



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:09 PM UTC

PDB ID : 7UWD / pdb_00007uwd
EMDB ID : EMD-26829
Title : Citrus V-ATPase State 2, H in contact with subunits AB
Authors : Keon, K.A.; Abdelaziz, R.A.; Schulze, W.X.; Schumacher, K.; Rubinstein, J.L.
Deposited on : 2022-05-03
Resolution : 4.10 Å (reported)

This is a Full wwPDB EM Validation 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:

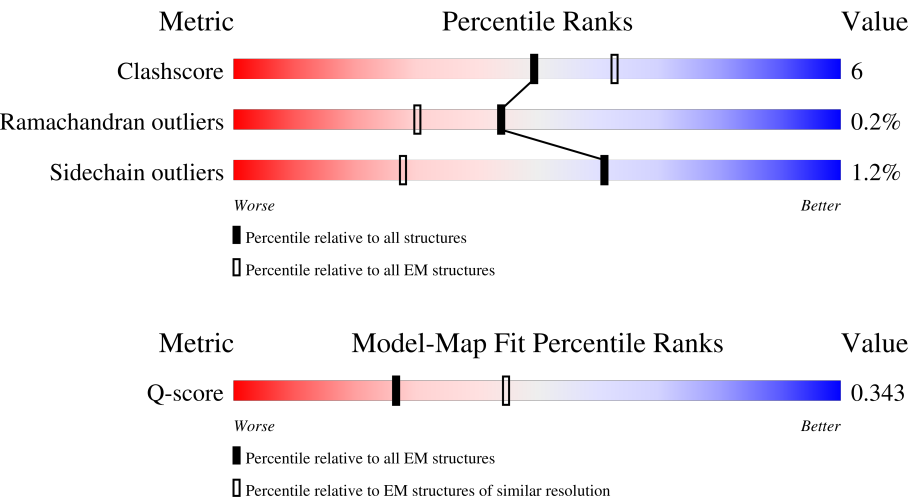
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.10 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	P	452	
2	A	623	
2	C	623	
2	E	623	

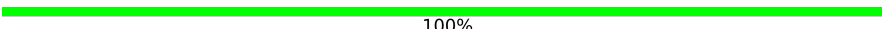
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Mol	Chain	Length	Quality of chain
3	B	488	
3	D	488	
3	F	488	
4	G	230	
4	I	230	
4	K	230	
5	H	110	
5	J	110	
5	L	110	
6	M	259	
7	N	130	
8	O	375	
9	a	823	
10	b	32	
11	c	182	
12	d	351	
13	e	70	
14	g	164	
14	h	164	
14	i	164	
14	j	164	
14	k	164	
14	l	164	
14	m	164	
14	n	164	

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Mol	Chain	Length	Quality of chain
14	o	164	 91% 7%
15	r	24	 100%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 46162 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 H.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	P	430	Total	C	N	O	0	0
			2137	1277	430	430		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	589	Total	C	N	O	S	0	0
			3935	2537	674	712	12		
2	C	603	Total	C	N	O	S	0	0
			4146	2671	714	746	15		
2	E	603	Total	C	N	O	S	0	0
			4252	2733	734	767	18		

- Molecule 3 is a protein called Vacuolar proton pump subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	460	Total	C	N	O	S	0	0
			3147	2040	544	555	8		
3	D	467	Total	C	N	O	S	0	0
			3213	2086	560	560	7		
3	F	463	Total	C	N	O	S	0	0
			3194	2069	547	569	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	204	Total	C	N	O	S	0	0
			1273	795	241	233	4		
4	I	207	Total	C	N	O	S	0	0
			1357	852	253	248	4		
4	K	217	Total	C	N	O	S	0	0
			1364	855	250	253	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	97	Total	C	N	O	S	0	0
			555	343	110	101	1		
5	J	96	Total	C	N	O	S	0	0
			517	316	100	100	1		
5	L	101	Total	C	N	O	S	0	0
			582	357	112	112	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	213	Total	C	N	O	0	0
			1096	660	216	220		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	107	Total	C	N	O	0	0
			545	331	107	107		

- Molecule 8 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	311	Total	C	N	O	0	0
			1571	947	312	312		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	a	713	Total	C	N	O	0	0
			3590	2161	715	714		

- Molecule 10 is a protein called V-type proton ATPase subunit AP1 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	b	32	Total	C	N	O	0	0
			160	96	32	32		

- Molecule 11 is a protein called Vacuolar membrane ATPase subunit c.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	c	168	Total	C	N	O	0	0
			833	497	168	168		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	d	268	Total	C	N	O	0	0
			1344	806	268	270		

- Molecule 13 is a protein called V-type proton ATPase subunit e1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	66	Total	C	N	O	0	0
			358	221	70	67		

- Molecule 14 is a protein called V-type proton ATPase subunit c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g	153	Total	C	N	O	S	0	0
			764	456	153	154	1		
14	h	155	Total	C	N	O		0	0
			763	452	155	156			
14	i	156	Total	C	N	O		0	0
			780	463	156	161			
14	j	155	Total	C	N	O		0	0
			777	465	155	157			
14	k	155	Total	C	N	O	S	0	0
			769	458	155	155	1		
14	l	153	Total	C	N	O		0	0
			752	446	153	153			
14	m	155	Total	C	N	O		0	0
			769	458	155	156			
14	n	155	Total	C	N	O		0	0
			762	452	155	155			
14	o	152	Total	C	N	O		0	0
			737	433	152	152			

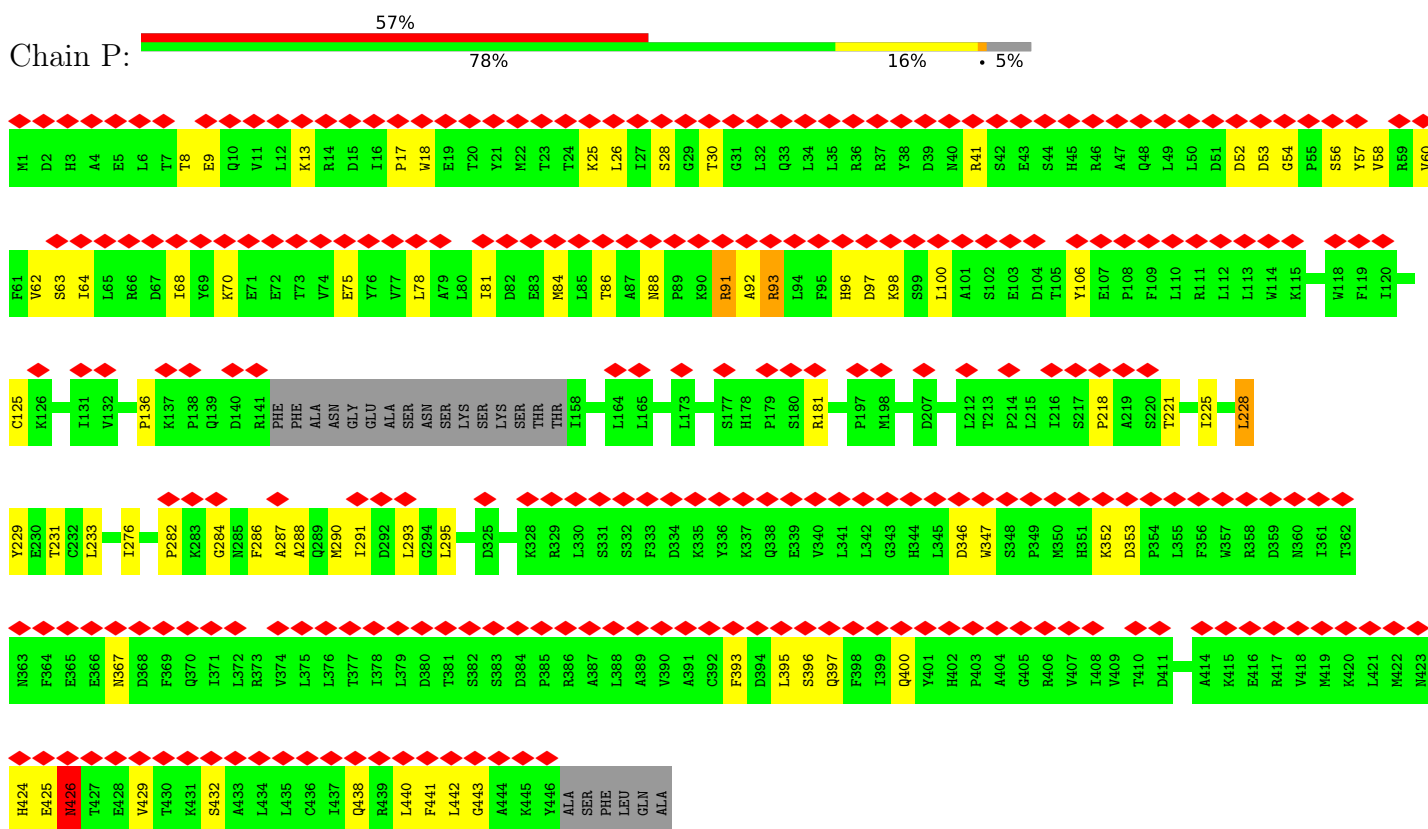
- Molecule 15 is a protein called V-type proton ATPase subunit AP2 fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	r	24	Total	C	N	O	0	0
			120	72	24	24		

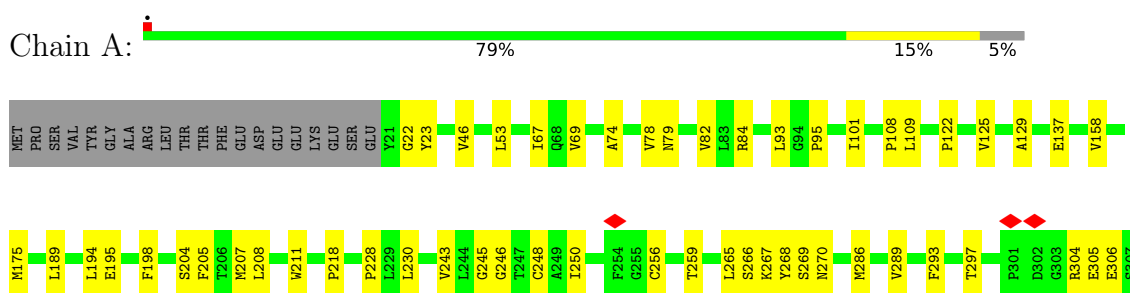
3 Residue-property plots

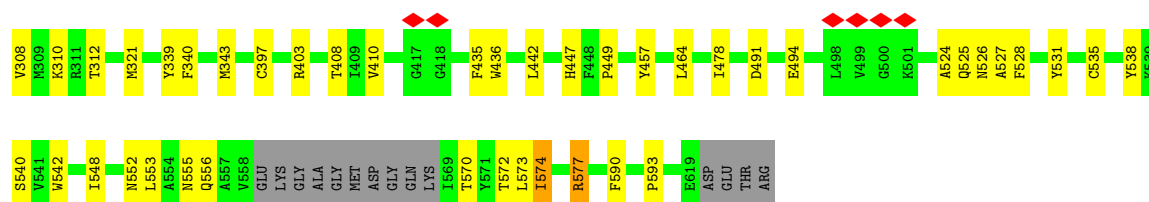
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

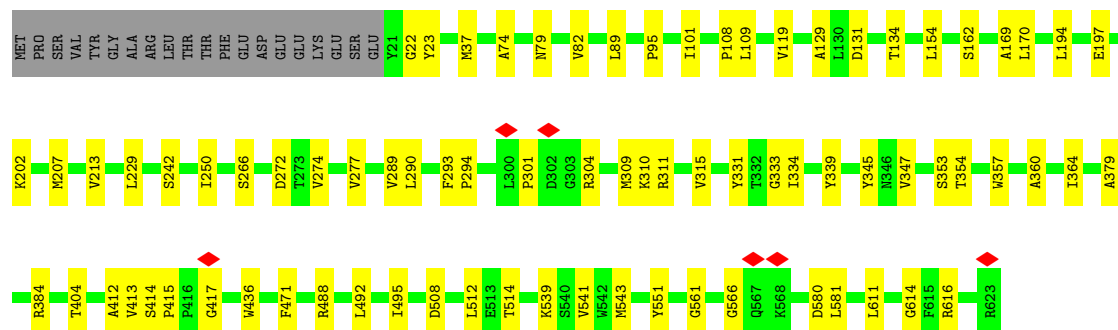
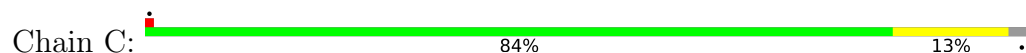


• Molecule 2: V-type proton ATPase catalytic subunit A

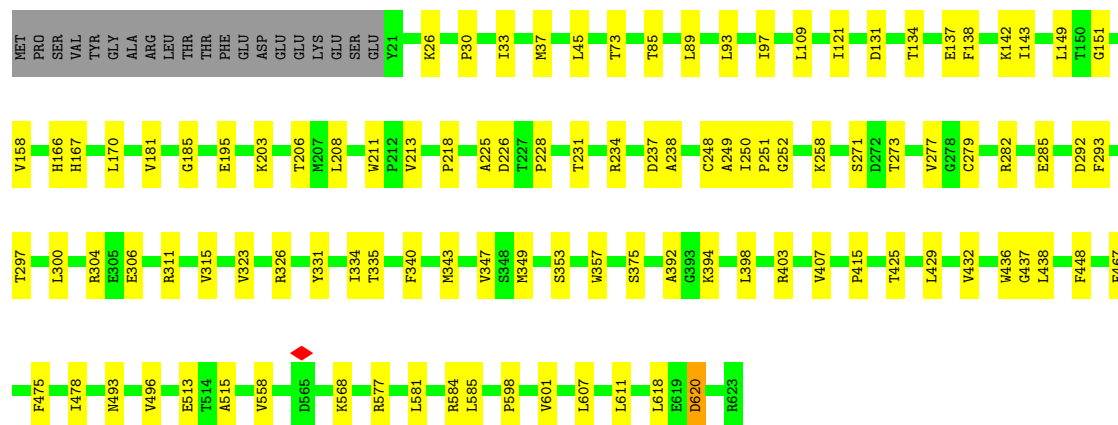
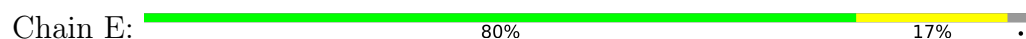




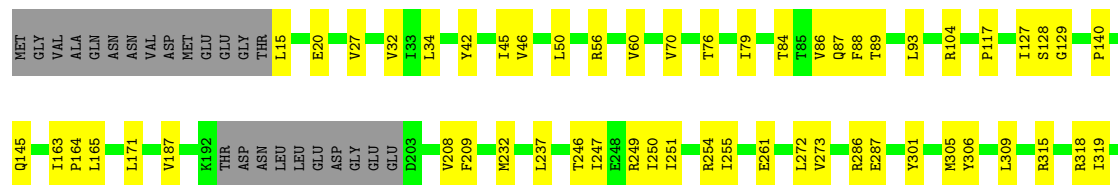
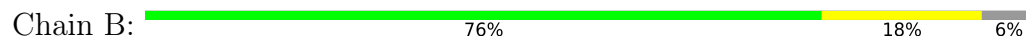
• Molecule 2: V-type proton ATPase catalytic subunit A

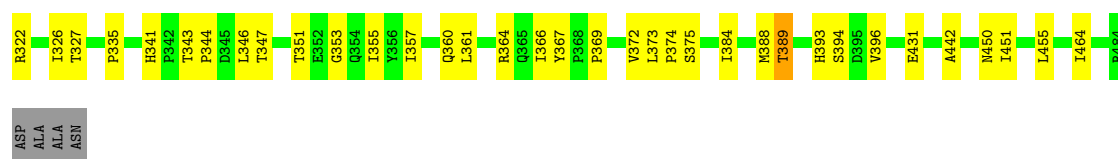


• Molecule 2: V-type proton ATPase catalytic subunit A



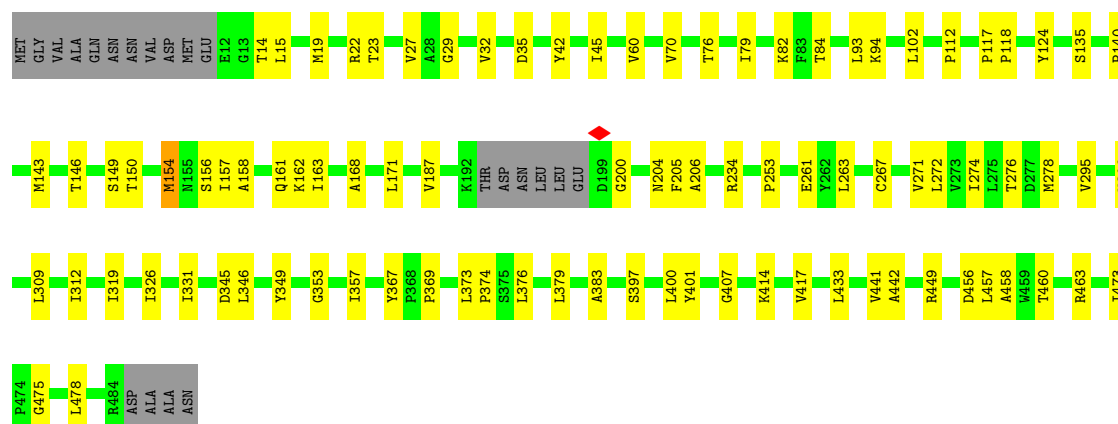
• Molecule 3: Vacuolar proton pump subunit B





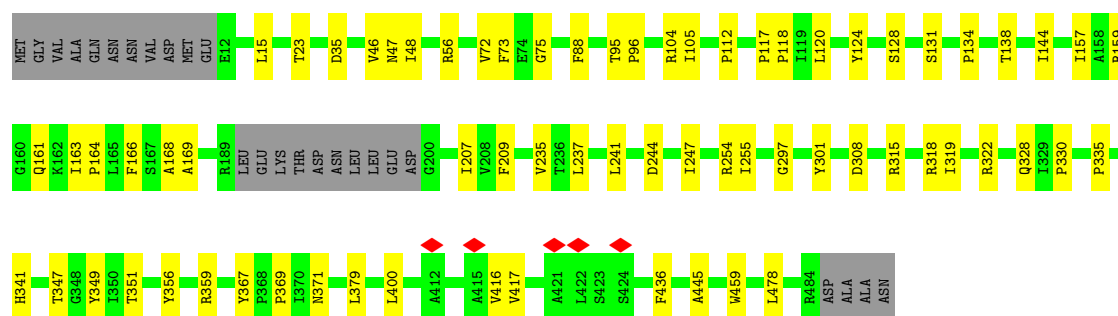
• Molecule 3: Vacuolar proton pump subunit B

Chain D: 77% 18% 5%



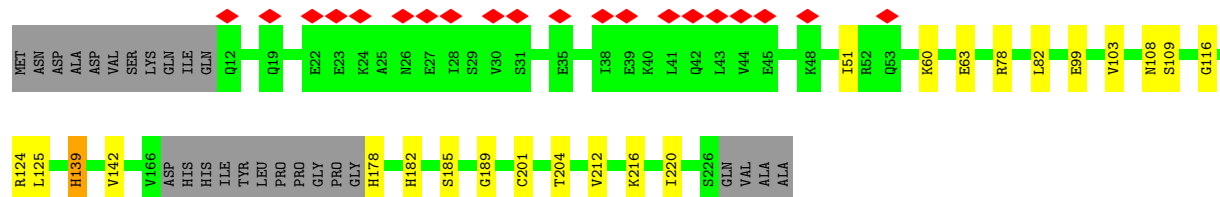
• Molecule 3: Vacuolar proton pump subunit B

Chain F: 81% 14% 5%



• Molecule 4: V-type proton ATPase subunit E

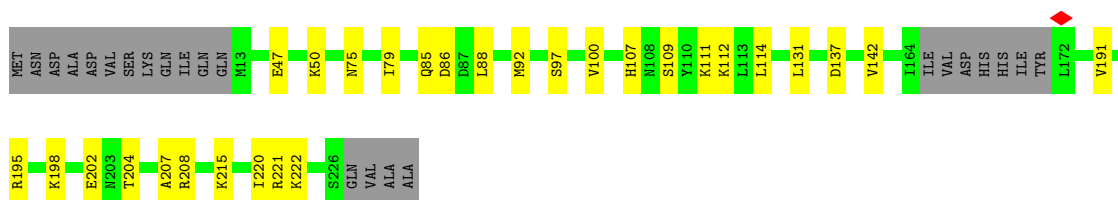
Chain G: 9% 79% 10% 11%



• Molecule 4: V-type proton ATPase subunit E

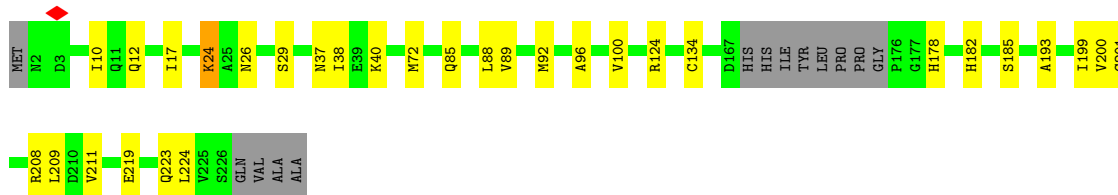
Chain I: 77% 13% 10%





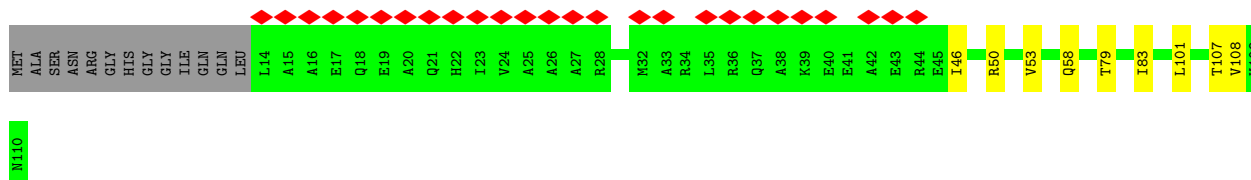
• Molecule 4: V-type proton ATPase subunit E

Chain K: 81% 13% 6%



• Molecule 5: V-type proton ATPase subunit G

Chain H: 24% 80% 8% 12%



• Molecule 5: V-type proton ATPase subunit G

Chain J: 72% 15% 13%



• Molecule 5: V-type proton ATPase subunit G

Chain L: 82% 10% 8%



• Molecule 6: V-type proton ATPase subunit D

Chain M: 78% 18% 4%



SER
ALA
GLY
GLY
LYS
ASP
GLU
ASP
ILE
PHE

- Molecule 7: V-type proton ATPase subunit F

Chain N:  74% 8% 18%

MET
ALA
GLY
ARG
ALA
GLN
ILE
PRO
THR
THR
LYS
SER
S12
M17
E21
A50
G31
V32
V35
I45
A58
F62
K101
L113
N118
LEU
PHE
SER
ALA
GLU
SER
VAL
ALA
SER
GLY
ARG
ARG

- Molecule 8: V-type proton ATPase subunit C

Chain O:  10% 80% 17%

MET
A2
A16
K29
T34
P35
L36
L44
N154
R155
K156
Q157
S158
G159
A162
V163
R164
D165
L166
S167
N168
K171
PRO
GLU
ASP
ILE
THR
SER
GLU
HIS
L181
P189
LYS
TYR
SER
GLN
LYS
ASP
TRP
LEU
ALA
SER
TYR
GLU
THR
LEU
T204
S211
S212
K213

L214
L215
Y216
E217
D218
ASN
TYR
ALA
L223
T227
I238
R241
E242
F245
Q246
I247
R248
D249
S254
E255
A256
Q257
E258
S259
S273
L274
S277
L278
L279
P322
G339
ASN
ALA
ASN
SER
THR
PHE
TRP
LYS
SER
GLU
ASP
ASP
GLY
GLY
MET
MET
ALA
GLY
LEU

GLY
GLY
ASP
ALA
ASP
SER
HIS
PRO
TYR
VAL
SER
PHE
THR
ILE
ASN
VAL

- Molecule 9: V-type proton ATPase subunit a

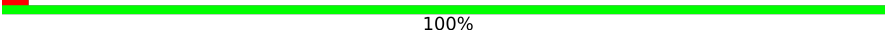
Chain a:  84% 13%

MET
ALA
GLU
LEU
GLN
SER
GLY
GLY
GLY
GLY
GLY
CYS
PRO
PRO
MET
ASP
LEU
PHE
ARG
SER
GLU
P23
M24
Q50
S69
T64
Y65
A66
K70
S93
SER
VAL
LYS
SER
THR
THR
ARG
ALA
ASP
ASN
ASN
THR
ASP
D107
Q161
ARG
GLU
MET
GLU
SER
GLN
GLN
THR

GLY
GLU
MET
THR
ILE
GLU
THR
PRO
LEU
LEU
THR
ASP
LYS
GLU
MET
MET
ALA
ASP
PRO
PHE
SER
LYS
GLN
ILE
K193
L200
Y201
P202
D229
V245
F246
A268
E348
P352
Y505
A506
C507
C512
I521
K522
V523
H669
GLN
ASP
ARG
GLU
HIS
GLN
GLY
GLN
SER
TYR

GLU
ALA
LEU
GLN
SER
THR
ASP
GLU
SER
LEU
GLN
PRO
ASP
THR
ASN
HIS
SER
HIS
GLY
HIS
GLU
GLU
PHE
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Y803
E804
P812
F815
D819
ASP
GLU
ASP
GLU

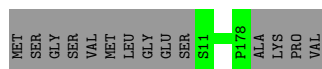
- Molecule 10: V-type proton ATPase subunit AP1 fragment

Chain b:  100%

X273
X288
X304

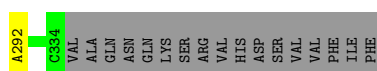
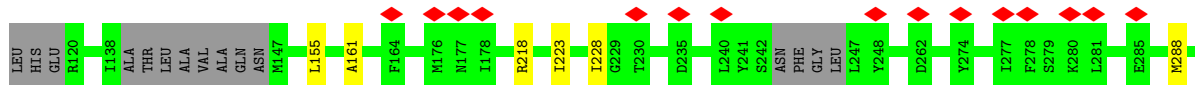
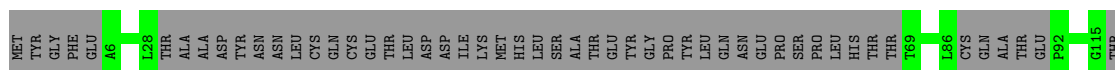
- Molecule 11: Vacuolar membrane ATPase subunit c

Chain c:  92% 8%



- Molecule 12: V-type proton ATPase subunit

Chain d: 74% 24%



- Molecule 13: V-type proton ATPase subunit e1

Chain e: 94% 6%



- Molecule 14: V-type proton ATPase subunit c1

Chain g: 91% 7%



- Molecule 14: V-type proton ATPase subunit c1

Chain h: 88% 6% 5%



- Molecule 14: V-type proton ATPase subunit c1

Chain i: 89% 6% 5%



- Molecule 14: V-type proton ATPase subunit c1

Chain j: 92% 5% 5%



- Molecule 14: V-type proton ATPase subunit c1

Chain k: 88% 6% 5%



- Molecule 14: V-type proton ATPase subunit c1

Chain l: 90% 7%



- Molecule 14: V-type proton ATPase subunit c1

Chain m: 89% 5% 5%



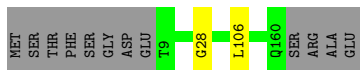
- Molecule 14: V-type proton ATPase subunit c1

Chain n: 90% 5% 5%



- Molecule 14: V-type proton ATPase subunit c1

Chain o: 91% 7%



- Molecule 15: V-type proton ATPase subunit AP2 fragment

Chain r: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51571	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 ($e^-/\text{\AA}^2$)	31	Depositor
Minimum defocus (nm)	677.558	Depositor
Maximum defocus (nm)	3414.211	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.698	Depositor
Minimum map value	-0.381	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	485.1, 485.1, 485.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.617, 1.617, 1.617	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	P	1.62	31/2135 (1.5%)	1.92	73/2978 (2.5%)
2	A	0.31	0/4023	0.50	0/5546
2	C	0.31	0/4244	0.60	1/5833 (0.0%)
2	E	0.21	0/4350	0.44	1/5958 (0.0%)
3	B	0.21	0/3207	0.43	0/4403
3	D	0.27	0/3277	0.50	0/4494
3	F	0.17	0/3257	0.38	0/4468
4	G	0.28	0/1283	0.47	0/1764
4	I	0.14	0/1374	0.38	0/1884
4	K	0.45	0/1377	0.74	0/1895
5	H	0.11	0/558	0.29	0/772
5	J	0.13	0/517	0.39	0/716
5	L	0.71	0/586	1.05	1/812 (0.1%)
6	M	0.12	0/1099	0.32	0/1530
7	N	0.14	0/549	0.43	0/769
8	O	0.24	0/1578	0.35	0/2203
9	a	0.11	0/3613	0.27	0/5044
11	c	0.10	0/837	0.21	0/1164
12	d	0.10	0/1345	0.29	0/1870
13	e	0.12	0/363	0.29	0/506
14	g	0.11	0/769	0.22	0/1064
14	h	0.12	0/767	0.33	0/1062
14	i	0.11	0/785	0.25	0/1086
14	j	0.11	0/783	0.22	0/1084
14	k	0.11	0/774	0.23	0/1071
14	l	0.11	0/756	0.21	0/1047
14	m	0.12	0/774	0.24	0/1071
14	n	0.10	0/766	0.22	0/1061
14	o	0.09	0/736	0.29	0/1015
All	All	0.42	31/46482 (0.1%)	0.60	76/64170 (0.1%)

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
2	E	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	64	ILE	CA-C	-7.66	1.43	1.52
1	P	91	ARG	CA-C	-7.21	1.43	1.52
1	P	9	GLU	CA-C	-7.11	1.43	1.52
1	P	286	PHE	N-CA	-7.06	1.37	1.46
1	P	78	LEU	CA-C	-6.72	1.44	1.52
1	P	28	SER	CA-C	-6.69	1.44	1.52
1	P	426	ASN	N-CA	-6.67	1.37	1.46
1	P	346	ASP	CA-C	-6.57	1.44	1.52
1	P	396	SER	CA-C	-6.35	1.44	1.52
1	P	352	LYS	CA-C	-6.24	1.44	1.52
1	P	291	ILE	N-CA	6.15	1.53	1.46
1	P	347	TRP	CA-C	-6.12	1.44	1.52
1	P	8	THR	C-N	5.91	1.42	1.33
1	P	70	LYS	CA-C	5.68	1.60	1.52
1	P	25	LYS	CA-C	-5.66	1.45	1.52
1	P	75	GLU	N-CA	5.60	1.53	1.46
1	P	57	TYR	N-CA	-5.56	1.38	1.46
1	P	30	THR	N-CA	-5.53	1.39	1.46
1	P	18	TRP	N-CA	5.52	1.52	1.46
1	P	432	SER	C-N	5.43	1.41	1.33
1	P	56	SER	C-N	5.42	1.42	1.33
1	P	287	ALA	C-N	5.41	1.40	1.33
1	P	443	GLY	C-N	5.39	1.41	1.33
1	P	60	VAL	N-CA	-5.38	1.40	1.46
1	P	290	MET	N-CA	-5.31	1.40	1.46
1	P	284	GLY	CA-C	-5.25	1.46	1.52
1	P	429	VAL	N-CA	-5.24	1.40	1.46
1	P	231	THR	N-CA	-5.14	1.40	1.46
1	P	424	HIS	C-N	5.07	1.40	1.33
1	P	441	PHE	C-N	5.07	1.40	1.33
1	P	397	GLN	C-N	5.04	1.40	1.33

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	98	LYS	CA-C-N	9.43	132.70	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	98	LYS	C-N-CA	9.43	132.70	120.44
1	P	290	MET	CA-C-N	8.45	131.03	120.72
1	P	290	MET	C-N-CA	8.45	131.03	120.72
1	P	18	TRP	CA-C-N	7.81	131.08	120.38
1	P	18	TRP	C-N-CA	7.81	131.08	120.38
1	P	93	ARG	CA-C-N	7.73	130.97	120.54
1	P	93	ARG	C-N-CA	7.73	130.97	120.54
1	P	400	GLN	CA-C-O	7.46	128.33	120.42
1	P	228	LEU	CA-C-N	7.42	130.53	120.44
1	P	228	LEU	C-N-CA	7.42	130.53	120.44
1	P	393	PHE	N-CA-C	-7.24	103.32	111.14
2	E	620	ASP	O-C-N	-6.99	113.60	122.34
1	P	400	GLN	CA-C-N	6.97	130.18	120.29
1	P	400	GLN	C-N-CA	6.97	130.18	120.29
1	P	62	VAL	CA-C-N	6.91	129.42	120.44
1	P	62	VAL	C-N-CA	6.91	129.42	120.44
1	P	233	LEU	N-CA-C	-6.60	104.08	111.28
1	P	57	TYR	CA-C-N	6.57	128.84	120.56
1	P	57	TYR	C-N-CA	6.57	128.84	120.56
1	P	28	SER	CA-C-N	6.56	128.34	120.14
1	P	28	SER	C-N-CA	6.56	128.34	120.14
1	P	81	ILE	CA-C-N	6.53	128.93	120.44
1	P	81	ILE	C-N-CA	6.53	128.93	120.44
1	P	395	LEU	CA-C-N	6.49	128.88	120.44
1	P	395	LEU	C-N-CA	6.49	128.88	120.44
1	P	86	THR	CA-C-N	6.25	130.19	120.75
1	P	86	THR	C-N-CA	6.25	130.19	120.75
1	P	125	CYS	CB-CA-C	-6.00	109.06	117.23
1	P	68	ILE	CA-C-O	-5.98	115.43	121.59
1	P	287	ALA	CA-C-O	-5.96	114.56	120.82
1	P	56	SER	CA-C-O	5.96	126.73	119.11
1	P	440	LEU	CA-C-O	5.95	126.83	120.70
1	P	78	LEU	N-CA-C	5.94	117.76	111.28
1	P	63	SER	CA-C-N	5.90	128.54	120.46
1	P	63	SER	C-N-CA	5.90	128.54	120.46
1	P	393	PHE	CA-C-N	5.82	128.01	120.44
1	P	393	PHE	C-N-CA	5.82	128.01	120.44
1	P	8	THR	CA-C-N	5.75	128.45	120.29
1	P	8	THR	C-N-CA	5.75	128.45	120.29
1	P	100	LEU	O-C-N	-5.73	116.17	122.07
1	P	26	LEU	N-CA-C	-5.68	98.69	110.80
1	P	88	ASN	CA-C-N	5.61	126.86	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	88	ASN	C-N-CA	5.61	126.86	119.84
1	P	58	VAL	CA-C-O	-5.60	115.23	121.17
1	P	432	SER	CA-C-N	5.59	127.78	120.28
1	P	432	SER	C-N-CA	5.59	127.78	120.28
5	L	43	GLU	N-CA-C	-5.59	105.19	111.28
1	P	353	ASP	CA-C-N	5.54	125.20	119.05
1	P	353	ASP	C-N-CA	5.54	125.20	119.05
1	P	438	GLN	CA-C-N	5.52	127.67	120.28
1	P	438	GLN	C-N-CA	5.52	127.67	120.28
1	P	288	ALA	N-CA-C	-5.49	105.19	111.07
1	P	78	LEU	CA-C-N	5.42	127.48	120.44
1	P	78	LEU	C-N-CA	5.42	127.48	120.44
1	P	96	HIS	CA-C-O	-5.38	115.17	120.82
1	P	97	ASP	CA-C-N	5.24	127.25	120.44
1	P	97	ASP	C-N-CA	5.24	127.25	120.44
1	P	442	LEU	CA-C-O	5.20	126.06	120.55
1	P	229	TYR	N-CA-C	-5.18	105.55	111.14
1	P	13	LYS	N-CA-C	5.16	116.59	111.07
1	P	106	TYR	N-CA-C	-5.14	105.30	112.45
1	P	92	ALA	CA-C-N	5.14	127.68	120.28
1	P	92	ALA	C-N-CA	5.14	127.68	120.28
1	P	64	ILE	CA-C-N	5.13	127.16	120.28
1	P	64	ILE	C-N-CA	5.13	127.16	120.28
1	P	284	GLY	CA-C-N	5.12	127.56	120.29
1	P	284	GLY	C-N-CA	5.12	127.56	120.29
2	C	339	TYR	CB-CA-C	-5.12	102.84	110.88
1	P	295	LEU	CA-C-O	5.09	123.72	118.73
1	P	293	LEU	CA-C-N	5.09	131.39	121.41
1	P	293	LEU	C-N-CA	5.09	131.39	121.41
1	P	276	ILE	CA-C-N	5.07	127.07	120.28
1	P	276	ILE	C-N-CA	5.07	127.07	120.28
1	P	426	ASN	CA-C-N	5.02	126.97	120.44
1	P	426	ASN	C-N-CA	5.02	126.97	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	620	ASP	Mainchain

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	P	2137	0	935	9	0
2	A	3935	0	3531	53	0
2	C	4146	0	3766	48	0
2	E	4252	0	3975	67	0
3	B	3147	0	2942	57	0
3	D	3213	0	3010	59	0
3	F	3194	0	2985	47	0
4	G	1273	0	1039	17	0
4	I	1357	0	1177	22	0
4	K	1364	0	1113	21	0
5	H	555	0	400	7	0
5	J	517	0	343	14	0
5	L	582	0	411	7	0
6	M	1096	0	579	7	0
7	N	545	0	280	5	0
8	O	1571	0	752	5	0
9	a	3590	0	1768	11	0
10	b	160	0	34	0	0
11	c	833	0	446	0	0
12	d	1344	0	632	4	0
13	e	358	0	170	0	0
14	g	764	0	446	2	0
14	h	763	0	432	6	0
14	i	780	0	460	6	0
14	j	777	0	448	3	0
14	k	769	0	439	6	0
14	l	752	0	425	3	0
14	m	769	0	439	5	0
14	n	762	0	429	4	0
14	o	737	0	393	1	0
15	r	120	0	26	0	0
All	All	46162	0	34225	457	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 6.

All (457) 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:P:84:MET:CB	1:P:91:ARG:CB	2.37	1.02
4:K:40:LYS:HE2	5:L:42:ALA:HB3	1.49	0.94
3:B:357:ILE:HG23	3:B:369:PRO:HG2	1.55	0.89
2:C:488:ARG:HE	2:C:492:LEU:HD23	1.39	0.85
2:E:334:ILE:HA	2:E:349:MET:HE1	1.62	0.79
4:G:139:HIS:CE1	4:G:178:HIS:CE1	2.72	0.77
2:E:206:THR:HG22	2:E:208:LEU:H	1.48	0.76
4:G:139:HIS:HE1	4:G:178:HIS:CE1	2.05	0.73
2:E:277:VAL:HG23	2:E:315:VAL:HB	1.69	0.72
2:E:167:HIS:H	2:E:343:MET:HE3	1.53	0.72
3:D:157:ILE:HG12	3:D:163:ILE:HG13	1.70	0.71
3:F:367:TYR:O	3:F:369:PRO:HD3	1.91	0.71
2:A:228:PRO:HB3	2:A:464:LEU:HD21	1.71	0.71
2:E:213:VAL:HG12	2:E:331:TYR:HB3	1.72	0.71
2:A:122:PRO:HG2	2:A:125:VAL:HB	1.72	0.71
2:C:492:LEU:HD11	2:C:512:LEU:HD21	1.72	0.70
3:B:45:ILE:HG13	3:B:93:LEU:HG	1.74	0.70
2:E:252:GLY:HA3	2:E:258:LYS:HD3	1.72	0.70
14:j:19:ALA:HB1	14:k:100:ALA:HB2	1.74	0.69
3:B:306:TYR:HA	3:B:346:LEU:HD21	1.72	0.69
2:E:282:ARG:NH1	2:E:285:GLU:OE2	2.26	0.68
3:D:94:LYS:HB3	3:D:124:TYR:HB3	1.74	0.68
1:P:53:ASP:O	1:P:93:ARG:CB	2.42	0.67
3:B:287:GLU:HA	2:C:379:ALA:HB1	1.77	0.67
1:P:84:MET:CA	1:P:91:ARG:CB	2.73	0.67
3:F:459:TRP:HE1	3:F:478:LEU:HB2	1.60	0.67
2:C:22:GLY:HA3	2:C:37:MET:HE1	1.76	0.67
3:D:19:MET:SD	4:G:124:ARG:NH2	2.68	0.66
2:C:580:ASP:OD1	2:C:581:LEU:N	2.28	0.66
4:I:208:ARG:NH2	5:J:106:THR:O	2.28	0.66
14:g:17:GLY:HA3	14:g:95:LEU:HA	1.78	0.66
3:B:50:LEU:HD11	3:B:56:ARG:HE	1.61	0.65
3:B:128:SER:HB3	3:B:254:ARG:HD3	1.79	0.65
2:A:553:LEU:HD13	2:A:556:GLN:HE22	1.58	0.65
3:D:276:THR:HG23	3:D:331:ILE:HD11	1.78	0.64
5:J:86:LEU:O	5:J:90:ALA:N	2.30	0.64
14:i:17:GLY:HA3	14:i:95:LEU:HA	1.78	0.64
5:J:85:HIS:O	5:J:89:GLY:N	2.29	0.64
2:A:248:CYS:HB2	2:A:410:VAL:HA	1.80	0.64
2:E:93:LEU:HA	2:E:97:ILE:HD11	1.80	0.63
8:O:159:GLY:HA2	8:O:165:ASP:HA	1.80	0.63
5:H:79:THR:O	5:H:83:ILE:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:89:GLY:O	5:J:93:ILE:N	2.30	0.63
14:n:28:GLY:HA3	14:n:106:LEU:HA	1.81	0.63
2:E:577:ARG:HD2	2:E:618:LEU:HD22	1.81	0.63
3:D:161:GLN:HE22	3:D:379:LEU:HB2	1.64	0.63
2:C:266:SER:O	2:C:311:ARG:NH1	2.32	0.62
3:F:46:VAL:HG12	3:F:88:PHE:HA	1.81	0.62
12:d:218:ARG:HA	12:d:292:ALA:HB3	1.79	0.62
3:B:140:PRO:HA	3:B:318:ARG:HD3	1.81	0.62
2:E:392:ALA:HA	2:E:407:VAL:HG13	1.82	0.62
2:E:429:LEU:HA	2:E:432:VAL:HG12	1.81	0.62
3:D:140:PRO:HG2	3:D:379:LEU:HG	1.81	0.62
2:E:279:CYS:HB2	2:E:326:ARG:HG3	1.82	0.61
14:n:32:GLY:HA2	14:n:113:GLY:HA3	1.82	0.61
2:A:22:GLY:O	2:A:82:VAL:N	2.33	0.61
4:K:219:GLU:O	4:K:223:GLN:HG2	2.00	0.61
14:o:28:GLY:HA3	14:o:106:LEU:HA	1.82	0.61
2:C:23:TYR:HB2	2:C:79:ASN:HA	1.81	0.61
4:G:124:ARG:NH1	4:G:201:CYS:SG	2.73	0.61
3:D:278:MET:HE1	3:D:312:ILE:HD13	1.83	0.61
4:I:107:HIS:O	4:I:111:LYS:HD2	2.00	0.61
3:F:104:ARG:NH1	3:F:117:PRO:O	2.25	0.61
5:J:83:ILE:O	5:J:87:ASN:N	2.33	0.61
2:E:398:LEU:O	2:E:403:ARG:NH1	2.31	0.60
3:F:328:GLN:HG3	3:F:330:PRO:HD3	1.82	0.60
3:B:15:LEU:O	4:K:208:ARG:NH2	2.33	0.60
5:J:84:HIS:O	5:J:88:ALA:N	2.24	0.60
2:C:213:VAL:HG22	2:C:331:TYR:HB3	1.82	0.60
3:D:400:LEU:HD11	3:D:458:ALA:HB1	1.82	0.60
7:N:58:ALA:O	7:N:62:PHE:N	2.35	0.60
9:a:506:ALA:O	9:a:522:LYS:N	2.34	0.60
5:J:88:ALA:O	5:J:92:LYS:N	2.30	0.60
3:D:206:ALA:HA	3:D:234:ARG:HG2	1.83	0.59
9:a:202:PRO:HG3	9:a:268:ALA:HB2	1.84	0.59
2:C:290:LEU:HD21	3:D:135:SER:HA	1.84	0.59
2:E:375:SER:H	6:M:195:LEU:HD11	1.66	0.59
8:O:273:SER:O	8:O:277:SER:N	2.31	0.59
3:F:254:ARG:NH1	3:F:308:ASP:OD1	2.34	0.59
3:B:127:ILE:HG21	3:B:255:ILE:HD13	1.84	0.59
2:A:266:SER:HB2	2:A:308:VAL:HG21	1.84	0.59
2:E:300:LEU:HD21	2:E:304:ARG:HB2	1.85	0.59
2:E:143:ILE:HG21	2:E:149:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:449:PRO:HG3	2:A:524:ALA:HA	1.83	0.58
7:N:31:GLY:O	7:N:32:VAL:CB	2.50	0.58
3:D:442:ALA:O	3:D:449:ARG:NH1	2.36	0.58
3:B:46:VAL:HG21	3:B:86:VAL:HG12	1.86	0.58
2:A:46:VAL:HG23	2:A:84:ARG:HA	1.86	0.58
3:B:127:ILE:HB	3:B:254:ARG:HG2	1.85	0.58
3:B:384:ILE:HG21	3:B:394:SER:HB3	1.85	0.58
2:C:561:GLY:HA2	2:C:566:GLY:HA3	1.86	0.58
4:G:108:ASN:OD1	4:G:109:SER:N	2.36	0.58
4:I:191:VAL:HG12	4:I:202:GLU:HA	1.86	0.58
14:h:10:ALA:HB1	14:h:91:GLY:HA3	1.85	0.58
2:C:277:VAL:HG11	2:C:333:GLY:HA3	1.86	0.57
12:d:155:LEU:HA	12:d:161:ALA:HB1	1.87	0.57
2:A:23:TYR:HB2	2:A:79:ASN:HA	1.86	0.57
3:B:79:ILE:HG23	3:B:84:THR:HG21	1.87	0.57
3:B:305:MET:HE2	3:B:346:LEU:HD13	1.84	0.57
4:I:114:LEU:HD21	4:I:142:VAL:HG22	1.86	0.57
3:D:168:ALA:H	3:D:171:LEU:HD12	1.68	0.57
3:B:384:ILE:HG23	3:B:393:HIS:HB3	1.85	0.57
14:k:28:GLY:HA3	14:k:106:LEU:HA	1.85	0.57
2:C:250:ILE:HG22	2:C:436:TRP:HB2	1.86	0.57
2:A:195:GLU:HA	2:A:204:SER:HA	1.87	0.56
3:B:46:VAL:HG23	3:B:88:PHE:HA	1.87	0.56
3:D:158:ALA:HB2	3:D:383:ALA:HB2	1.86	0.56
4:K:124:ARG:HH11	4:K:201:CYS:HB3	1.68	0.56
3:D:102:LEU:O	4:G:78:ARG:NH1	2.39	0.56
3:B:306:TYR:HB2	3:B:346:LEU:HD11	1.87	0.56
1:P:84:MET:O	1:P:91:ARG:CB	2.54	0.56
3:D:143:MET:HB2	3:D:383:ALA:HB1	1.88	0.56
2:E:581:LEU:HD13	2:E:611:LEU:HA	1.86	0.56
1:P:84:MET:C	1:P:91:ARG:CB	2.80	0.55
3:B:367:TYR:O	3:B:369:PRO:HD3	2.07	0.55
3:F:169:ALA:O	3:F:359:ARG:NH1	2.38	0.55
2:A:526:ASN:O	2:A:528:PHE:N	2.40	0.55
2:A:101:ILE:HG23	2:A:109:LEU:HB2	1.88	0.55
4:K:40:LYS:HD3	5:L:39:LYS:HA	1.88	0.55
2:E:598:PRO:HA	2:E:601:VAL:HG12	1.89	0.55
3:D:295:VAL:HG22	6:M:203:LEU:HD21	1.88	0.55
14:k:17:GLY:HA3	14:k:95:LEU:HA	1.89	0.55
3:D:253:PRO:HB2	3:D:312:ILE:HD11	1.88	0.54
3:F:56:ARG:NH2	3:F:75:GLY:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:581:LEU:HD13	2:C:611:LEU:HA	1.90	0.54
3:D:276:THR:HA	3:D:331:ILE:HG12	1.87	0.54
5:H:53:VAL:O	5:H:58:GLN:NE2	2.39	0.54
2:A:306:GLU:HG2	2:A:310:LYS:HD3	1.90	0.54
3:F:128:SER:HA	3:F:315:ARG:NH1	2.23	0.54
2:A:304:ARG:CZ	2:A:305:GLU:H	2.19	0.54
5:H:46:ILE:O	5:H:50:ARG:HG2	2.07	0.54
2:E:26:LYS:HB3	2:E:33:ILE:HB	1.88	0.54
4:G:116:GLY:HA3	5:H:108:VAL:HG21	1.90	0.54
2:A:250:ILE:HD11	2:A:436:TRP:HE3	1.72	0.54
3:F:297:GLY:N	3:F:301:TYR:O	2.39	0.54
3:B:286:ARG:HE	3:B:301:TYR:HA	1.72	0.53
4:G:125:LEU:HD11	4:G:201:CYS:HB2	1.90	0.53
4:K:89:VAL:O	4:K:92:MET:HG3	2.07	0.53
2:A:478:ILE:HG23	2:A:548:ILE:HG13	1.89	0.53
3:B:27:VAL:HG22	3:B:32:VAL:HG12	1.90	0.53
2:C:301:PRO:HG2	2:C:304:ARG:HB2	1.89	0.53
2:E:109:LEU:HD23	3:F:134:PRO:HD2	1.90	0.53
2:A:574:ILE:HA	2:A:577:ARG:HD3	1.90	0.53
3:B:388:MET:HG2	3:B:389:THR:HG22	1.91	0.53
1:P:52:ASP:C	1:P:54:GLY:H	2.16	0.53
2:C:354:THR:OG1	2:C:412:ALA:O	2.27	0.53
3:F:207:ILE:HB	3:F:235:VAL:HG22	1.90	0.53
9:a:66:ALA:O	9:a:70:LYS:N	2.38	0.53
3:D:309:LEU:HA	3:D:312:ILE:HG22	1.91	0.52
3:F:209:PHE:HB3	3:F:237:LEU:HD23	1.91	0.52
2:E:151:GLY:HA2	2:E:170:LEU:HD23	1.91	0.52
2:E:225:ALA:HA	2:E:394:LYS:HD3	1.91	0.52
7:N:17:MET:HA	7:N:45:ILE:HA	1.92	0.52
3:D:171:LEU:HD13	3:D:357:ILE:HG22	1.92	0.52
2:A:289:VAL:HG22	2:A:293:PHE:CE2	2.45	0.52
3:F:117:PRO:HB2	4:I:86:ASP:OD2	2.10	0.52
5:J:97:VAL:O	5:J:101:LEU:HD23	2.09	0.52
4:I:220:ILE:HG12	5:J:100:MET:HG2	1.92	0.51
2:A:265:LEU:HA	2:A:269:SER:HB3	1.91	0.51
3:D:22:ARG:NH2	3:D:82:LYS:O	2.41	0.51
3:F:356:TYR:HD2	3:F:371:ASN:HB3	1.76	0.51
2:A:108:PRO:HD3	2:A:129:ALA:HA	1.93	0.51
2:A:228:PRO:HA	2:A:243:VAL:HA	1.92	0.51
3:B:232:MET:HE1	4:K:72:MET:SD	2.50	0.51
2:A:531:TYR:CE1	2:A:590:PHE:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:164:PRO:HG3	3:B:351:THR:HG21	1.92	0.51
2:A:95:PRO:HG2	2:A:207:MET:HE2	1.92	0.51
2:C:154:LEU:HD23	2:C:169:ALA:HB2	1.92	0.51
2:E:251:PRO:HD2	2:E:437:GLY:HA2	1.91	0.51
2:E:248:CYS:SG	2:E:249:ALA:N	2.83	0.51
5:J:85:HIS:HA	5:J:88:ALA:HB3	1.92	0.51
3:F:112:PRO:HG2	3:F:118:PRO:HA	1.91	0.51
3:D:29:GLY:O	3:D:76:THR:OG1	2.25	0.50
3:D:161:GLN:HG3	3:D:162:LYS:N	2.25	0.50
3:B:247:ILE:HA	3:B:250:ILE:HD13	1.92	0.50
3:D:15:LEU:HD23	3:D:15:LEU:H	1.75	0.50
8:O:274:LEU:O	8:O:279:LEU:N	2.38	0.50
2:E:231:THR:N	2:E:237:ASP:OD2	2.44	0.50
2:A:286:MET:HA	2:A:289:VAL:HG12	1.92	0.50
3:F:23:THR:HG22	4:I:198:LYS:HB3	1.93	0.50
3:D:407:GLY:C	3:D:433:LEU:HD11	2.37	0.50
2:E:213:VAL:HA	2:E:335:THR:HG21	1.94	0.50
3:B:360:GLN:HG2	3:B:361:LEU:HD12	1.94	0.49
5:L:96:ASP:OD1	5:L:97:VAL:N	2.45	0.49
4:K:208:ARG:HA	4:K:211:VAL:HG12	1.93	0.49
3:D:161:GLN:NE2	3:D:379:LEU:HB2	2.28	0.49
4:I:137:ASP:OD1	4:I:137:ASP:N	2.44	0.49
2:C:89:LEU:HD23	2:C:213:VAL:HG11	1.95	0.49
2:C:170:LEU:HD21	2:C:194:LEU:HD22	1.93	0.49
3:F:241:LEU:N	3:F:244:ASP:OD2	2.46	0.49
2:C:108:PRO:HD3	2:C:129:ALA:HA	1.93	0.49
2:E:584:ARG:HH12	2:E:607:LEU:HA	1.76	0.49
3:B:165:LEU:HD12	3:B:355:ILE:HB	1.95	0.49
2:C:289:VAL:HG13	2:C:293:PHE:CD2	2.47	0.49
3:B:208:VAL:HB	3:B:273:VAL:HG12	1.94	0.49
3:B:343:THR:HB	3:B:344:PRO:HD3	1.94	0.49
3:D:45:ILE:HD11	3:D:93:LEU:HG	1.95	0.49
3:D:143:MET:HE2	3:D:187:VAL:HG11	1.95	0.49
3:F:459:TRP:HE1	3:F:478:LEU:HD13	1.77	0.49
3:B:246:THR:O	3:B:250:ILE:HD12	2.12	0.49
3:D:60:VAL:HG22	3:D:70:VAL:HG22	1.95	0.48
3:B:431:GLU:OE2	3:B:464:ILE:HG21	2.13	0.48
2:C:508:ASP:O	2:C:512:LEU:HD23	2.13	0.48
3:B:20:GLU:HA	3:B:87:GLN:HA	1.94	0.48
2:C:131:ASP:OD1	2:C:134:THR:N	2.44	0.48
3:D:27:VAL:HG22	3:D:32:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:100:VAL:HG11	4:K:209:LEU:HD12	1.94	0.48
3:D:306:TYR:HD2	3:D:346:LEU:HD22	1.79	0.48
3:F:73:PHE:HA	3:F:247:ILE:HG21	1.96	0.48
3:F:400:LEU:HD23	3:F:436:PHE:HE1	1.78	0.48
3:F:416:VAL:HG23	3:F:417:VAL:HG23	1.95	0.48
4:G:216:LYS:O	4:G:220:ILE:HG12	2.14	0.48
14:i:28:GLY:HA3	14:i:106:LEU:HA	1.96	0.48
2:E:415:PRO:O	3:F:349:TYR:OH	2.27	0.48
2:A:137:GLU:O	2:A:158:VAL:HG13	2.14	0.48
4:I:109:SER:HA	4:I:112:LYS:NZ	2.28	0.48
9:a:505:TYR:HA	9:a:523:VAL:HA	1.95	0.48
2:E:357:TRP:CG	2:E:357:TRP:O	2.67	0.48
14:k:41:ALA:HB2	14:l:118:ALA:HB1	1.95	0.48
3:B:45:ILE:O	3:B:89:THR:OG1	2.24	0.47
2:E:300:LEU:HD23	2:E:300:LEU:H	1.79	0.47
2:E:558:VAL:HG22	2:E:568:LYS:HA	1.95	0.47
3:F:164:PRO:HD3	3:F:351:THR:OG1	2.14	0.47
14:h:28:GLY:HA3	14:h:106:LEU:HA	1.96	0.47
2:C:380:TYR:O	2:C:384:ARG:HG2	2.14	0.47
3:B:104:ARG:NH1	3:B:117:PRO:O	2.40	0.47
3:B:145:GLN:HB2	3:B:187:VAL:HG22	1.96	0.47
3:D:149:SER:HB2	3:D:449:ARG:HD2	1.95	0.47
3:D:414:LYS:HA	3:D:417:VAL:HG22	1.96	0.47
2:E:273:THR:HB	2:E:347:VAL:HG23	1.97	0.47
3:F:95:THR:HG21	3:F:255:ILE:HG23	1.97	0.47
4:I:204:THR:HG23	4:I:207:ALA:H	1.80	0.47
3:D:112:PRO:HG3	3:D:118:PRO:HA	1.95	0.47
4:I:92:MET:HE1	5:J:100:MET:HE2	1.96	0.47
5:J:38:ALA:O	5:J:41:GLU:HG3	2.14	0.47
2:C:614:GLY:C	2:C:616:ARG:H	2.22	0.47
2:E:493:ASN:HA	2:E:496:VAL:HG12	1.97	0.47
4:I:85:GLN:O	4:I:88:LEU:HG	2.13	0.47
4:I:215:LYS:HD2	4:I:215:LYS:C	2.40	0.47
4:K:193:ALA:HB2	4:K:200:VAL:HG12	1.96	0.47
14:l:17:GLY:HA3	14:l:95:LEU:HA	1.97	0.47
2:A:297:THR:OG1	2:A:306:GLU:O	2.31	0.47
3:F:144:ILE:HD12	3:F:157:ILE:HG13	1.96	0.47
4:I:222:LYS:C	4:I:222:LYS:HD3	2.40	0.47
2:C:331:TYR:HA	2:C:334:ILE:HG22	1.96	0.47
3:D:475:GLY:HA2	3:D:478:LEU:HD12	1.97	0.47
2:E:30:PRO:HA	2:E:73:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:VAL:HG12	2:E:315:VAL:O	2.15	0.47
4:G:99:GLU:O	4:G:103:VAL:HG23	2.15	0.47
14:n:10:ALA:HB2	14:n:88:LEU:HA	1.97	0.47
1:P:425:GLU:O	1:P:426:ASN:CB	2.63	0.46
2:E:279:CYS:O	2:E:353:SER:OG	2.34	0.46
2:E:292:ASP:OD1	2:E:293:PHE:N	2.48	0.46
2:C:101:ILE:HG22	2:C:109:LEU:HD12	1.97	0.46
3:F:335:PRO:HG2	3:F:341:HIS:CD2	2.49	0.46
3:D:373:LEU:HB3	3:D:374:PRO:HD3	1.97	0.46
3:D:272:LEU:HD21	3:D:274:ILE:HD11	1.97	0.46
3:D:345:ASP:O	3:D:349:TYR:HD1	1.98	0.46
2:A:246:GLY:O	2:A:408:THR:OG1	2.32	0.46
2:A:397:CYS:SG	2:A:403:ARG:HD3	2.56	0.46
2:A:340:PHE:HA	2:A:343:MET:HE3	1.98	0.46
2:C:294:PRO:HA	2:C:309:MET:HG2	1.97	0.46
2:C:492:LEU:HA	2:C:495:ILE:HD13	1.97	0.46
2:E:513:GLU:C	2:E:515:ALA:H	2.24	0.46
2:A:74:ALA:HA	3:B:42:TYR:HD2	1.79	0.46
3:D:200:GLY:O	3:D:204:ASN:N	2.47	0.46
2:E:131:ASP:OD2	2:E:134:THR:N	2.47	0.46
2:E:347:VAL:O	2:E:407:VAL:HA	2.16	0.46
3:F:48:ILE:HD13	3:F:72:VAL:HG12	1.98	0.46
3:F:105:ILE:HG23	3:F:237:LEU:HB2	1.97	0.46
4:K:124:ARG:NH1	4:K:201:CYS:HB3	2.31	0.46
2:E:45:LEU:O	2:E:85:THR:OG1	2.28	0.45
2:E:211:TRP:CZ2	2:E:218:PRO:HD3	2.51	0.45
14:h:10:ALA:N	14:h:11:PRO:HD2	2.31	0.45
2:A:194:LEU:O	2:A:205:PHE:N	2.45	0.45
3:B:272:LEU:HD12	3:B:327:THR:O	2.16	0.45
3:D:143:MET:SD	3:D:156:SER:OG	2.69	0.45
4:G:60:LYS:O	4:G:63:GLU:HG2	2.16	0.45
14:h:19:ALA:HB1	14:i:100:ALA:HB2	1.96	0.45
3:D:163:ILE:HD13	3:D:353:GLY:HA3	1.97	0.45
5:J:87:ASN:O	5:J:91:GLU:N	2.49	0.45
3:F:459:TRP:NE1	3:F:478:LEU:HB2	2.29	0.45
4:G:51:ILE:HD11	5:H:53:VAL:HG11	1.99	0.45
14:m:17:GLY:HA3	14:m:95:LEU:HA	1.98	0.45
3:F:144:ILE:HD11	3:F:159:ARG:HA	1.98	0.45
2:C:471:PHE:HE2	2:C:541:VAL:HG11	1.81	0.45
2:E:415:PRO:HB3	2:E:425:THR:HG21	1.99	0.45
3:F:138:THR:OG1	3:F:318:ARG:O	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:GLN:CD	3:F:379:LEU:HB2	2.42	0.45
4:G:212:VAL:HG12	5:H:101:LEU:HD13	1.99	0.45
2:E:475:PHE:HA	2:E:478:ILE:HG12	1.98	0.45
4:K:134:CYS:HB2	4:K:178:HIS:HB3	1.99	0.45
2:C:197:GLU:HA	2:C:202:LYS:HA	1.98	0.45
2:C:514:THR:HG21	2:C:551:TYR:HB2	1.98	0.45
2:E:323:VAL:HG13	2:E:326:ARG:HH22	1.82	0.45
4:K:182:HIS:HB2	4:K:185:SER:HB2	1.99	0.45
6:M:66:SER:O	6:M:70:ILE:HG12	2.17	0.45
9:a:200:LEU:HA	9:a:246:PHE:H	1.81	0.45
4:K:24:LYS:HB3	4:K:24:LYS:HE3	1.64	0.44
2:C:360:ALA:O	2:C:364:ILE:HG12	2.17	0.44
4:K:85:GLN:O	4:K:88:LEU:HG	2.17	0.44
3:B:309:LEU:HD12	3:B:346:LEU:HD22	1.99	0.44
4:I:47:GLU:O	4:I:50:LYS:HG3	2.18	0.44
3:B:129:GLY:H	3:B:315:ARG:HH12	1.65	0.44
2:C:22:GLY:O	2:C:82:VAL:N	2.33	0.44
2:C:413:VAL:HG12	2:C:414:SER:H	1.82	0.44
2:E:89:LEU:O	2:E:213:VAL:HG23	2.17	0.44
14:l:28:GLY:HA3	14:l:106:LEU:HA	1.99	0.44
3:D:14:THR:HG22	5:H:107:THR:HG23	1.99	0.44
2:E:340:PHE:HD1	2:E:343:MET:SD	2.40	0.44
9:a:802:PHE:O	9:a:804:GLU:N	2.49	0.44
2:A:531:TYR:O	2:A:593:PRO:HD3	2.18	0.44
2:A:552:ASN:O	2:A:555:ASN:N	2.50	0.44
8:O:35:PRO:HD2	8:O:322:PRO:HB3	2.00	0.44
14:g:28:GLY:HA3	14:g:106:LEU:HA	1.99	0.44
14:n:17:GLY:HA3	14:n:95:LEU:HA	2.00	0.44
3:B:261:GLU:HA	3:B:326:ILE:HD11	2.00	0.44
9:a:24:MET:HA	9:a:352:PRO:HA	2.00	0.44
2:A:230:LEU:HB3	2:A:270:ASN:OD1	2.18	0.44
4:G:189:GLY:HA3	4:G:204:THR:HA	2.00	0.44
5:J:93:ILE:O	5:J:97:VAL:HG23	2.18	0.44
2:E:167:HIS:H	2:E:343:MET:CE	2.27	0.43
3:F:128:SER:HA	3:F:315:ARG:HH12	1.82	0.43
14:i:32:GLY:HA2	14:i:113:GLY:HA3	1.99	0.43
3:B:247:ILE:O	3:B:251:ILE:HG23	2.18	0.43
3:F:96:PRO:HB3	3:F:124:TYR:CE1	2.53	0.43
4:K:224:LEU:HG	5:L:93:ILE:HD11	2.00	0.43
2:A:175:MET:O	2:A:198:PHE:HB2	2.17	0.43
4:K:96:ALA:O	4:K:100:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:538:TYR:O	2:A:542:TRP:HD1	2.01	0.43
3:B:145:GLN:NE2	3:B:450:ASN:HA	2.33	0.43
1:P:225:ILE:HA	1:P:228:LEU:CB	2.48	0.43
3:B:209:PHE:HD2	3:B:237:LEU:HD13	1.84	0.43
3:B:360:GLN:O	3:B:364:ARG:HG3	2.18	0.43
2:A:78:VAL:HG12	2:A:79:ASN:OD1	2.19	0.43
3:D:79:ILE:HG23	3:D:84:THR:HG21	2.00	0.43
3:F:15:LEU:HD11	4:I:208:ARG:HG3	2.01	0.43
4:I:92:MET:HE3	4:I:92:MET:HB3	1.89	0.43
14:k:10:ALA:N	14:k:11:PRO:HD2	2.33	0.43
3:B:171:LEU:HD13	3:B:357:ILE:HG22	1.99	0.43
2:C:492:LEU:HD21	2:C:512:LEU:HD21	2.01	0.43
3:F:47:ASN:OD1	3:F:47:ASN:N	2.48	0.43
3:B:344:PRO:HA	3:B:347:THR:HG22	2.01	0.43
2:C:413:VAL:HG12	2:C:414:SER:N	2.34	0.43
3:D:23:THR:OG1	3:D:35:ASP:O	2.35	0.43
2:E:226:ASP:OD1	2:E:226:ASP:N	2.50	0.43
3:F:157:ILE:HD13	3:F:163:ILE:HG22	2.01	0.43
9:a:507:CYS:HA	9:a:521:ILE:HA	2.01	0.43
14:m:21:ALA:HB2	14:m:98:GLY:HA2	2.01	0.43
2:C:119:VAL:HG21	3:D:319:ILE:HD11	2.01	0.43
2:C:539:LYS:O	2:C:543:MET:HG3	2.19	0.43
6:M:95:VAL:O	7:N:12:SER:N	2.52	0.43
9:a:200:LEU:HA	9:a:245:VAL:HA	2.00	0.43
14:m:28:GLY:HA3	14:m:106:LEU:HA	1.99	0.43
2:A:211:TRP:CZ2	2:A:218:PRO:HD3	2.54	0.43
2:A:308:VAL:HG22	2:A:312:THR:OG1	2.19	0.42
2:C:415:PRO:O	2:C:417:GLY:N	2.48	0.42
3:D:117:PRO:HG2	4:G:82:LEU:HG	2.01	0.42
3:D:460:THR:HA	3:D:463:ARG:HE	1.83	0.42
3:F:23:THR:OG1	3:F:35:ASP:O	2.28	0.42
4:K:193:ALA:HA	4:K:199:ILE:O	2.19	0.42
3:B:60:VAL:HG22	3:B:70:VAL:HG22	2.00	0.42
14:h:56:VAL:N	14:h:57:PRO:HD2	2.34	0.42
2:C:272:ASP:HB2	2:C:345:TYR:HB3	2.02	0.42
3:D:154:MET:HE2	3:D:154:MET:HB2	1.74	0.42
4:I:97:SER:O	4:I:100:VAL:HG12	2.19	0.42
14:m:10:ALA:HB2	14:m:88:LEU:HA	2.01	0.42
2:A:53:LEU:HB3	2:A:69:VAL:HG11	2.02	0.42
2:C:162:SER:OG	2:C:310:LYS:NZ	2.30	0.42
2:E:109:LEU:CD2	3:F:134:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:353:SER:O	2:C:354:THR:OG1	2.36	0.42
3:D:367:TYR:O	3:D:369:PRO:HD3	2.20	0.42
3:D:456:ASP:O	3:D:460:THR:HG23	2.19	0.42
2:A:53:LEU:HD23	2:A:53:LEU:HA	1.86	0.42
3:F:164:PRO:HG2	3:F:166:PHE:HE1	1.84	0.42
3:F:319:ILE:HG23	3:F:322:ARG:HB2	2.01	0.42
14:i:30:ALA:HB1	14:j:111:ALA:HB2	2.01	0.42
3:B:373:LEU:HB3	3:B:374:PRO:HD3	2.02	0.42
2:E:158:VAL:HG13	2:E:166:HIS:HB3	2.00	0.42
7:N:113:LEU:H	7:N:113:LEU:HD12	1.84	0.42
2:A:93:LEU:HD12	2:A:339:TYR:CD2	2.54	0.42
2:C:74:ALA:HA	3:D:42:TYR:HD1	1.83	0.42
2:E:584:ARG:NH2	2:E:607:LEU:HG	2.35	0.42
8:O:29:LYS:NZ	8:O:36:LEU:O	2.50	0.42
2:A:46:VAL:HG11	2:A:67:ILE:HD13	2.01	0.42
2:A:245:GLY:H	2:A:408:THR:HB	1.85	0.42
2:E:271:SER:O	2:E:311:ARG:NH2	2.53	0.42
4:G:182:HIS:O	4:G:185:SER:OG	2.36	0.42
2:A:256:CYS:O	2:A:259:THR:OG1	2.32	0.41
3:B:319:ILE:HG22	3:B:322:ARG:H	1.84	0.41
3:D:407:GLY:O	3:D:433:LEU:HD11	2.20	0.41
2:E:37:MET:HE2	2:E:37:MET:HB2	1.82	0.41
2:E:250:ILE:HD11	2:E:436:TRP:HE3	1.85	0.41
4:I:131:LEU:HD12	4:I:195:ARG:HE	1.84	0.41
14:h:32:GLY:HA2	14:h:113:GLY:HA3	2.01	0.41
2:A:267:LYS:HE3	2:A:268:TYR:CZ	2.55	0.41
4:I:75:ASN:O	4:I:79:ILE:HG12	2.20	0.41
4:K:88:LEU:HD13	5:L:90:ALA:HB2	2.02	0.41
3:B:163:ILE:HD12	3:B:353:GLY:HA3	2.02	0.41
2:C:266:SER:HA	2:C:274:VAL:HG21	2.01	0.41
9:a:50:GLN:HA	9:a:812:PRO:HA	2.02	0.41
2:A:442:LEU:HB3	2:A:447:HIS:HB2	2.02	0.41
3:B:34:LEU:HD21	3:B:86:VAL:HG11	2.03	0.41
3:F:120:LEU:HG	4:I:221:ARG:HD2	2.02	0.41
4:I:109:SER:HA	4:I:112:LYS:HZ2	1.86	0.41
12:d:223:ILE:O	12:d:228:ILE:N	2.54	0.41
3:B:128:SER:HA	3:B:315:ARG:HH22	1.86	0.41
3:B:246:THR:O	3:B:249:ARG:N	2.54	0.41
3:B:366:ILE:HG23	3:B:442:ALA:HB2	2.01	0.41
2:C:229:LEU:N	2:C:242:SER:O	2.46	0.41
2:E:297:THR:OG1	2:E:306:GLU:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:331:TYR:HA	2:E:334:ILE:HG22	2.01	0.41
9:a:815:PHE:O	9:a:819:ASP:N	2.50	0.41
3:D:357:ILE:HG23	3:D:369:PRO:HB2	2.03	0.41
2:E:585:LEU:HD11	2:E:611:LEU:HD22	2.02	0.41
3:F:168:ALA:HB3	3:F:359:ARG:HH11	1.86	0.41
3:F:367:TYR:CE2	3:F:445:ALA:HA	2.55	0.41
2:A:535:CYS:SG	2:A:540:SER:OG	2.64	0.41
2:C:95:PRO:HG2	2:C:207:MET:HE2	2.01	0.41
3:D:205:PHE:O	3:D:271:VAL:HA	2.21	0.41
2:E:121:ILE:HG12	3:F:131:SER:O	2.21	0.41
2:E:234:ARG:O	2:E:238:ALA:HB3	2.21	0.41
2:E:142:LYS:HA	2:E:142:LYS:HE2	2.02	0.41
2:E:340:PHE:O	2:E:343:MET:HB2	2.21	0.41
2:A:189:LEU:HD23	2:A:208:LEU:HD12	2.02	0.41
2:A:449:PRO:HD3	2:A:525:GLN:H	1.85	0.41
3:F:347:THR:O	3:F:351:THR:N	2.52	0.41
3:B:76:THR:HB	3:B:79:ILE:HD12	2.02	0.41
3:B:396:VAL:HG21	3:B:455:LEU:HD22	2.03	0.41
2:E:138:PHE:HB3	2:E:185:GLY:O	2.21	0.41
14:i:10:ALA:HB1	14:i:91:GLY:HA3	2.03	0.41
2:C:315:VAL:HG12	2:C:315:VAL:O	2.21	0.40
6:M:51:ILE:HA	6:M:54:THR:HG22	2.03	0.40
14:k:32:GLY:HA2	14:k:113:GLY:HA3	2.03	0.40
2:E:195:GLU:HA	2:E:203:LYS:O	2.21	0.40
2:E:252:GLY:HA2	2:E:438:LEU:HD12	2.03	0.40
6:M:126:ALA:O	12:d:288:MET:N	2.33	0.40
14:j:28:GLY:HA3	14:j:106:LEU:HA	2.03	0.40
14:m:10:ALA:N	14:m:11:PRO:HD2	2.36	0.40
1:P:41:ARG:HA	1:P:52:ASP:CB	2.50	0.40
2:A:491:ASP:HA	2:A:494:GLU:OE1	2.21	0.40
2:E:228:PRO:HG3	2:E:467:PHE:CE2	2.57	0.40
4:K:40:LYS:NZ	5:L:39:LYS:O	2.53	0.40
6:M:131:GLN:O	6:M:135:CYS:N	2.50	0.40
2:A:435:PHE:HB3	2:A:457:TYR:CE1	2.56	0.40
3:B:393:HIS:CE1	3:B:451:ILE:HD11	2.56	0.40
3:D:146:THR:HG21	3:D:157:ILE:HD12	2.03	0.40
3:D:150:THR:HG21	3:D:441:VAL:HG13	2.03	0.40
2:E:137:GLU:O	2:E:158:VAL:HG23	2.21	0.40
2:A:321:MET:HE3	2:A:321:MET:HB3	1.88	0.40
3:B:335:PRO:HD2	3:B:341:HIS:CG	2.57	0.40
2:C:354:THR:HA	2:C:357:TRP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:GLU:HA	3:D:326:ILE:HD11	2.03	0.40
3:D:263:LEU:O	3:D:267:CYS:HB3	2.21	0.40
3:D:457:LEU:O	3:D:460:THR:OG1	2.32	0.40
4:G:139:HIS:HE1	4:G:178:HIS:ND1	2.19	0.40
4:K:100:VAL:HG12	5:L:102:LEU:HD11	2.03	0.40

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	P	426/452 (94%)	399 (94%)	19 (4%)	8 (2%)	6	34
2	A	585/623 (94%)	565 (97%)	19 (3%)	1 (0%)	43	76
2	C	601/623 (96%)	563 (94%)	38 (6%)	0	100	100
2	E	601/623 (96%)	562 (94%)	38 (6%)	1 (0%)	43	76
3	B	456/488 (93%)	423 (93%)	32 (7%)	1 (0%)	43	76
3	D	463/488 (95%)	435 (94%)	28 (6%)	0	100	100
3	F	459/488 (94%)	433 (94%)	26 (6%)	0	100	100
4	G	200/230 (87%)	193 (96%)	7 (4%)	0	100	100
4	I	203/230 (88%)	195 (96%)	8 (4%)	0	100	100
4	K	213/230 (93%)	203 (95%)	10 (5%)	0	100	100
5	H	95/110 (86%)	94 (99%)	1 (1%)	0	100	100
5	J	94/110 (86%)	91 (97%)	3 (3%)	0	100	100
5	L	99/110 (90%)	99 (100%)	0	0	100	100
6	M	211/259 (82%)	196 (93%)	15 (7%)	0	100	100
7	N	105/130 (81%)	76 (72%)	25 (24%)	4 (4%)	2	21
8	O	303/375 (81%)	283 (93%)	20 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	a	705/823 (86%)	661 (94%)	43 (6%)	1 (0%)	48	81
11	c	166/182 (91%)	161 (97%)	5 (3%)	0	100	100
12	d	256/351 (73%)	235 (92%)	21 (8%)	0	100	100
13	e	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
14	g	151/164 (92%)	148 (98%)	3 (2%)	0	100	100
14	h	153/164 (93%)	147 (96%)	6 (4%)	0	100	100
14	i	154/164 (94%)	148 (96%)	6 (4%)	0	100	100
14	j	153/164 (93%)	151 (99%)	2 (1%)	0	100	100
14	k	153/164 (93%)	152 (99%)	1 (1%)	0	100	100
14	l	151/164 (92%)	149 (99%)	2 (1%)	0	100	100
14	m	153/164 (93%)	151 (99%)	2 (1%)	0	100	100
14	n	153/164 (93%)	151 (99%)	2 (1%)	0	100	100
14	o	150/164 (92%)	141 (94%)	9 (6%)	0	100	100
All	All	7676/8471 (91%)	7267 (95%)	393 (5%)	16 (0%)	44	76

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	282	PRO
1	P	367	ASN
2	A	527	ALA
2	E	448	PHE
7	N	32	VAL
1	P	136	PRO
1	P	181	ARG
1	P	218	PRO
1	P	221	THR
1	P	426	ASN
7	N	21	GLU
1	P	17	PRO
3	B	389	THR
7	N	101	LYS
7	N	35	VAL
9	a	59	SER

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	
2	A	328/517 (63%)	323 (98%)	5 (2%)	57	70
2	C	357/517 (69%)	355 (99%)	2 (1%)	78	80
2	E	387/517 (75%)	386 (100%)	1 (0%)	86	85
3	B	272/413 (66%)	270 (99%)	2 (1%)	76	79
3	D	275/413 (67%)	270 (98%)	5 (2%)	51	67
3	F	279/413 (68%)	279 (100%)	0	100	100
4	G	87/206 (42%)	85 (98%)	2 (2%)	44	64
4	I	108/206 (52%)	108 (100%)	0	100	100
4	K	96/206 (47%)	88 (92%)	8 (8%)	10	32
5	H	21/87 (24%)	21 (100%)	0	100	100
5	J	14/87 (16%)	14 (100%)	0	100	100
5	L	25/87 (29%)	22 (88%)	3 (12%)	5	20
6	M	15/225 (7%)	15 (100%)	0	100	100
7	N	6/111 (5%)	6 (100%)	0	100	100
8	O	13/336 (4%)	13 (100%)	0	100	100
9	a	27/715 (4%)	27 (100%)	0	100	100
11	c	5/139 (4%)	5 (100%)	0	100	100
12	d	9/312 (3%)	9 (100%)	0	100	100
13	e	4/63 (6%)	4 (100%)	0	100	100
14	g	8/115 (7%)	8 (100%)	0	100	100
14	h	6/115 (5%)	6 (100%)	0	100	100
14	i	11/115 (10%)	11 (100%)	0	100	100
14	j	8/115 (7%)	8 (100%)	0	100	100
14	k	7/115 (6%)	7 (100%)	0	100	100
14	l	5/115 (4%)	5 (100%)	0	100	100
14	m	7/115 (6%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	n	5/115 (4%)	5 (100%)	0	100	100
All	All	2385/6490 (37%)	2357 (99%)	28 (1%)	61	73

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	570	THR
2	A	572	THR
2	A	573	LEU
2	A	574	ILE
2	A	577	ARG
3	B	372	VAL
3	B	375	SER
2	C	347	VAL
2	C	404	THR
3	D	154	MET
3	D	376	LEU
3	D	397	SER
3	D	401	TYR
3	D	473	ILE
2	E	181	VAL
4	G	139	HIS
4	G	142	VAL
4	K	10	ILE
4	K	12	GLN
4	K	17	ILE
4	K	24	LYS
4	K	26	ASN
4	K	29	SER
4	K	37	ASN
4	K	38	ILE
5	L	23	ILE
5	L	49	HIS
5	L	52	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	447	HIS
2	A	576	HIS
2	C	166	HIS

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Mol	Chain	Res	Type
2	C	233	GLN
2	C	447	HIS
3	D	161	GLN
3	D	362	GLN
2	E	86	HIS
2	E	166	HIS
2	E	447	HIS
4	G	139	HIS
4	G	178	HIS
4	K	179	HIS

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](#)

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.

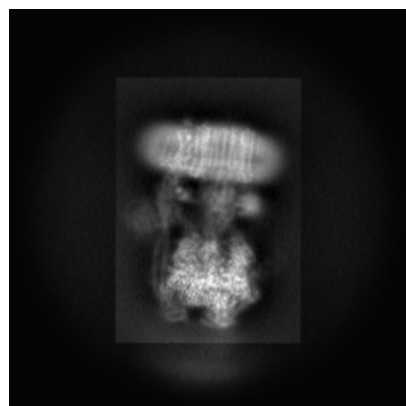
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26829. These allow visual inspection of the internal detail of the map and identification of artifacts.

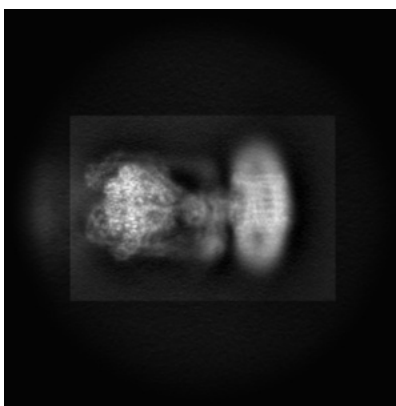
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

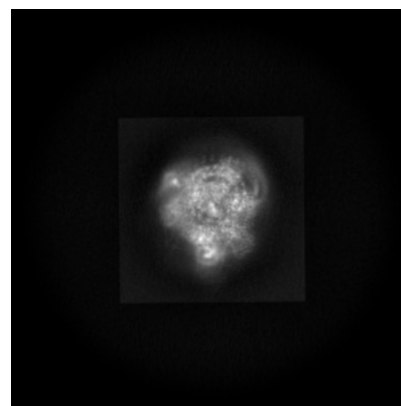
6.1.1 Primary map



X

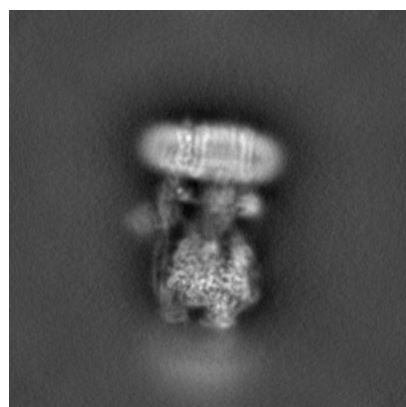


Y

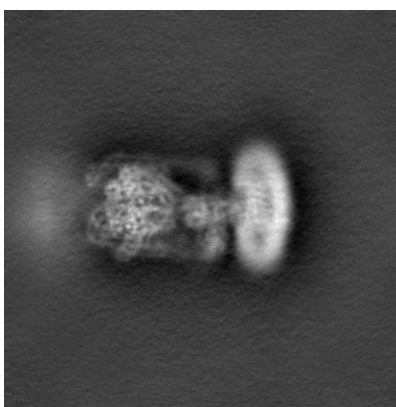


Z

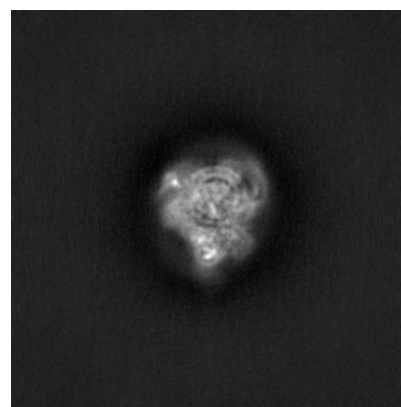
6.1.2 Raw map



X



Y

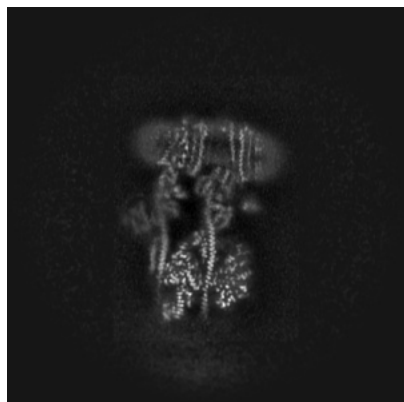


Z

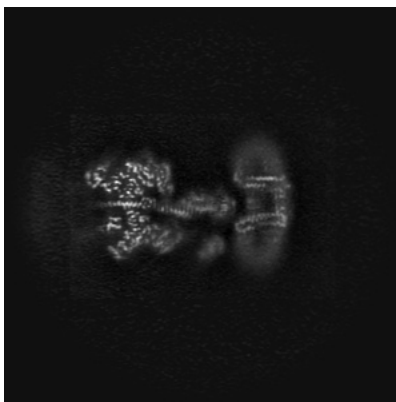
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

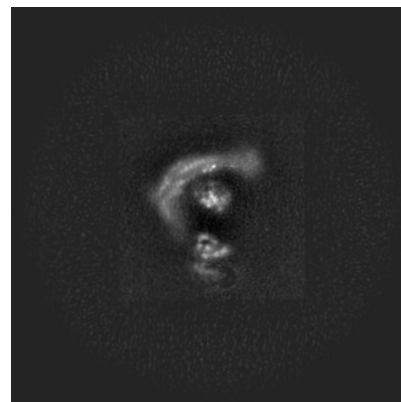
6.2.1 Primary map



X Index: 150

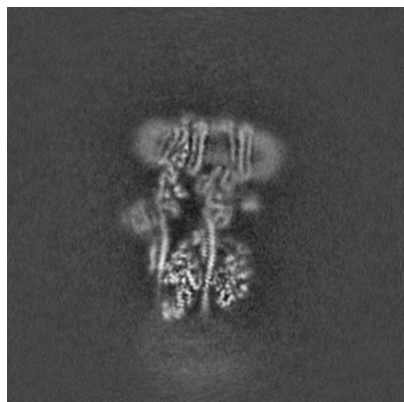


Y Index: 150

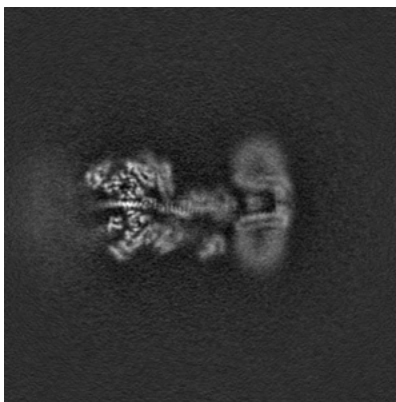


Z Index: 150

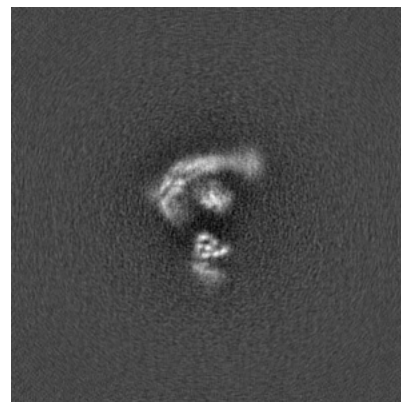
6.2.2 Raw map



X Index: 150



Y Index: 150

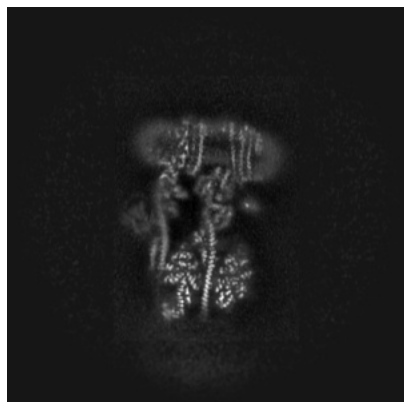


Z Index: 150

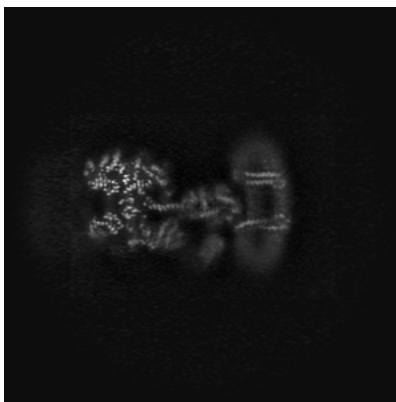
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

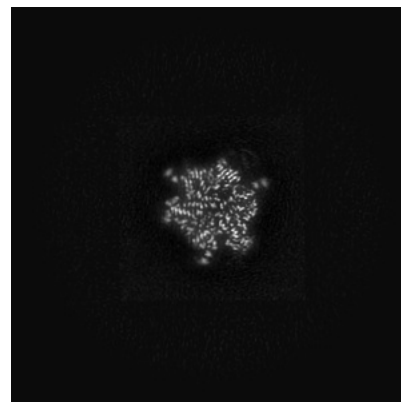
6.3.1 Primary map



X Index: 151

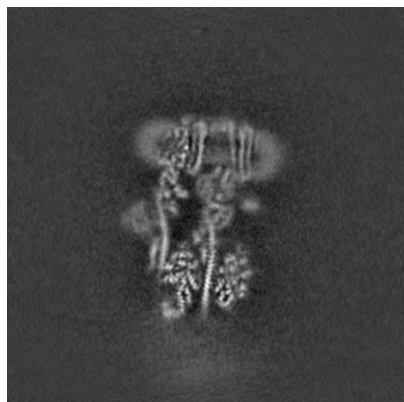


Y Index: 155

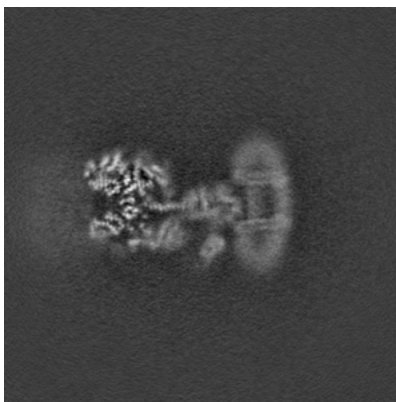


Z Index: 96

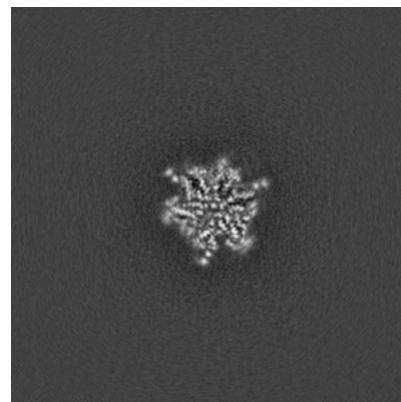
6.3.2 Raw map



X Index: 151



Y Index: 155

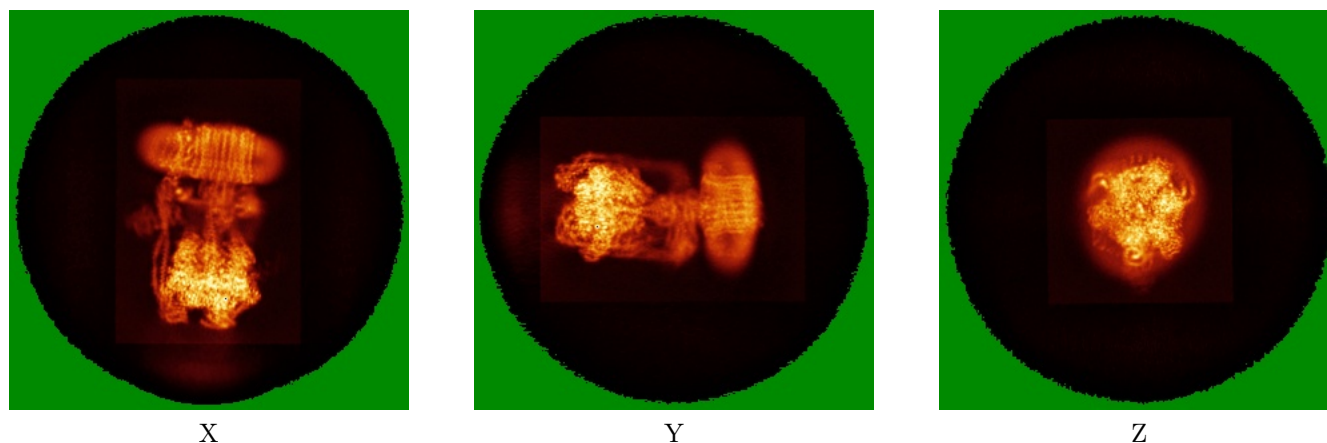


Z Index: 96

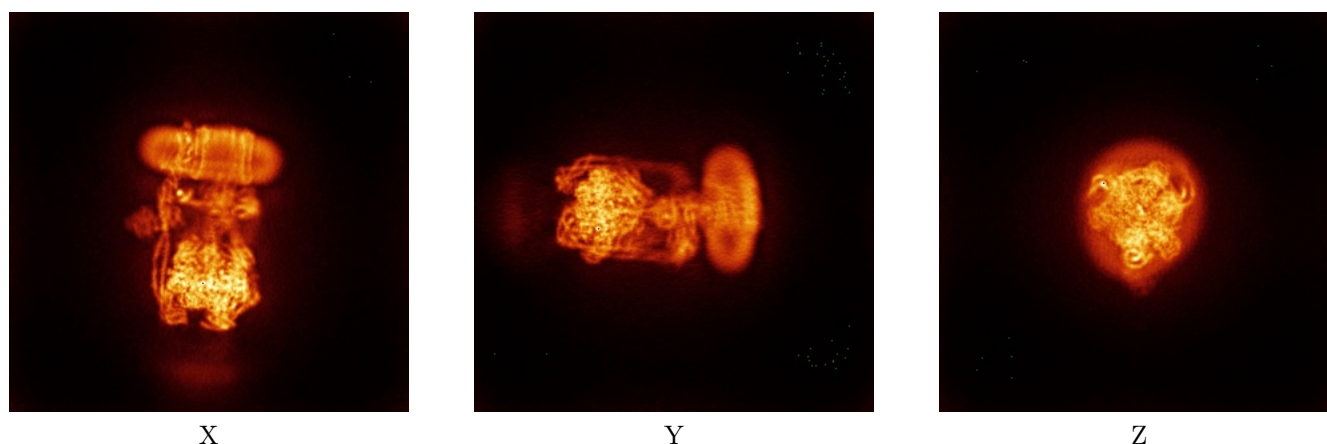
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

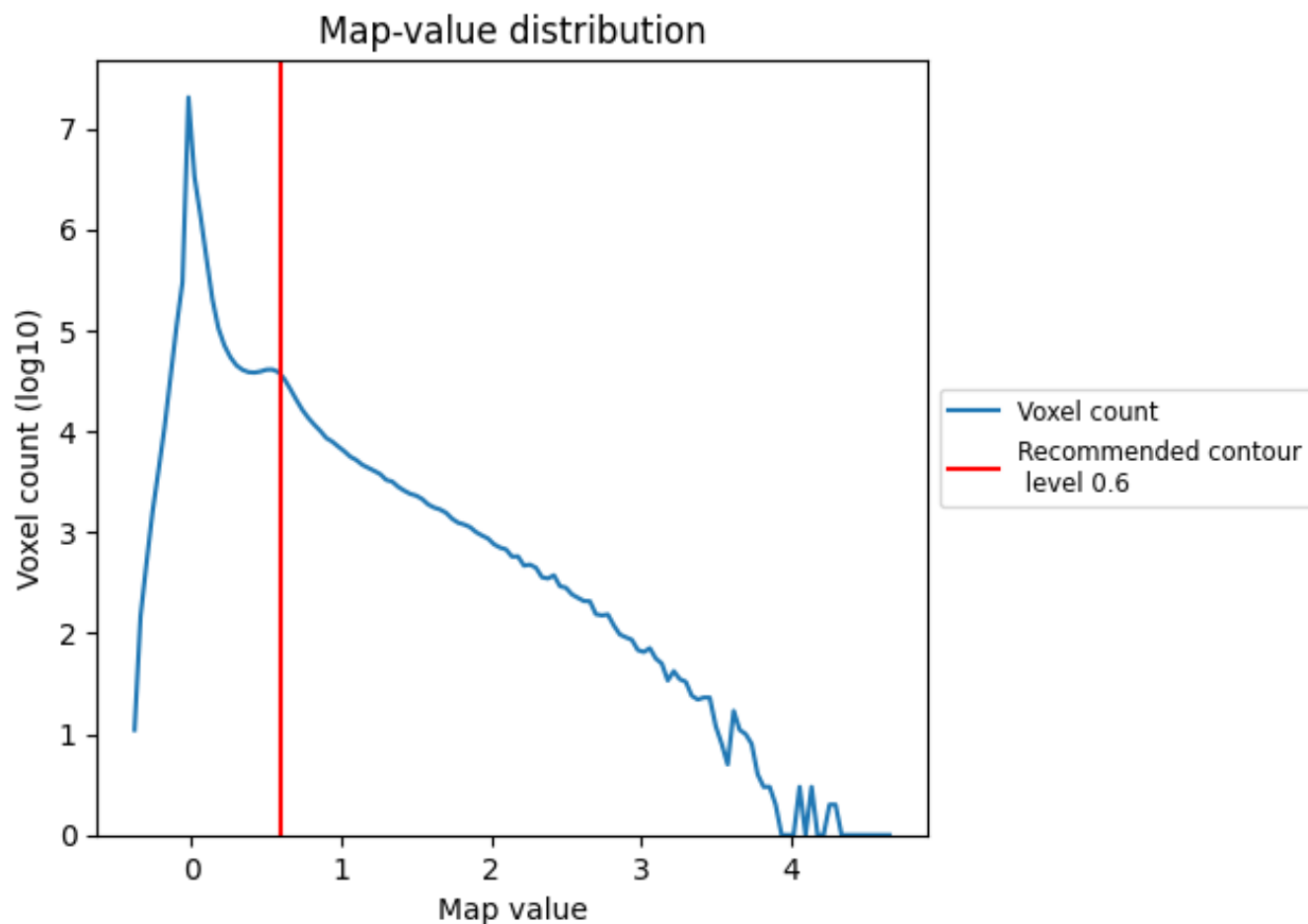
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

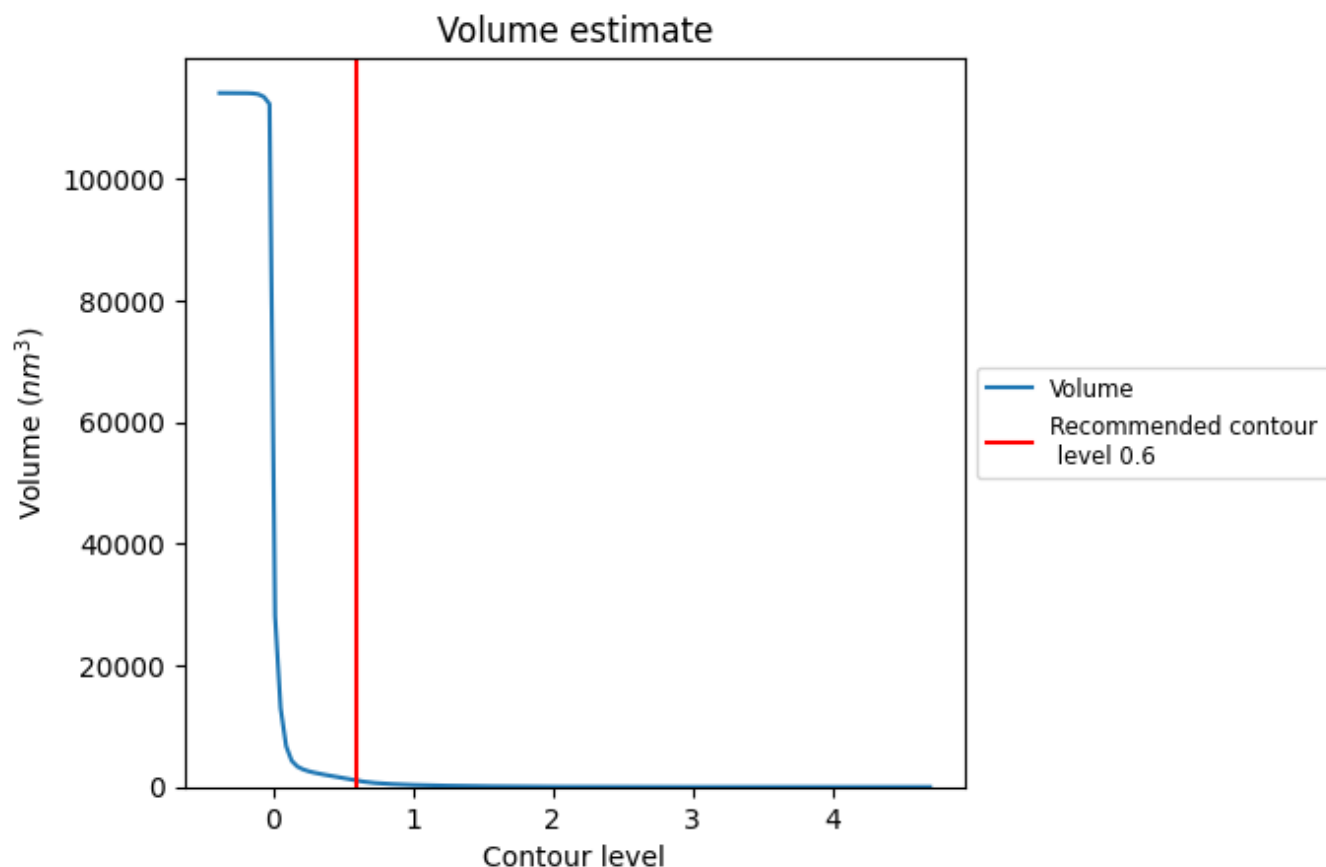
This section contains the results of statistical analysis of the map.

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.

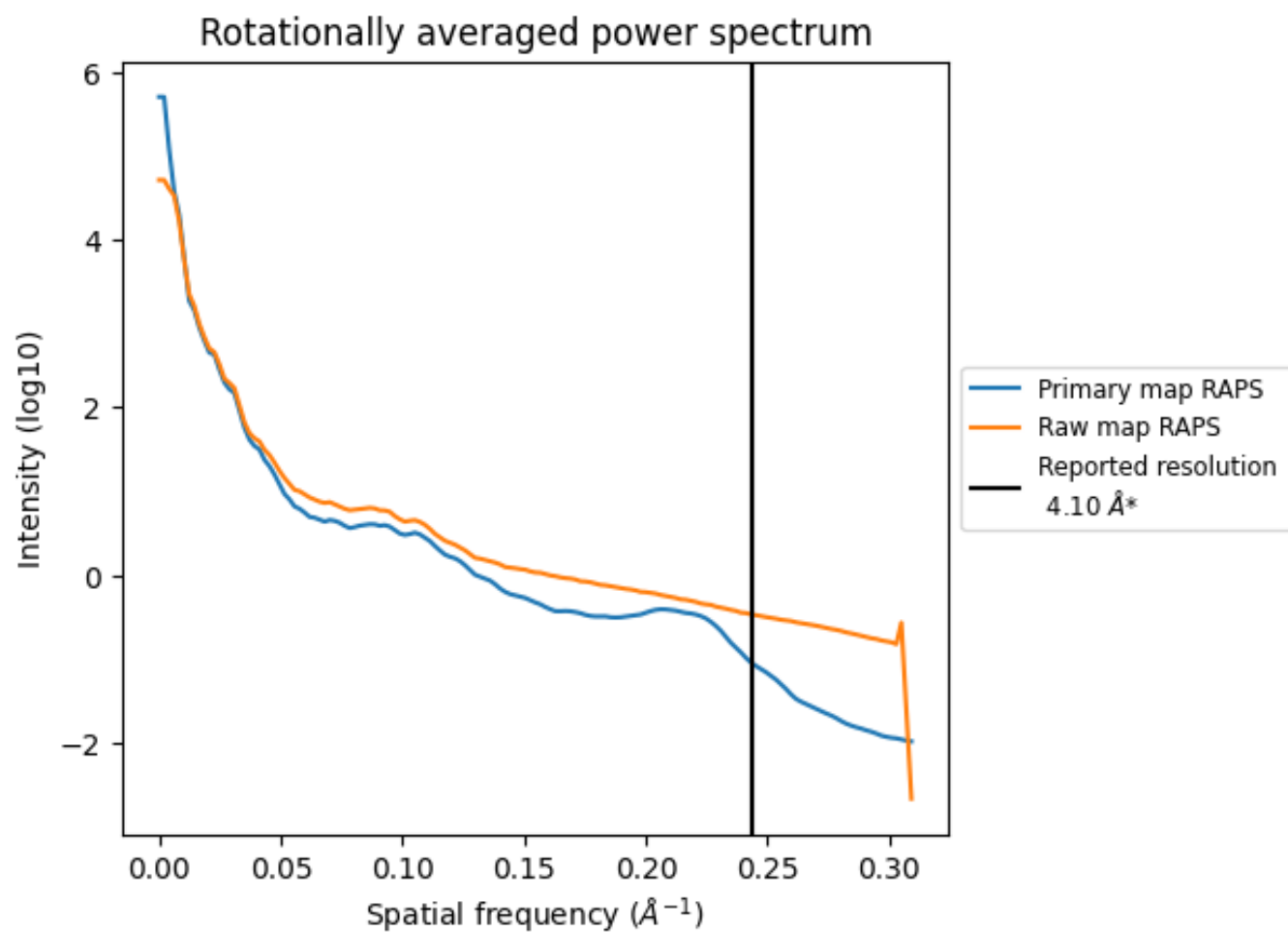
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1052 nm^3 ; this corresponds to an approximate mass of 950 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 ⓘ

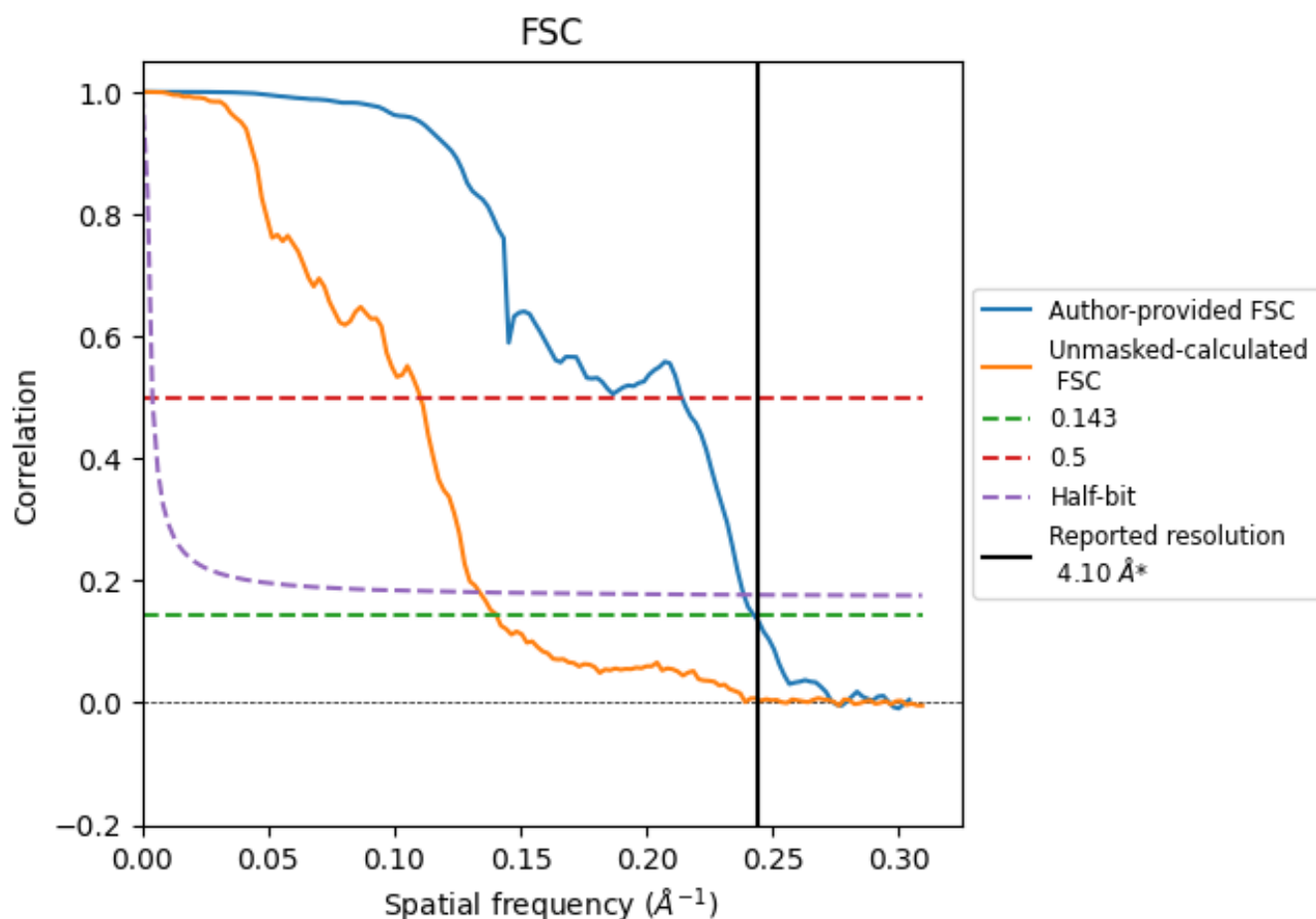


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

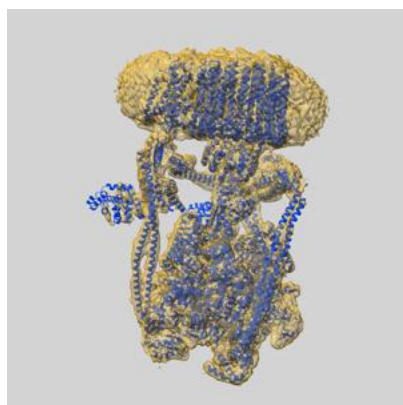
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.12	4.68	4.19
Unmasked-calculated*	7.12	9.07	7.48

*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 7.12 differs from the reported value 4.1 by more than 10 %

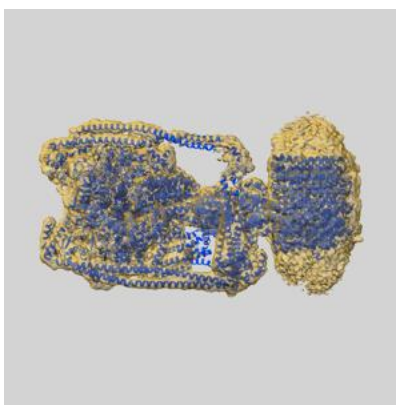
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26829 and PDB model 7UWD. Per-residue inclusion information can be found in section [3](#) on page [8](#).

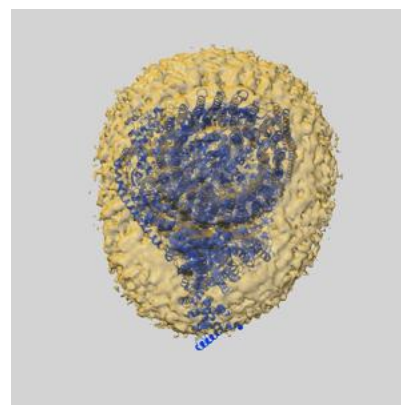
9.1 Map-model overlay [i](#)



X



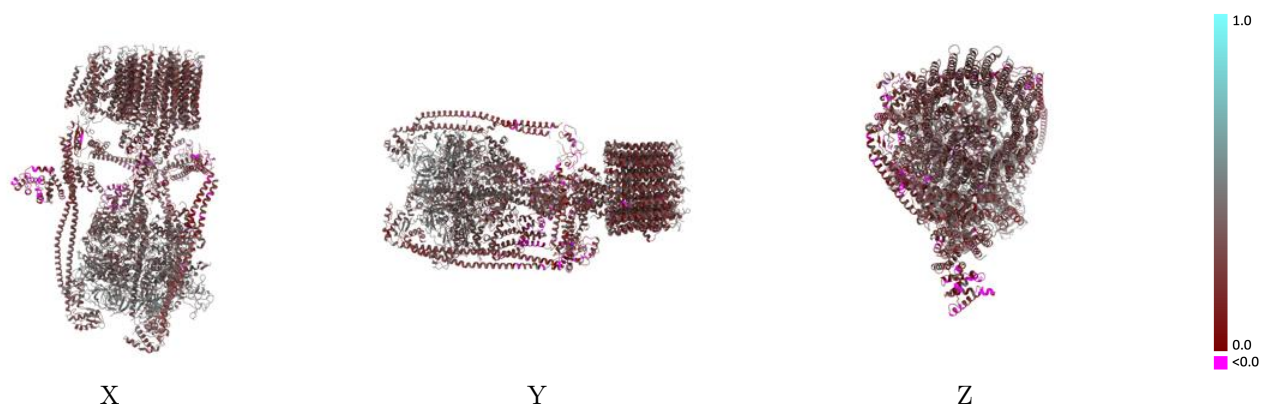
Y



Z

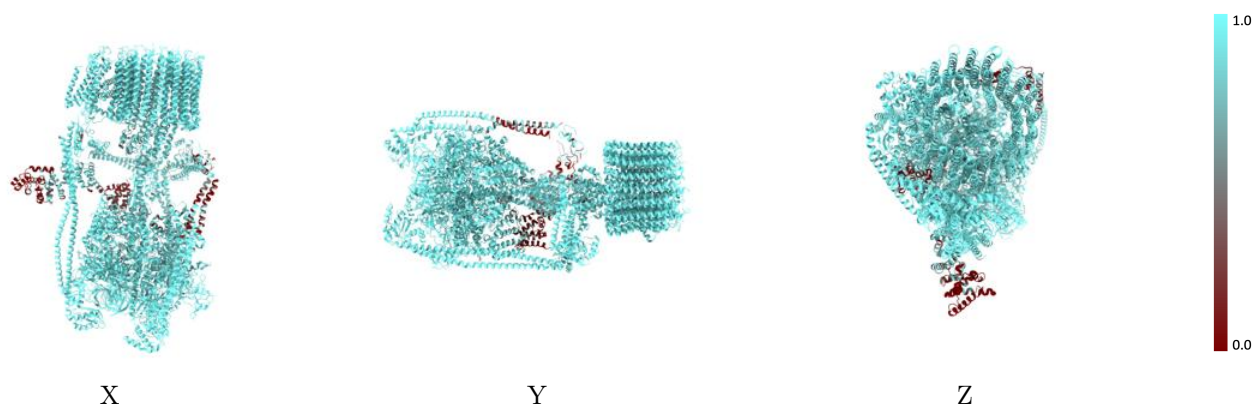
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



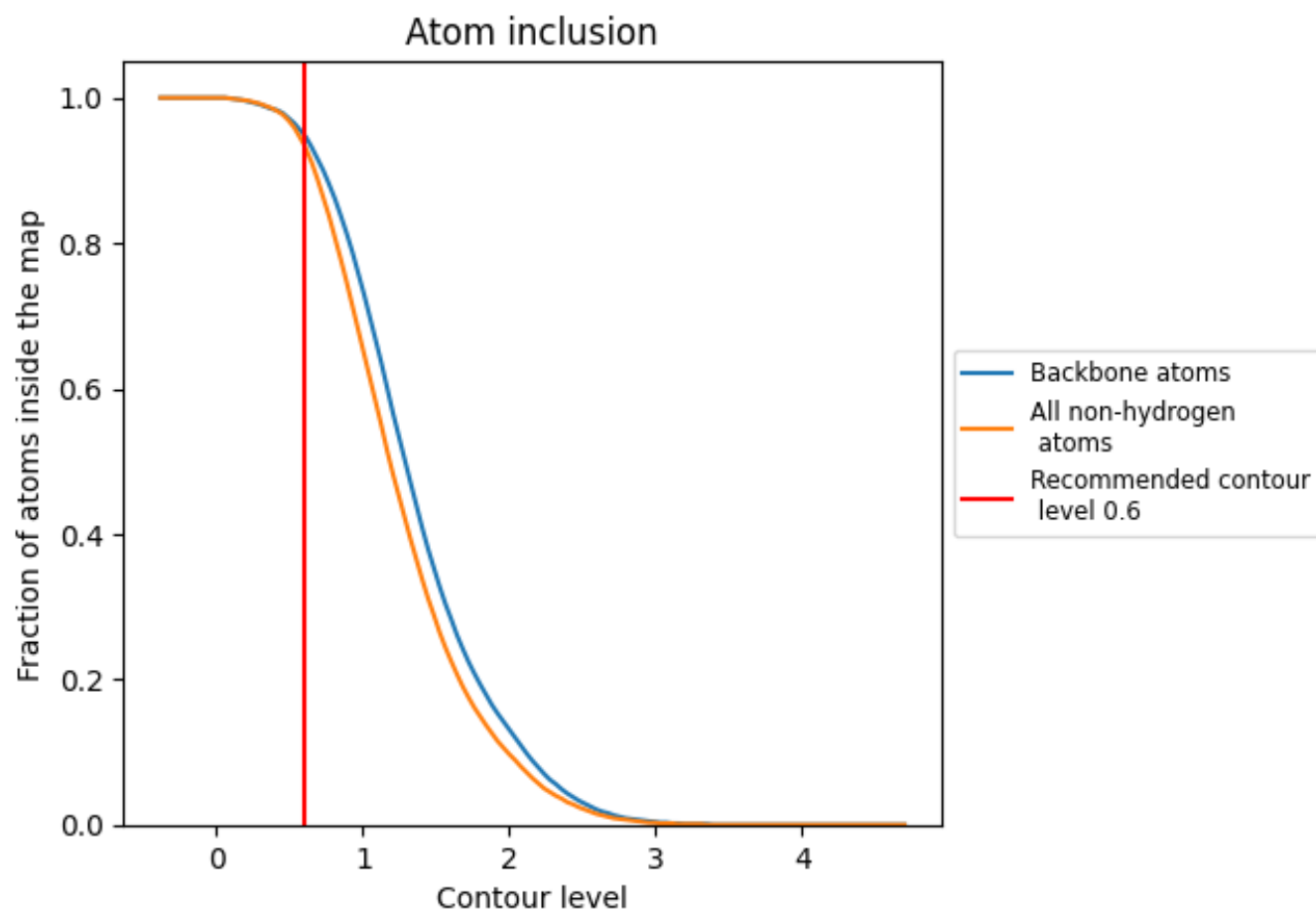
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9350	 0.3430
A	 0.9530	 0.3610
B	 0.9810	 0.4110
C	 0.9790	 0.4140
D	 0.9840	 0.4320
E	 0.9830	 0.4160
F	 0.9680	 0.3960
G	 0.8820	 0.3250
H	 0.7560	 0.2800
I	 0.9660	 0.3090
J	 0.9900	 0.2700
K	 0.9790	 0.3270
L	 0.9900	 0.2950
M	 0.9820	 0.3420
N	 0.9560	 0.2800
O	 0.8570	 0.2230
P	 0.3710	 0.1600
a	 0.9800	 0.2830
b	 0.8870	 0.3110
c	 0.9770	 0.2950
d	 0.8990	 0.2870
e	 0.9890	 0.3460
g	 0.9780	 0.3020
h	 0.9700	 0.3060
i	 0.9760	 0.3110
j	 0.9920	 0.3160
k	 0.9750	 0.3020
l	 0.9730	 0.3210
m	 0.9830	 0.3240
n	 0.9590	 0.3150
o	 0.9550	 0.3100
r	 0.9420	 0.3380

