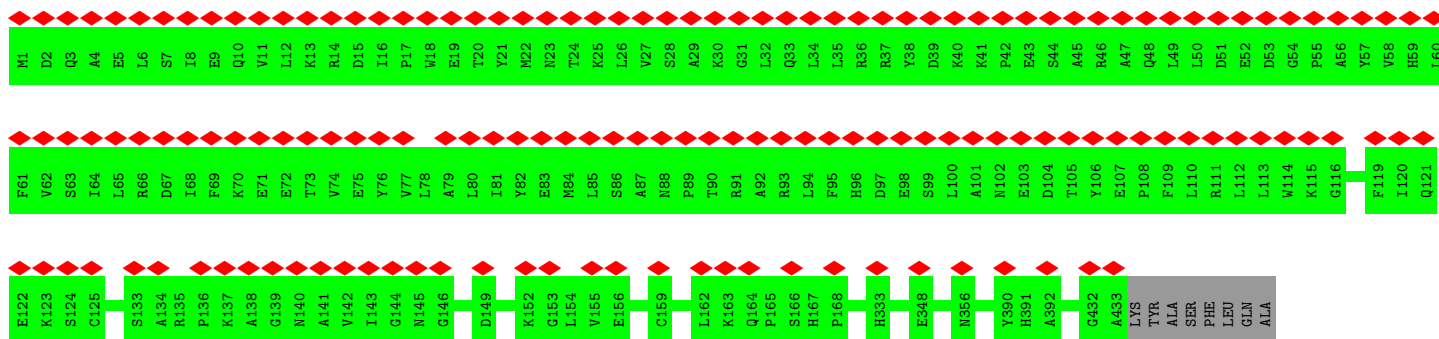
- Molecule 5: V-type proton ATPase subunit F

Chain N:  5% 79% 21%

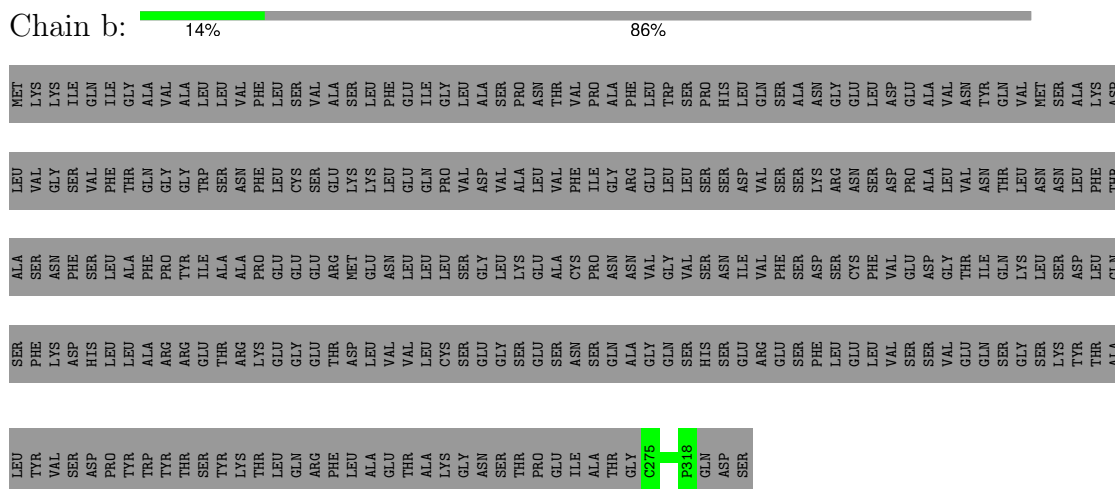


- Molecule 6: V-type proton ATPase subunit H

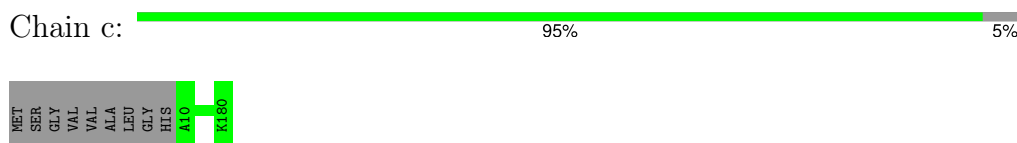
Chain P:  35% 98% •



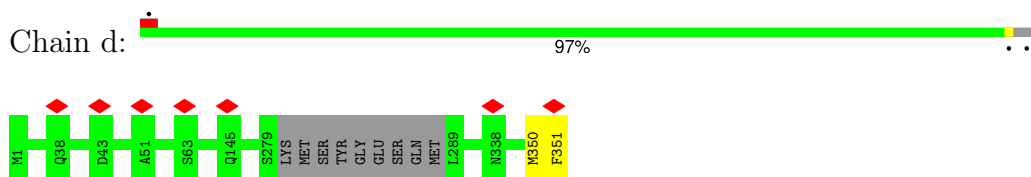
- Molecule 7: V-type proton ATPase subunit AP1 fragment



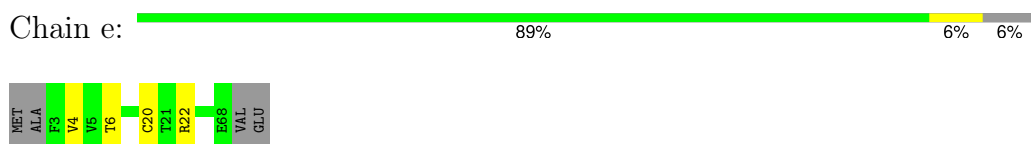
- Molecule 8: V-type proton ATPase subunit c'1



- Molecule 9: V-type proton ATPase subunit d1

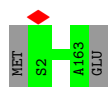


- Molecule 10: V-type proton ATPase subunit e2



- Molecule 11: V-type proton ATPase subunit c1

Chain g:  99%

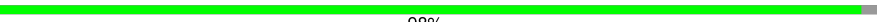


- Molecule 11: V-type proton ATPase subunit c1

Chain h:  99%

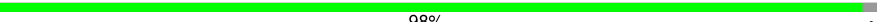


- Molecule 11: V-type proton ATPase subunit c1

Chain i:  98%

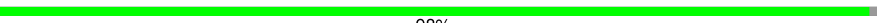


- Molecule 11: V-type proton ATPase subunit c1

Chain j:  98%

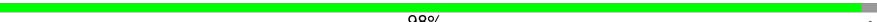


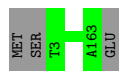
- Molecule 11: V-type proton ATPase subunit c1

Chain k:  98%

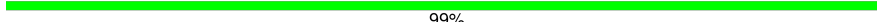


- Molecule 11: V-type proton ATPase subunit c1

Chain l:  98%



- Molecule 11: V-type proton ATPase subunit c1

Chain m:  99%

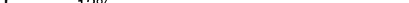


- Molecule 11: V-type proton ATPase subunit c1

MET S2 A163 GLU

- Chain 0: 97%

MET
SER
THR
PHE
S5
A163
GLU

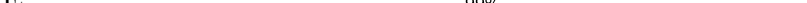
- Chain r:  13% 87%

[illegible]

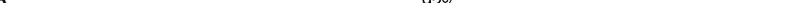
SER
ALA
ARG
SER
MET
VAL
GLU
VAL
GLU
GLY
ILE
PRO
S314
K354
S360
N361
VAL
LYS
LEU
ASP

- Chain C:  97%

MET
 PRO
 ALA
 PHE
 TYR
 GLY
 GLY
 K8
 G400
 G417
 G418
 R560
 ALA
 ALA
 GLY
 MET
 ASP
 GLY
 GLN
 K568
 E621
 THR
 ARG

- Chain E:  99%

MET
PRO
ALA
PHE
Y5
G563
MET
ASP
GLY
Q567
R623

- Chain A:  92% 7%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.772	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.194	Depositor
Map size ($\text{\AA}$)	476.16, 476.16, 476.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	B	0.23	0/1830	0.50	0/2284
1	D	0.24	0/1846	0.55	0/2304
1	F	0.15	0/1822	0.37	0/2274
2	G	0.60	0/818	1.10	1/1019 (0.1%)
2	I	0.63	0/853	1.18	2/1061 (0.2%)
2	K	0.38	0/862	0.72	0/1074
3	H	0.41	0/419	0.81	0/522
3	J	0.52	0/440	1.02	3/547 (0.5%)
3	L	0.50	0/428	0.89	0/534
4	M	0.58	0/761	1.11	2/946 (0.2%)
5	N	0.58	0/403	1.10	0/502
6	P	0.17	0/1731	0.37	0/2162
7	b	0.17	0/175	0.29	0/217
8	c	0.20	0/684	0.38	0/852
9	d	0.31	0/1367	0.67	0/1704
10	e	0.30	0/263	0.91	4/327 (1.2%)
11	g	0.19	0/647	0.32	0/807
11	h	0.18	0/647	0.33	0/807
11	i	0.18	0/643	0.33	0/802
11	j	0.18	0/643	0.35	0/802
11	k	0.18	0/643	0.38	0/802
11	l	0.20	0/643	0.35	0/802
11	m	0.20	0/647	0.34	0/807
11	n	0.19	0/647	0.35	0/807
11	o	0.20	0/635	0.34	0/792
12	r	0.15	0/191	0.27	0/237
13	A	0.19	0/2305	0.48	1/2876 (0.0%)
13	C	0.16	0/2426	0.41	0/3029
13	E	0.17	0/2463	0.39	0/3074
14	O	0.20	0/1366	0.47	0/1703
15	a	0.19	0/2933	0.43	0/3661
All	All	0.28	0/32181	0.57	13/40137 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	137	GLU	CA-C-N	6.74	131.39	120.60
2	I	137	GLU	C-N-CA	6.74	131.39	120.60
13	A	529	THR	N-CA-C	6.71	118.16	109.64
10	e	4	VAL	N-CA-C	-6.68	103.97	110.72
10	e	6	THR	N-CA-C	6.58	118.53	111.36

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	B	1832	0	504	5	0
1	D	1848	0	508	1	0
1	F	1824	0	502	0	0
2	G	820	0	208	0	0
2	I	856	0	219	0	0
2	K	864	0	221	4	0
3	H	420	0	112	0	0
3	J	441	0	120	0	0
3	L	429	0	115	0	0
4	M	764	0	205	0	0
5	N	404	0	101	0	0
6	P	1732	0	450	0	0
7	b	176	0	49	0	0
8	c	685	0	202	0	0
9	d	1369	0	364	1	0
10	e	264	0	66	0	0
11	g	648	0	204	0	0
11	h	648	0	204	0	0
11	i	644	0	203	0	0
11	j	644	0	203	0	0
11	k	644	0	203	0	0
11	l	644	0	203	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	m	648	0	204	0	0
11	n	648	0	204	0	0
11	o	636	0	201	0	0
12	r	192	0	50	0	0
13	A	2308	0	635	0	0
13	C	2428	0	668	0	0
13	E	2465	0	683	0	0
14	O	1369	0	348	0	0
15	a	2936	0	789	1	0
16	E	27	0	11	0	0
17	E	1	0	0	0	0
All	All	32258	0	8959	8	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 0.

The worst 5 of 8 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:K:200:VAL:N	1:B:18:GLU:O	2.05	0.88
2:K:198:LYS:O	1:B:19:TYR:CA	2.33	0.77
2:K:200:VAL:O	1:B:18:GLU:N	2.31	0.57
15:a:719:GLY:O	15:a:720:ALA:C	2.49	0.55
2:K:198:LYS:O	1:B:20:ARG:N	2.44	0.51

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	B	454/486 (93%)	436 (96%)	18 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	458/486 (94%)	444 (97%)	14 (3%)	0	100	100
1	F	452/486 (93%)	438 (97%)	14 (3%)	0	100	100
2	G	201/230 (87%)	196 (98%)	5 (2%)	0	100	100
2	I	208/230 (90%)	207 (100%)	1 (0%)	0	100	100
2	K	212/230 (92%)	208 (98%)	4 (2%)	0	100	100
3	H	103/110 (94%)	101 (98%)	2 (2%)	0	100	100
3	J	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
3	L	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
4	M	185/261 (71%)	181 (98%)	3 (2%)	1 (0%)	24	60
5	N	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
6	P	431/441 (98%)	423 (98%)	8 (2%)	0	100	100
7	b	42/321 (13%)	42 (100%)	0	0	100	100
8	c	169/180 (94%)	168 (99%)	1 (1%)	0	100	100
9	d	338/351 (96%)	327 (97%)	11 (3%)	0	100	100
10	e	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
11	g	160/164 (98%)	158 (99%)	2 (1%)	0	100	100
11	h	160/164 (98%)	158 (99%)	2 (1%)	0	100	100
11	i	159/164 (97%)	158 (99%)	1 (1%)	0	100	100
11	j	159/164 (97%)	158 (99%)	1 (1%)	0	100	100
11	k	159/164 (97%)	157 (99%)	2 (1%)	0	100	100
11	l	159/164 (97%)	155 (98%)	4 (2%)	0	100	100
11	m	160/164 (98%)	157 (98%)	3 (2%)	0	100	100
11	n	160/164 (98%)	157 (98%)	3 (2%)	0	100	100
11	o	157/164 (96%)	156 (99%)	1 (1%)	0	100	100
12	r	46/364 (13%)	45 (98%)	1 (2%)	0	100	100
13	A	571/623 (92%)	552 (97%)	19 (3%)	0	100	100
13	C	603/623 (97%)	587 (97%)	16 (3%)	0	100	100
13	E	612/623 (98%)	592 (97%)	20 (3%)	0	100	100
14	O	336/375 (90%)	317 (94%)	19 (6%)	0	100	100
15	a	728/821 (89%)	704 (97%)	24 (3%)	0	100	100
All	All	7958/9135 (87%)	7745 (97%)	212 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	129	GLY

5.3.2 Protein sidechains [i](#)

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

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	ADP	E	701	17	28,29,29	3.01	10 (35%)	43,45,45	2.31	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	ADP	E	701	17	-	3/16/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	701	ADP	O4'-C1'	8.64	1.62	1.42
16	E	701	ADP	C2'-C1'	-7.14	1.31	1.53
16	E	701	ADP	O4'-C4'	-6.19	1.31	1.45
16	E	701	ADP	PA-O3A	4.53	1.64	1.59
16	E	701	ADP	C6-N6	4.27	1.45	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	E	701	ADP	N6-C6-N1	-7.29	102.14	118.38
16	E	701	ADP	C5-C6-N6	5.79	137.62	123.29
16	E	701	ADP	C5-C4-N3	-5.49	119.16	126.72
16	E	701	ADP	N3-C2-N1	-5.30	120.56	128.58
16	E	701	ADP	N9-C8-N7	-3.72	108.66	113.94

There are no chirality outliers.

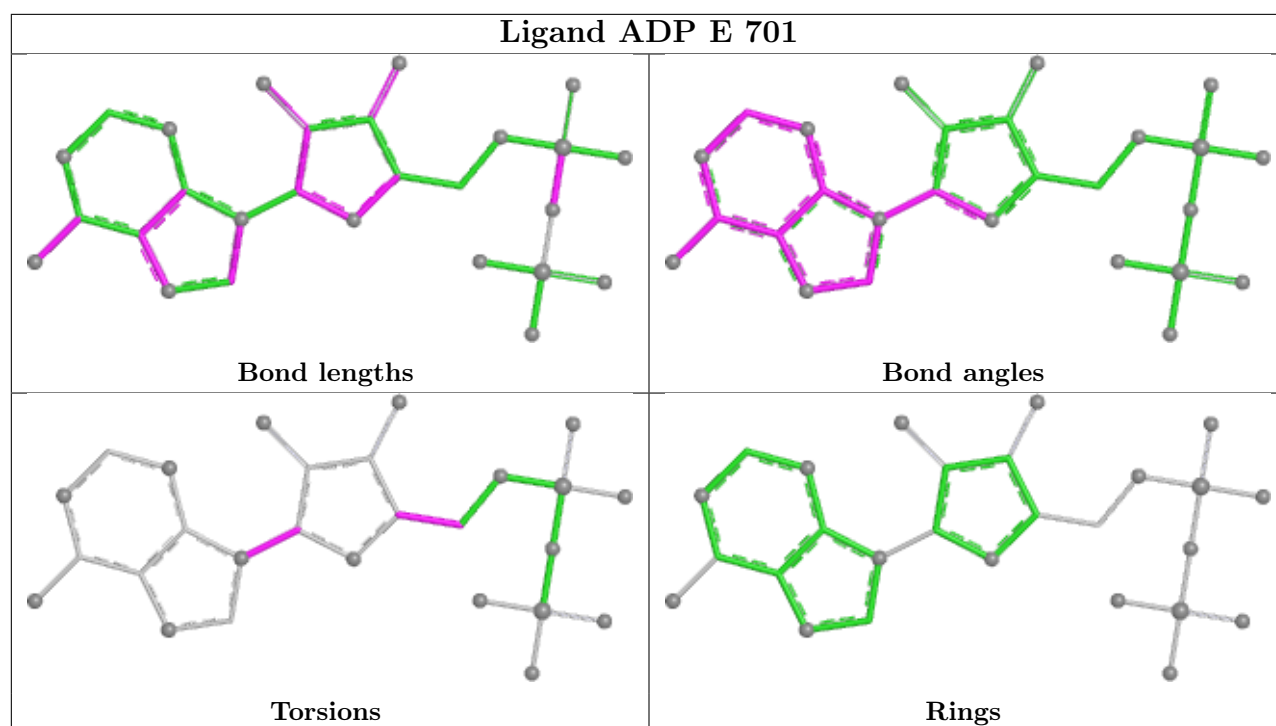
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	E	701	ADP	O4'-C1'-N9-C8
16	E	701	ADP	O4'-C1'-N9-C4
16	E	701	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

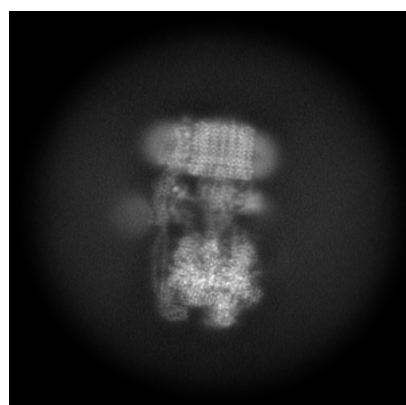
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77787. These allow visual inspection of the internal detail of the map and identification of artifacts.

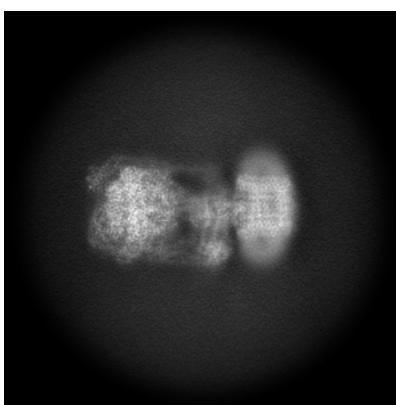
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

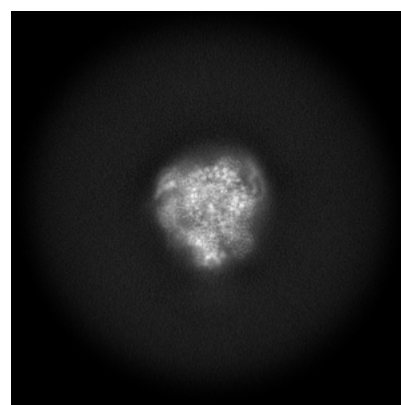
6.1.1 Primary map



X



Y

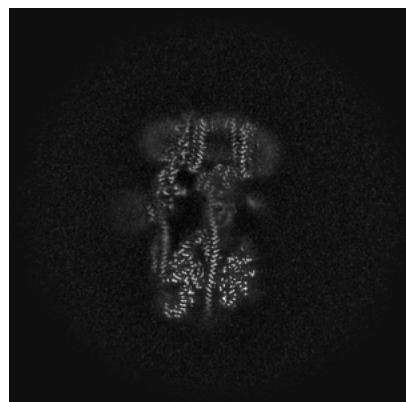


Z

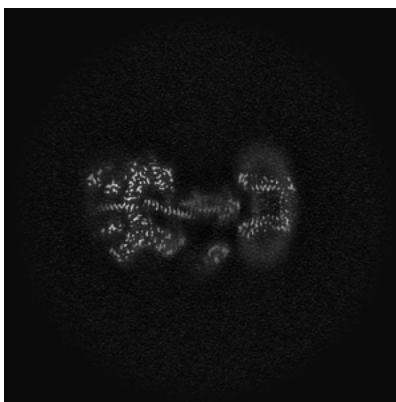
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

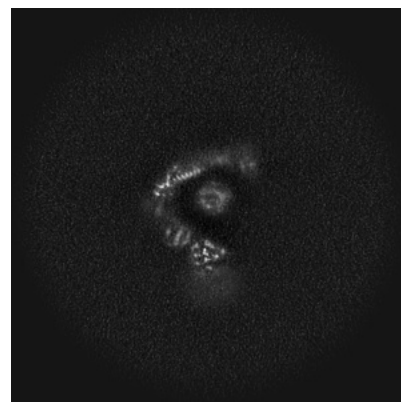
6.2.1 Primary map



X Index: 256



Y Index: 256

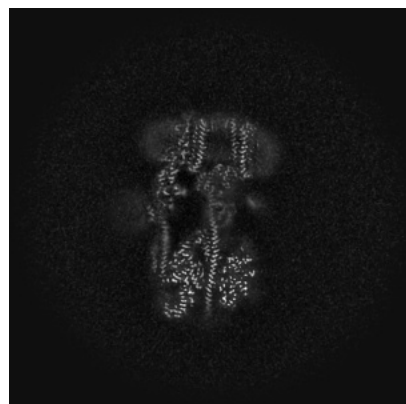


Z Index: 256

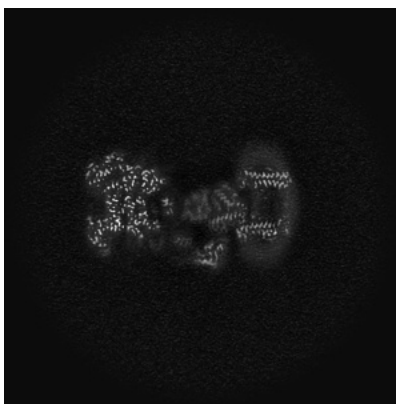
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

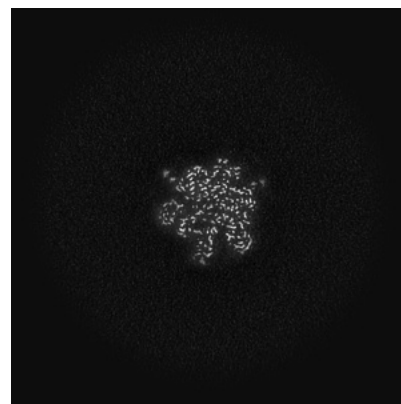
6.3.1 Primary map



X Index: 256



Y Index: 273

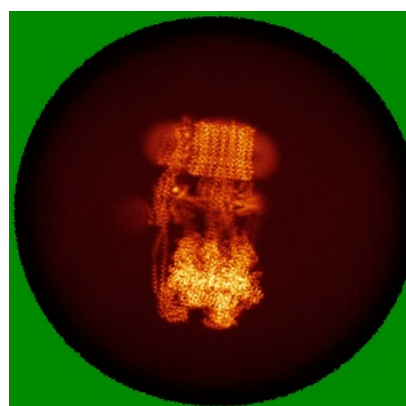


Z Index: 162

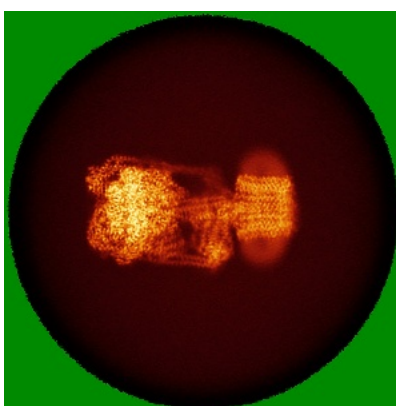
The images above show the largest variance slices of the map in three orthogonal directions.

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

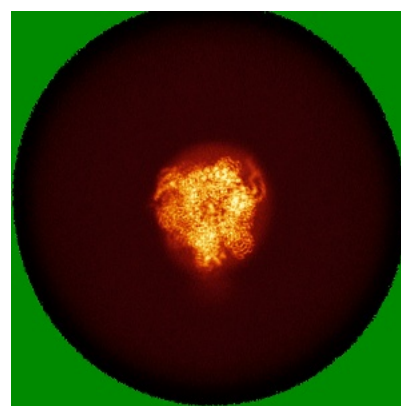
6.4.1 Primary map



X



Y

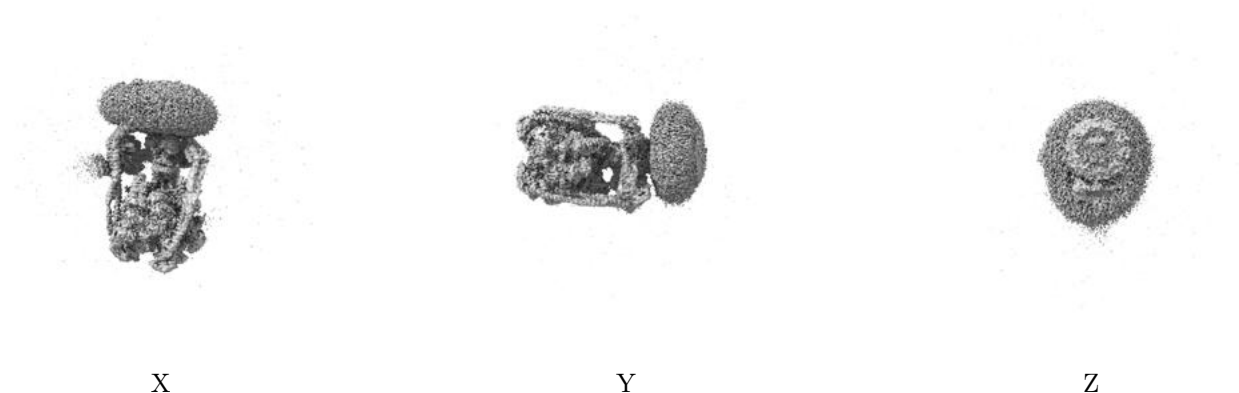


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

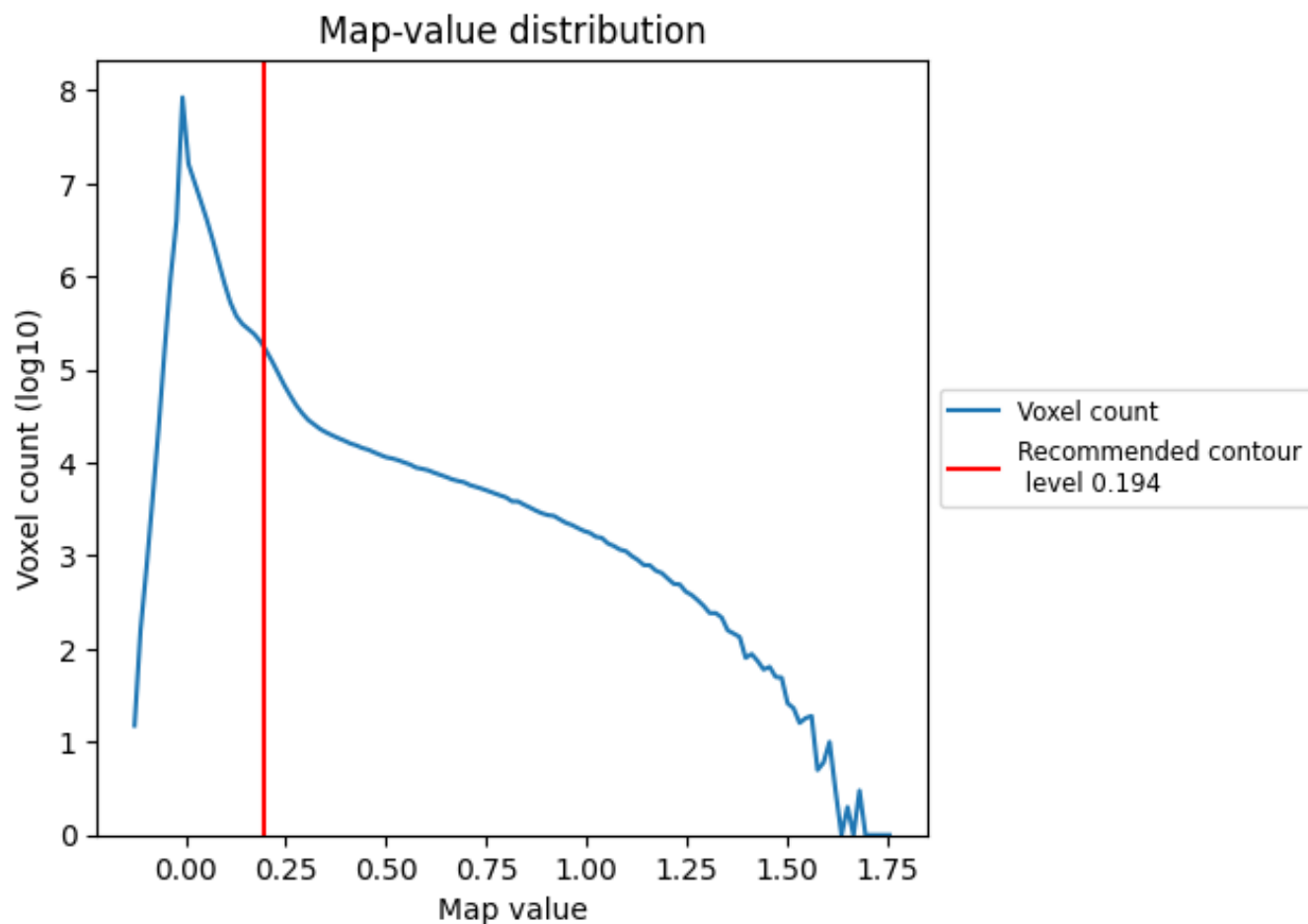
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

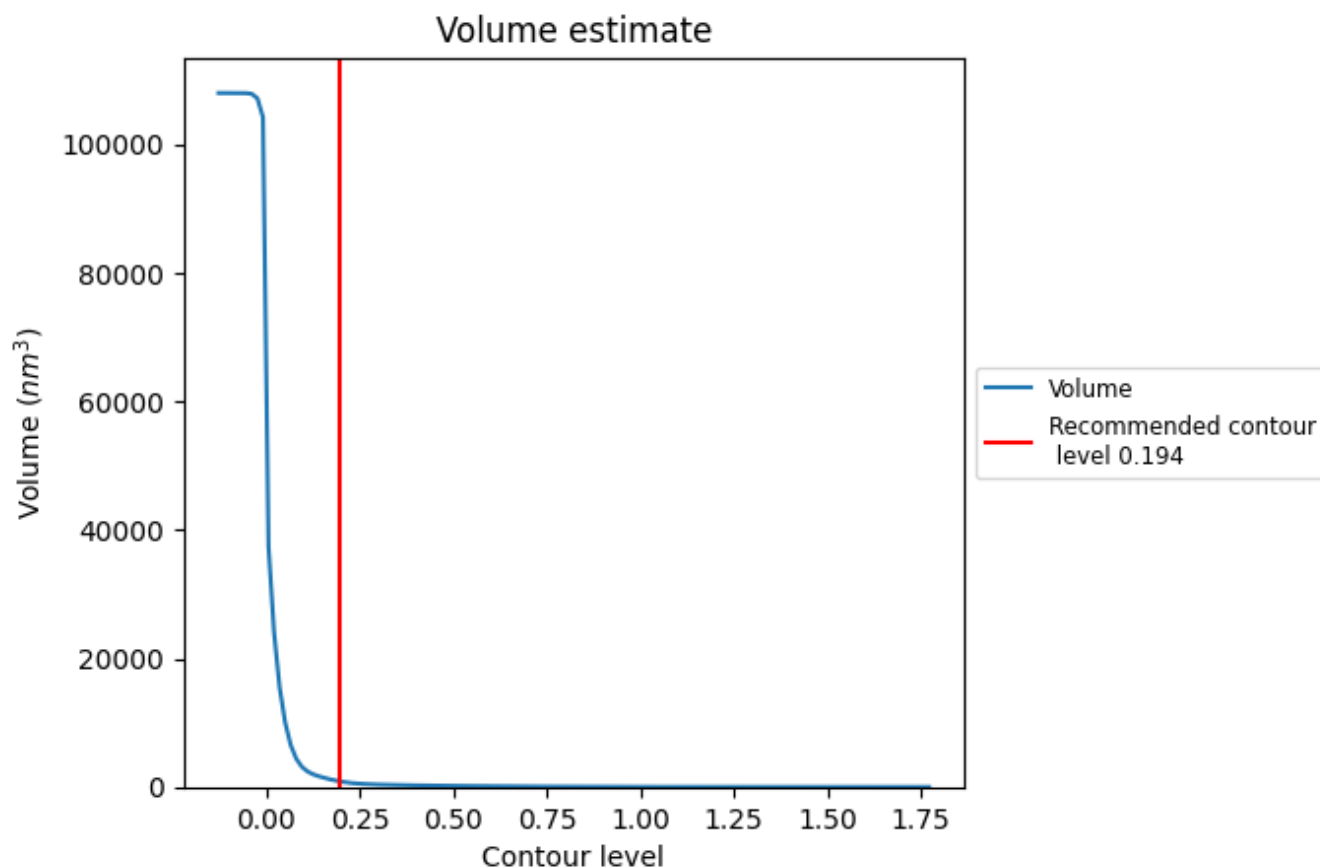
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

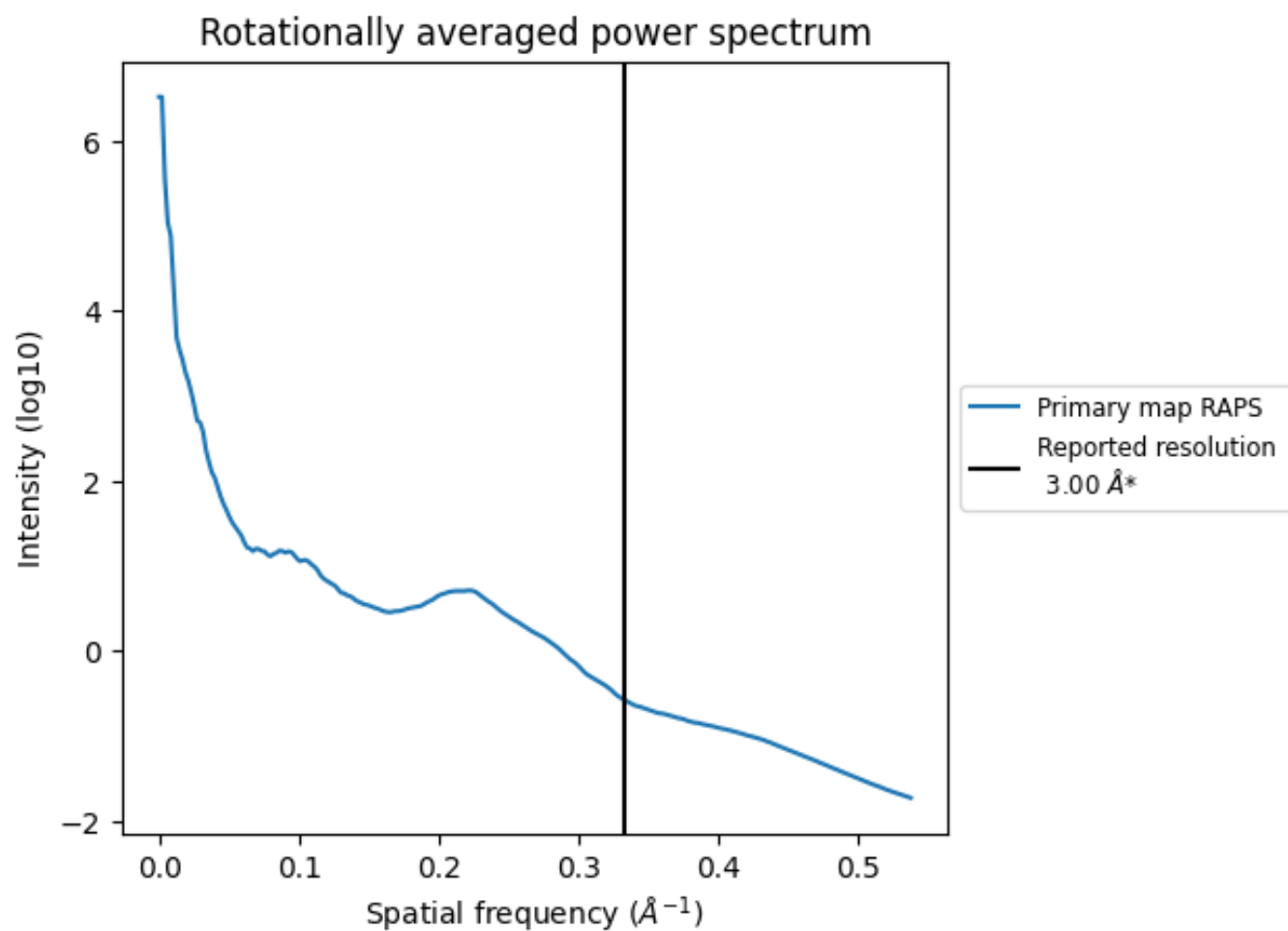
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 899 nm³; this corresponds to an approximate mass of 812 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 0.333 Å⁻¹

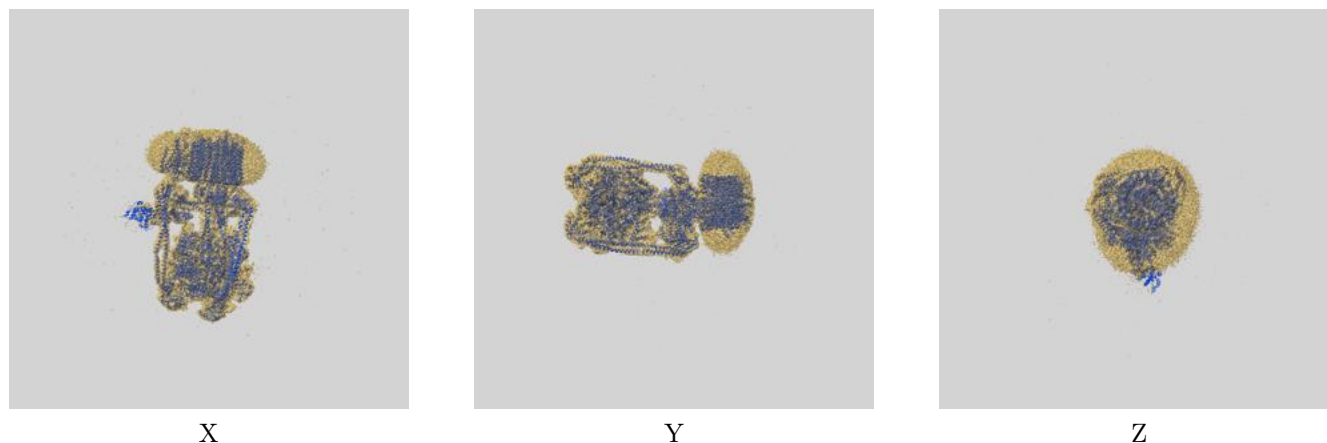
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

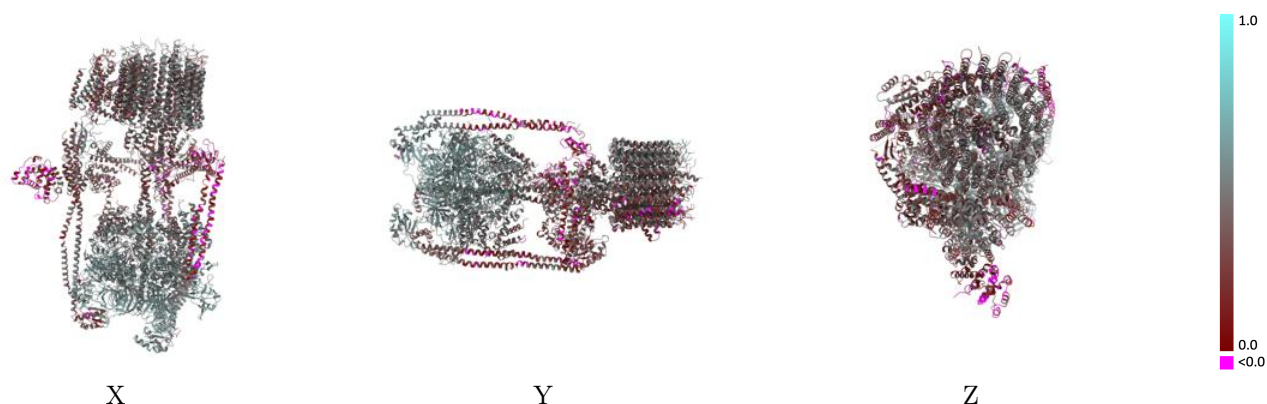
This section contains information regarding the fit between EMDB map EMD-77787 and PDB model 36QV. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



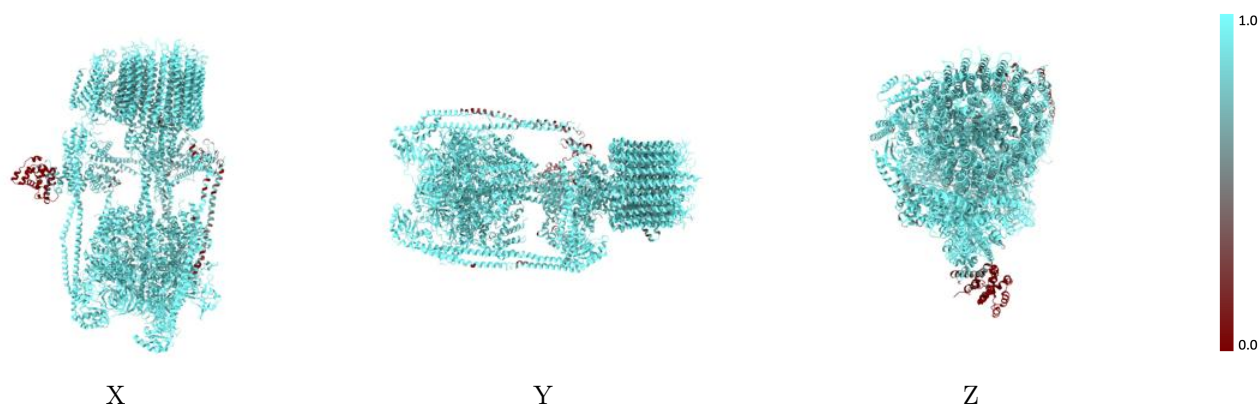
The images above show the 3D surface view of the map at the recommended contour level 0.194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



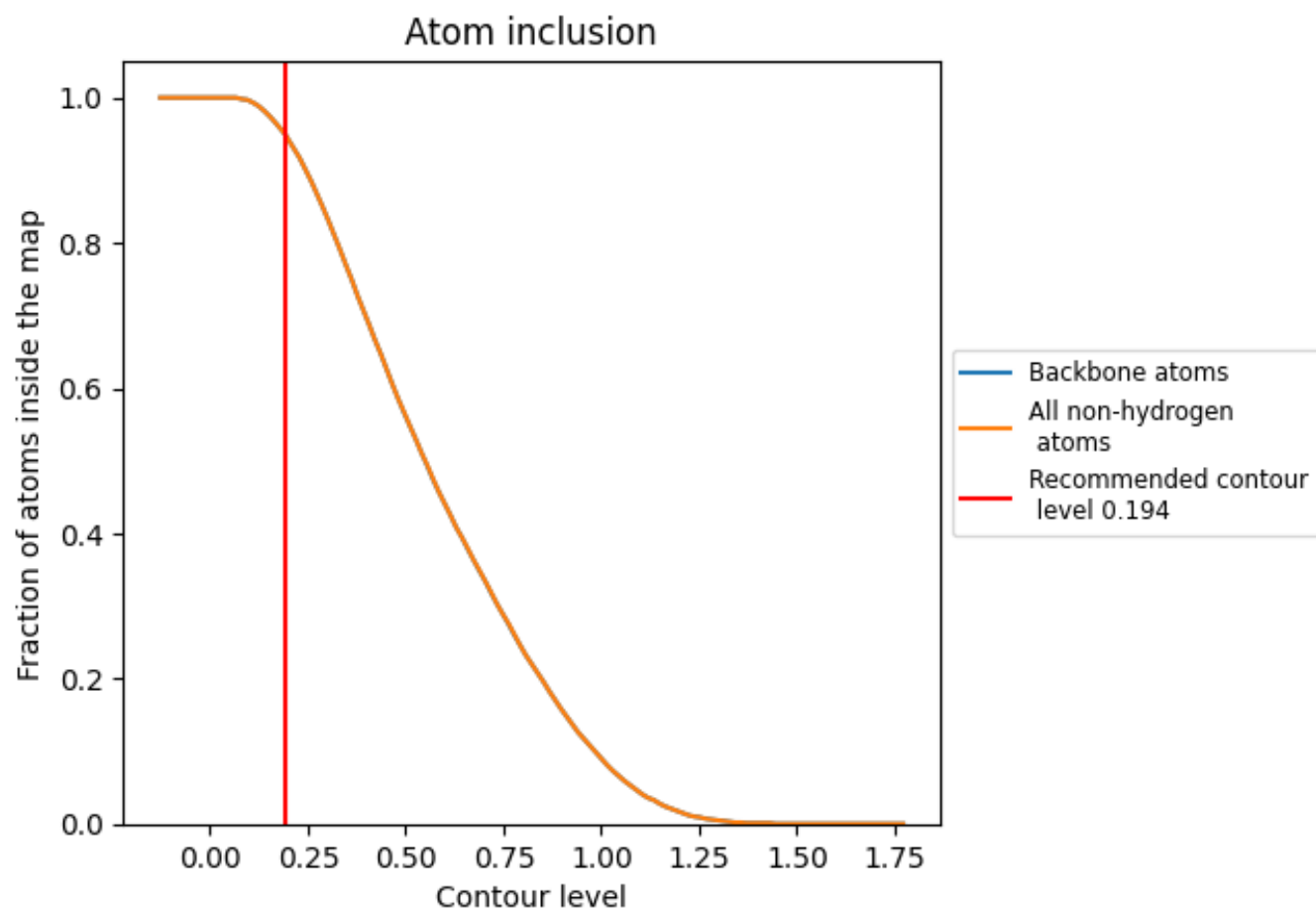
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.194).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.4150
A	 0.9910	 0.4520
B	 0.9980	 0.5450
C	 0.9900	 0.5080
D	 0.9950	 0.5440
E	 0.9970	 0.5410
F	 0.9940	 0.5160
G	 0.9520	 0.4130
H	 0.7710	 0.2600
I	 0.9950	 0.3830
J	 0.9360	 0.2950
K	 0.9760	 0.3630
L	 0.9580	 0.3540
M	 0.9870	 0.4330
N	 0.8640	 0.2120
O	 0.8690	 0.2340
P	 0.6130	 0.2180
a	 0.9760	 0.3490
b	 0.8690	 0.4010
c	 0.9460	 0.3140
d	 0.9280	 0.3650
e	 0.9770	 0.3930
g	 0.9520	 0.3180
h	 0.9780	 0.4180
i	 0.9780	 0.4550
j	 0.9580	 0.4390
k	 0.9580	 0.4320
l	 0.9550	 0.4150
m	 0.9650	 0.4090
n	 0.9440	 0.3790
o	 0.9530	 0.3360
r	 0.8910	 0.4590

