Full wwPDB EM Validation Report ⓘ

Jan 11, 2024 – 01:59 AM EST

PDB ID	:	7UWB
EMDB ID	:	EMD-26827
Title	:	Citrus V-ATPase State 2, Highest-Resolution Class
Authors	:	Keon, K.A.; Abdelaziz, R.A.; Schulze, W.X.; Schumacher, K.; Rubinstein, J.L.
Deposited on	:	2022-05-03
Resolution	:	3.90 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:

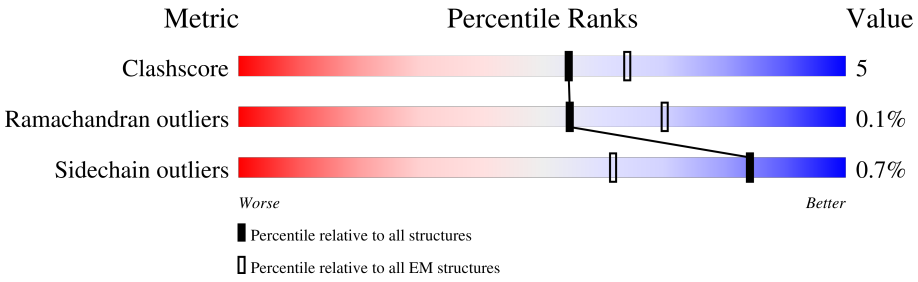
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	81% 14% 5%
1	C	623	84% 13%
1	E	623	81% 16%
2	B	488	76% 18% 6%
2	D	488	79% 17%
2	F	488	82% 13% 5%
3	G	230	17% 80% 8% 11%
3	I	230	78% 11% 10%

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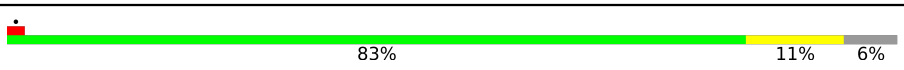
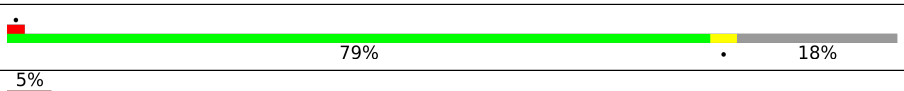
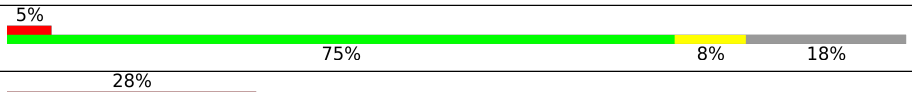
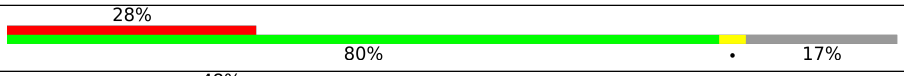
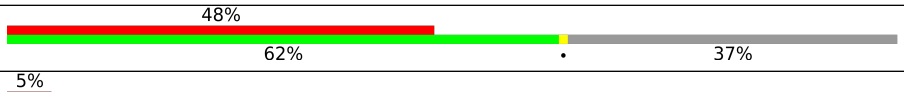
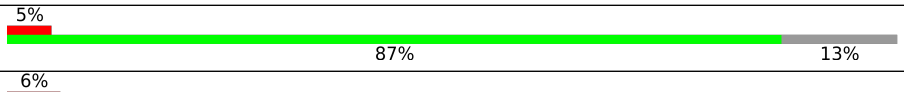
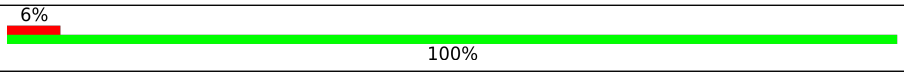
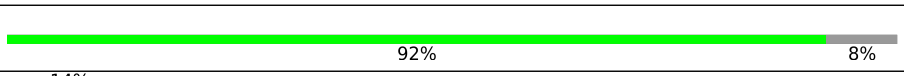
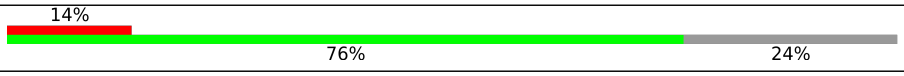
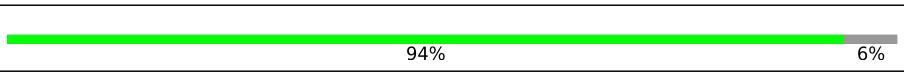
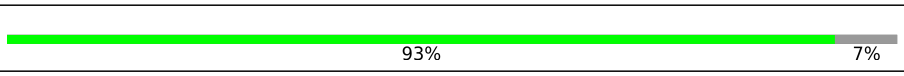
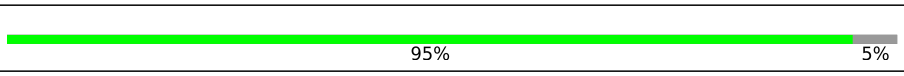
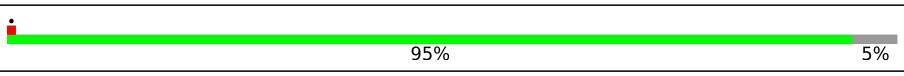
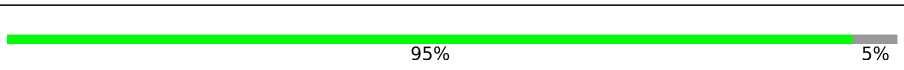
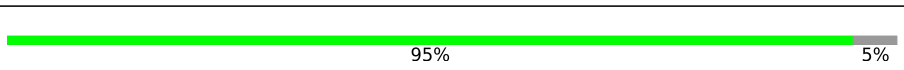
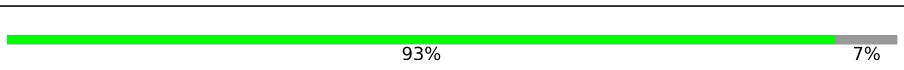
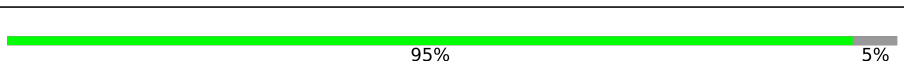
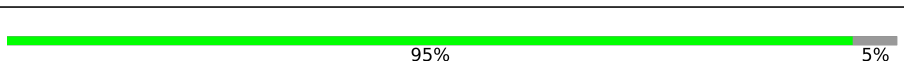
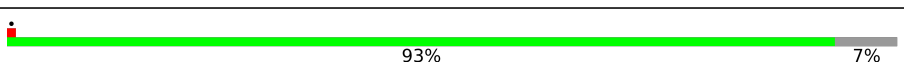
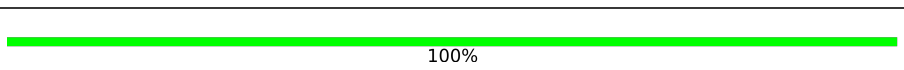
Mol	Chain	Length	Quality of chain
3	K	230	
4	H	110	
4	J	110	
4	L	110	
5	M	259	
6	N	130	
7	O	375	
8	P	452	
9	a	823	
10	b	32	
11	c	182	
12	d	351	
13	e	70	
14	g	164	
14	h	164	
14	i	164	
14	j	164	
14	k	164	
14	l	164	
14	m	164	
14	n	164	
14	o	164	
15	r	24	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 45475 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 catalytic subunit A.

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

- Molecule 2 is a protein called V-type proton ATPase subunit B2.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	97	Total	C	N	O	S	0	0
			555	343	110	101	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	96	Total	C	N	O	S	0	0
			517	316	100	100	1		
4	L	101	Total	C	N	O	S	0	0
			582	357	112	112	1		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	107	Total	C	N	O	0	0
			544	330	107	107		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	285	Total	C	N	O	0	0
			1451	878	285	288		

- Molecule 9 is a protein called V-type proton ATPase subunit a3.

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 V-type proton 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 d2.

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 c.

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.

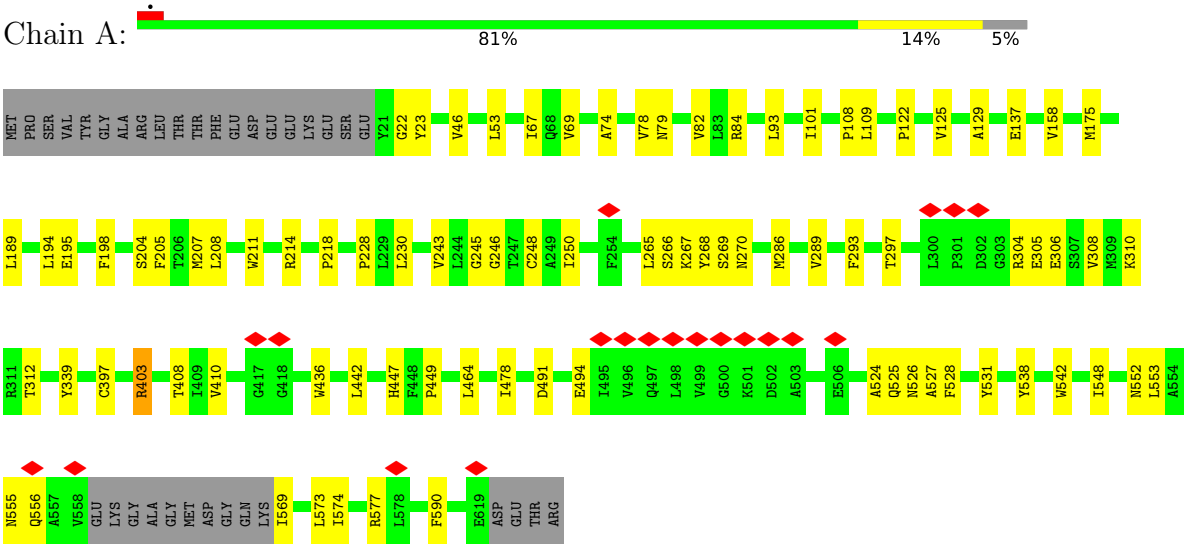
Mol	Chain	Residues	Atoms				AltConf	Trace
15	r	24	Total	C	N	O	0	0
			120	72	24	24		

3 Residue-property plots (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.

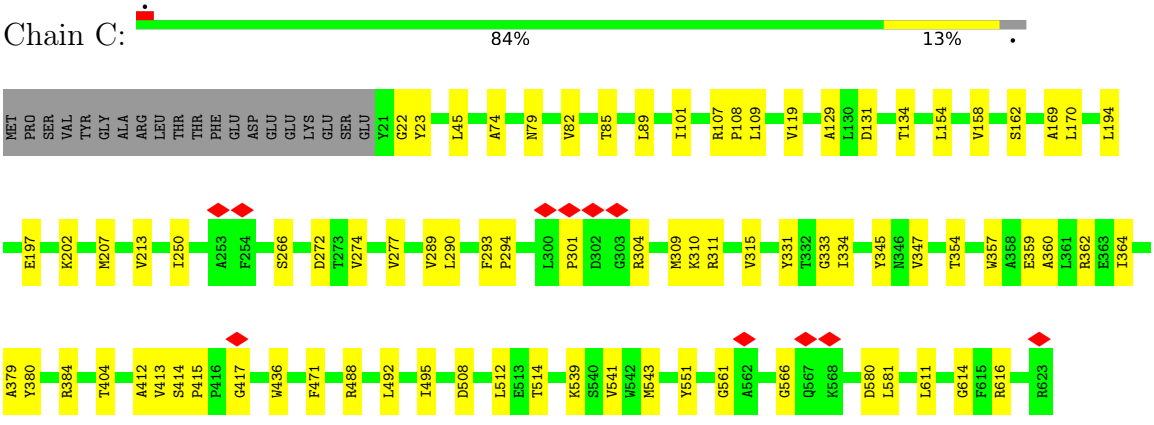
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain A:



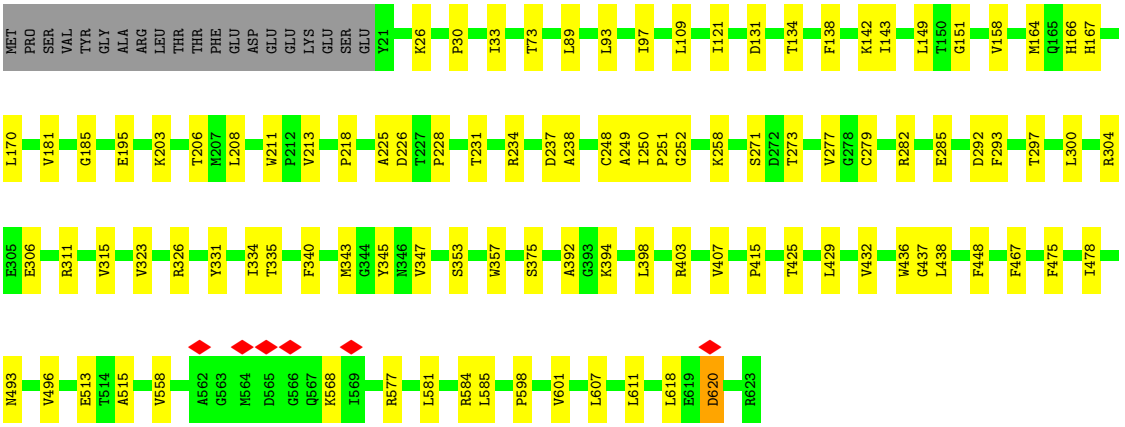
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain C:



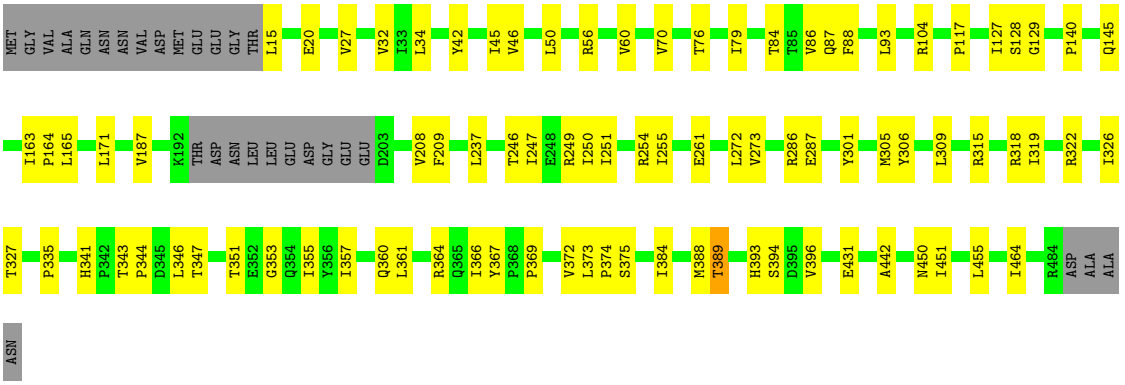
• Molecule 1: V-type proton ATPase catalytic subunit A

Chain E:



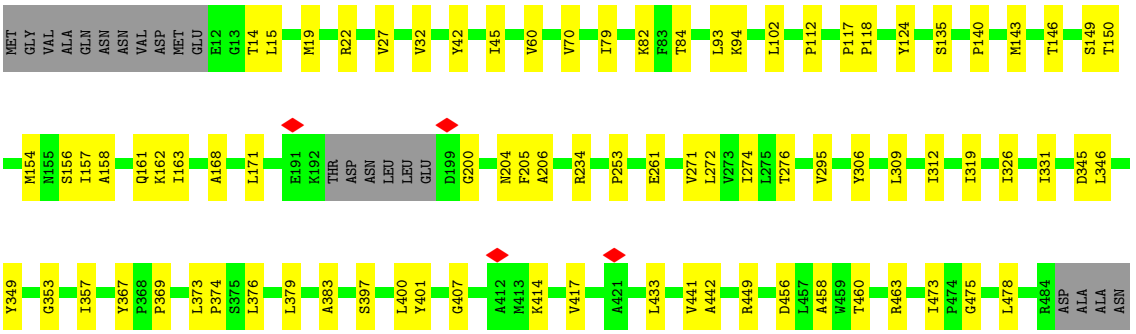
• Molecule 2: V-type proton ATPase subunit B2

Chain B:



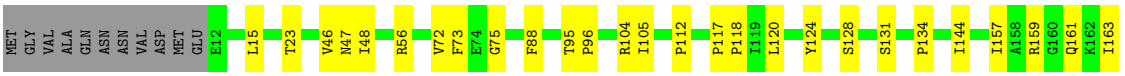
• Molecule 2: V-type proton ATPase subunit B2

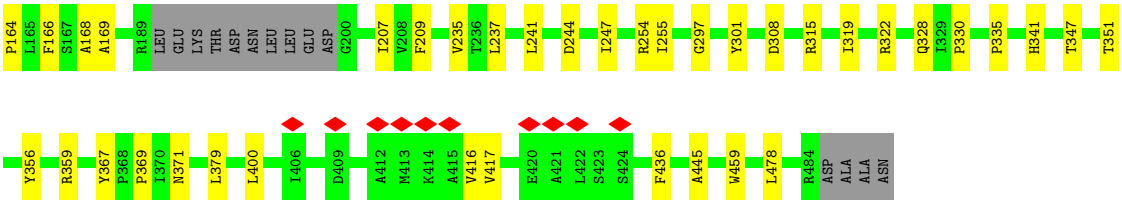
Chain D:



• Molecule 2: V-type proton ATPase subunit B2

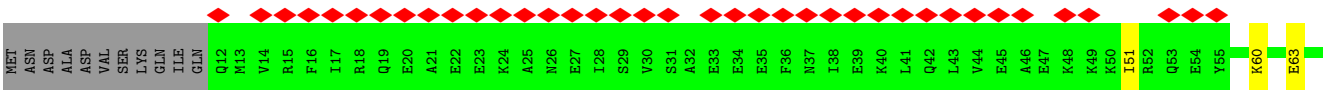
Chain F:

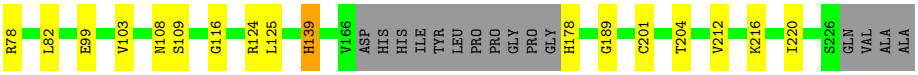




• Molecule 3: V-type proton ATPase subunit E

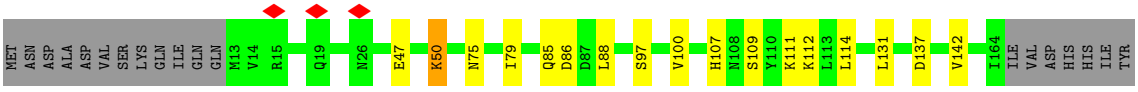
Chain G:

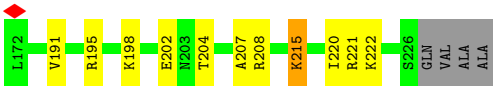




• Molecule 3: V-type proton ATPase subunit E

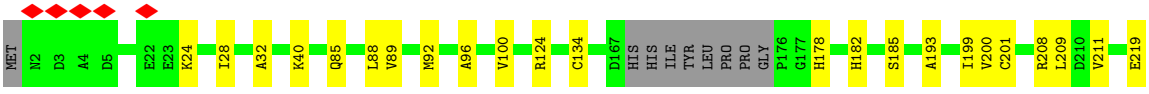
Chain I:





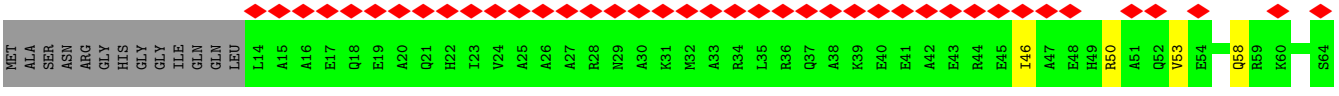
• Molecule 3: V-type proton ATPase subunit E

Chain K:



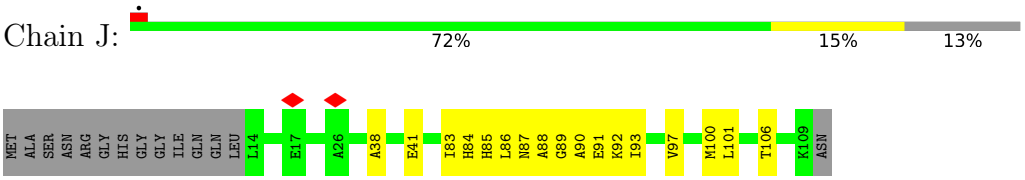
• Molecule 4: V-type proton ATPase subunit G

Chain H:



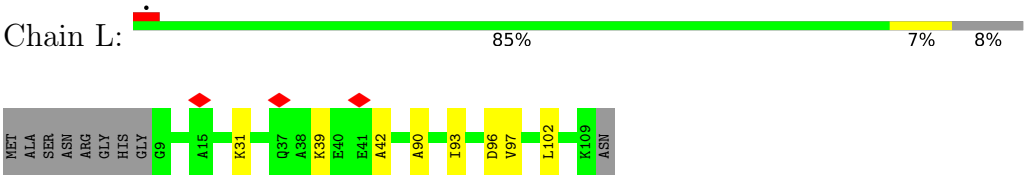
• Molecule 4: V-type proton ATPase subunit G

Chain J:



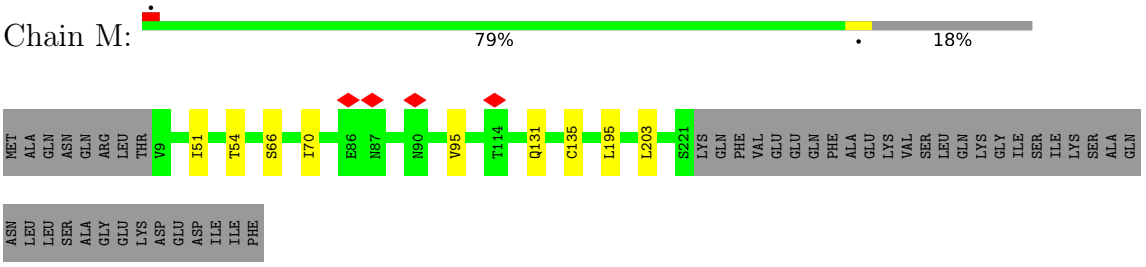
• Molecule 4: V-type proton ATPase subunit G

Chain L:



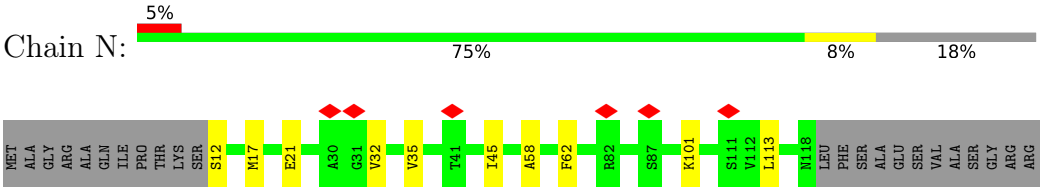
• Molecule 5: V-type proton ATPase subunit D

Chain M:



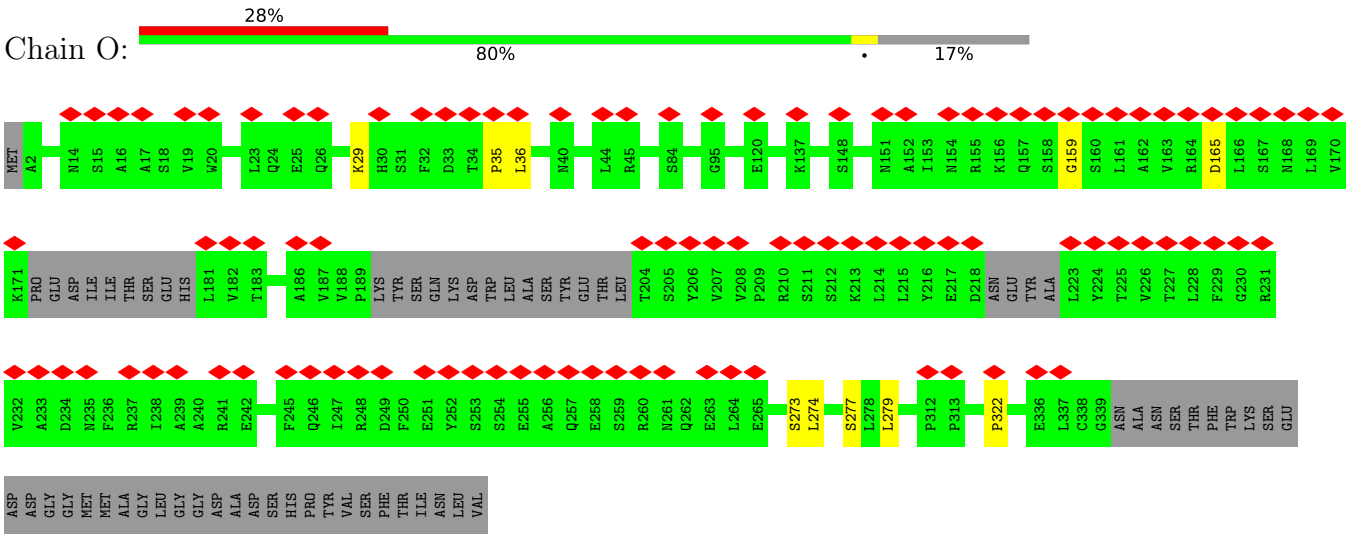
• Molecule 6: V-type proton ATPase subunit F

Chain N:



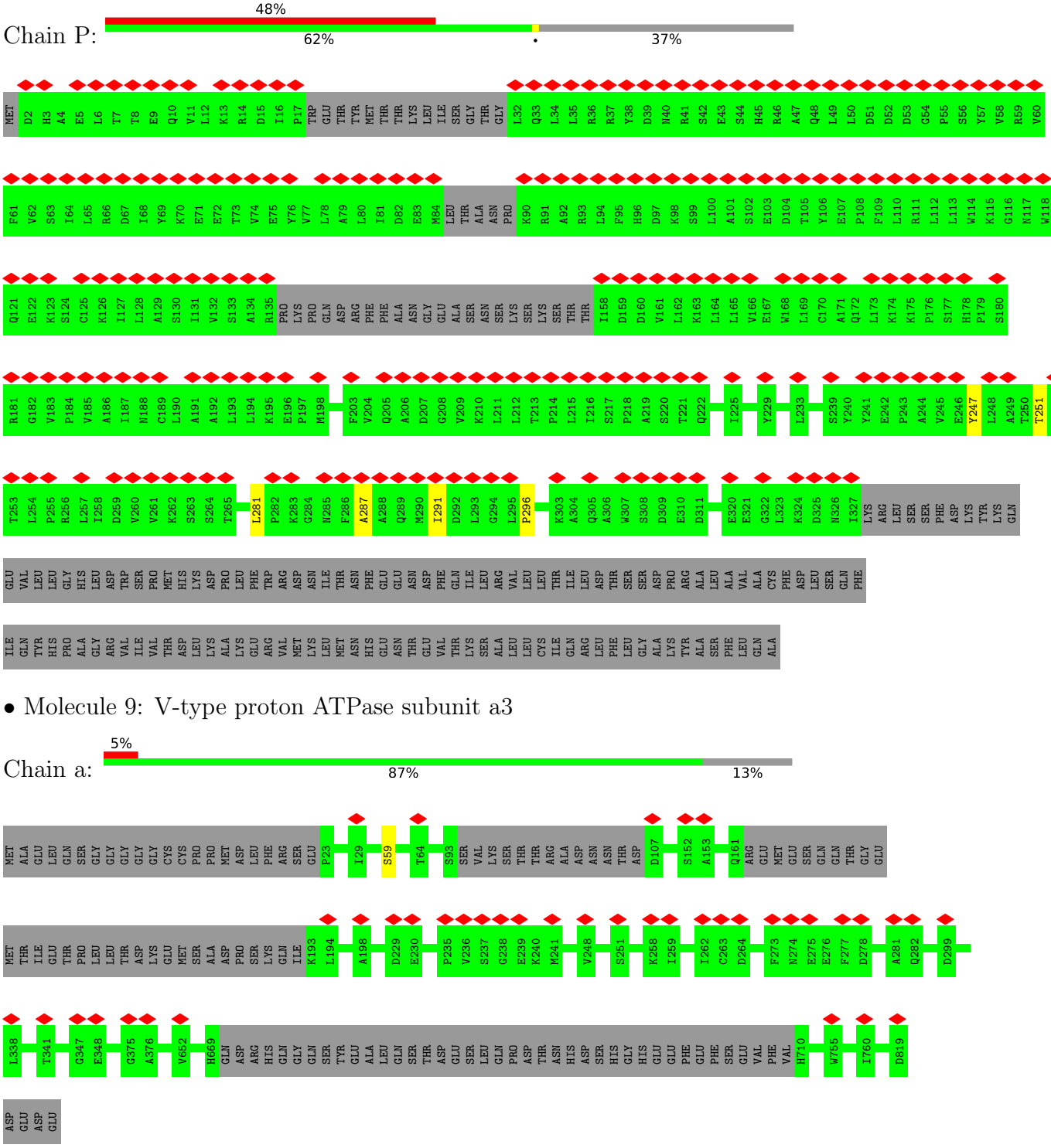
• Molecule 7: V-type proton ATPase subunit C

Chain O:



• Molecule 8: V-type proton ATPase subunit H

Chain P:

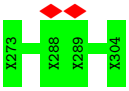


• Molecule 9: V-type proton ATPase subunit a3

Chain a:

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

Chain b:

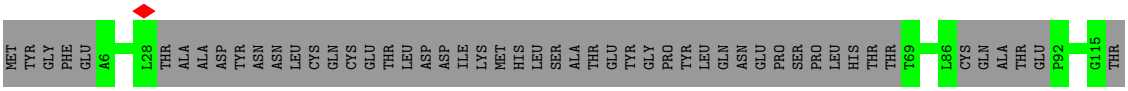


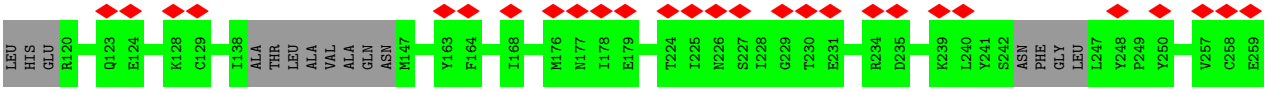
• Molecule 11: V-type proton ATPase subunit c"

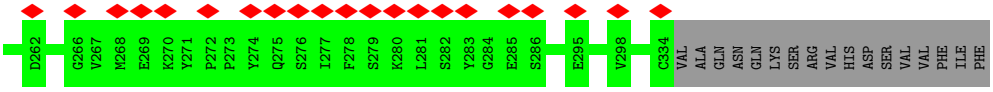
Chain c:

• Molecule 12: V-type proton ATPase subunit d2

Chain d:

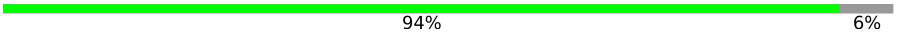


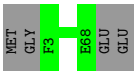




• Molecule 13: V-type proton ATPase subunit e1

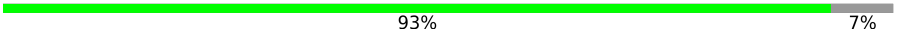
Chain e:

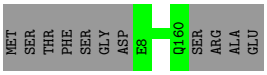




• Molecule 14: V-type proton ATPase subunit c

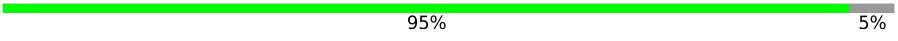
Chain g:





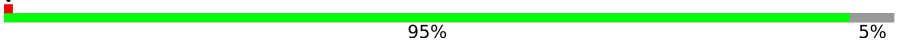
• Molecule 14: V-type proton ATPase subunit c

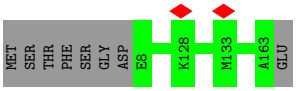
Chain h:



• Molecule 14: V-type proton ATPase subunit c

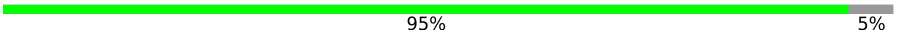
Chain i:





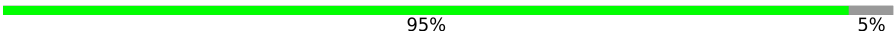
• Molecule 14: V-type proton ATPase subunit c

Chain j:



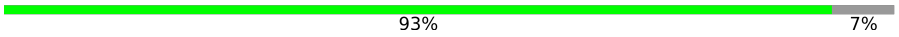
• Molecule 14: V-type proton ATPase subunit c

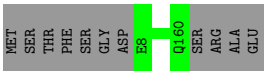
Chain k:



• Molecule 14: V-type proton ATPase subunit c

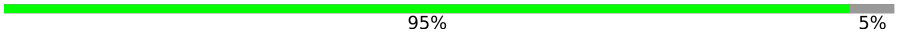
Chain l:





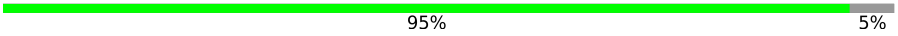
• Molecule 14: V-type proton ATPase subunit c

Chain m:



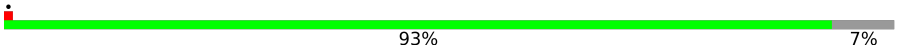
• Molecule 14: V-type proton ATPase subunit c

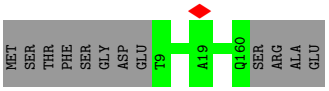
Chain n:



• Molecule 14: V-type proton ATPase subunit c

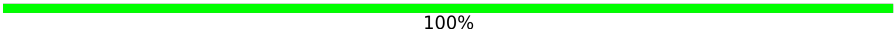
Chain o:





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

Chain r:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104874	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 ($e^-/Å^2$)	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	5.696	Depositor
Minimum map value	-0.463	Depositor
Average map value	0.126	Depositor
Map value standard deviation	0.290	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	226.38, 226.38, 323.4	wwPDB
Map dimensions	140, 140, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.617, 1.617, 1.617	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/4023	0.46	0/5546
1	C	0.34	0/4244	0.57	0/5833
1	E	0.29	0/4350	0.50	1/5958 (0.0%)
2	B	0.28	0/3207	0.49	0/4403
2	D	0.31	0/3277	0.51	0/4494
2	F	0.28	0/3257	0.48	0/4468
3	G	0.28	0/1283	0.47	0/1764
3	I	0.25	0/1374	0.45	0/1884
3	K	0.25	0/1377	0.45	0/1895
4	H	0.23	0/558	0.40	0/772
4	J	0.23	0/517	0.39	0/716
4	L	0.25	0/586	0.35	0/812
5	M	0.24	0/1099	0.40	0/1530
6	N	0.23	0/548	0.47	0/767
7	O	0.27	0/1578	0.42	0/2203
8	P	0.23	0/1460	0.40	0/2043
9	a	0.23	0/3613	0.38	0/5044
11	c	0.23	0/837	0.36	0/1164
12	d	0.23	0/1345	0.41	0/1870
13	e	0.23	0/363	0.33	0/506
14	g	0.25	0/769	0.38	0/1064
14	h	0.24	0/767	0.39	0/1062
14	i	0.25	0/785	0.40	0/1086
14	j	0.25	0/783	0.38	0/1084
14	k	0.25	0/774	0.39	0/1071
14	l	0.24	0/756	0.38	0/1047
14	m	0.25	0/774	0.38	0/1071
14	n	0.24	0/766	0.38	0/1061
14	o	0.24	0/736	0.37	0/1015
All	All	0.27	0/45806	0.45	1/63233 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	620	ASP	O-C-N	-5.69	113.60	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	620	ASP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3935	0	3531	49	0
1	C	4146	0	3766	47	0
1	E	4252	0	3975	63	0
2	B	3147	0	2942	55	0
2	D	3213	0	3010	53	0
2	F	3194	0	2985	44	0
3	G	1273	0	1039	16	0
3	I	1357	0	1177	19	0
3	K	1364	0	1113	20	0
4	H	555	0	400	7	0
4	J	517	0	343	13	0
4	L	582	0	411	7	0
5	M	1096	0	579	6	0
6	N	544	0	279	4	0
7	O	1571	0	752	5	0
8	P	1451	0	718	3	0
9	a	3590	0	1768	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	b	160	0	34	0	0
11	c	833	0	446	0	0
12	d	1344	0	632	0	0
13	e	358	0	170	0	0
14	g	764	0	446	0	0
14	h	763	0	432	0	0
14	i	780	0	460	0	0
14	j	777	0	448	0	0
14	k	769	0	439	0	0
14	l	752	0	425	0	0
14	m	769	0	439	0	0
14	n	762	0	429	0	0
14	o	737	0	393	0	0
15	r	120	0	26	0	0
All	All	45475	0	34007	380	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 5.

All (380) 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:B:357:ILE:HG23	2:B:369:PRO:HG2	1.55	0.89
1:C:488:ARG:HE	1:C:492:LEU:HD23	1.39	0.85
3:G:139:HIS:CE1	3:G:178:HIS:CE1	2.72	0.77
1:E:206:THR:HG22	1:E:208:LEU:H	1.48	0.76
3:G:139:HIS:HE1	3:G:178:HIS:CE1	2.05	0.73
1:E:277:VAL:HG23	1:E:315:VAL:HB	1.69	0.72
2:D:157:ILE:HG12	2:D:163:ILE:HG13	1.70	0.71
2:F:367:TYR:O	2:F:369:PRO:HD3	1.91	0.71
1:A:228:PRO:HB3	1:A:464:LEU:HD21	1.71	0.71
1:E:213:VAL:HG12	1:E:331:TYR:HB3	1.72	0.71
1:A:122:PRO:HG2	1:A:125:VAL:HB	1.72	0.71
1:C:492:LEU:HD11	1:C:512:LEU:HD21	1.72	0.70
2:B:45:ILE:HG13	2:B:93:LEU:HG	1.74	0.70
1:E:252:GLY:HA3	1:E:258:LYS:HD3	1.72	0.70
2:B:306:TYR:HA	2:B:346:LEU:HD21	1.73	0.69
1:E:282:ARG:NH1	1:E:285:GLU:OE2	2.26	0.68
2:D:94:LYS:HB3	2:D:124:TYR:HB3	1.74	0.68
2:B:287:GLU:HA	1:C:379:ALA:HB1	1.77	0.67
2:F:459:TRP:HE1	2:F:478:LEU:HB2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:281:LEU:HA	8:P:287:ALA:HB2	1.77	0.67
1:C:580:ASP:OD1	1:C:581:LEU:N	2.28	0.66
2:D:19:MET:SD	3:G:124:ARG:NH2	2.68	0.66
3:I:208:ARG:NH2	4:J:106:THR:O	2.28	0.66
2:B:50:LEU:HD11	2:B:56:ARG:HE	1.61	0.65
1:A:553:LEU:HD13	1:A:556:GLN:HE22	1.58	0.65
2:B:128:SER:HB3	2:B:254:ARG:HD3	1.79	0.65
2:D:276:THR:HG23	2:D:331:ILE:HD11	1.78	0.65
4:J:86:LEU:O	4:J:90:ALA:N	2.30	0.64
4:J:85:HIS:O	4:J:89:GLY:N	2.29	0.64
1:A:248:CYS:HB2	1:A:410:VAL:HA	1.80	0.64
1:E:93:LEU:HA	1:E:97:ILE:HD11	1.80	0.63
4:H:79:THR:O	4:H:83:ILE:HG12	1.98	0.63
4:J:89:GLY:O	4:J:93:ILE:N	2.30	0.63
7:O:159:GLY:HA2	7:O:165:ASP:HA	1.80	0.63
2:D:161:GLN:HE22	2:D:379:LEU:HB2	1.64	0.63
1:E:577:ARG:HD2	1:E:618:LEU:HD22	1.81	0.63
2:F:46:VAL:HG12	2:F:88:PHE:HA	1.81	0.63
2:B:140:PRO:HA	2:B:318:ARG:HD3	1.81	0.62
1:C:266:SER:O	1:C:311:ARG:NH1	2.32	0.62
1:E:167:HIS:H	1:E:343:MET:HE3	1.65	0.62
1:E:392:ALA:HA	1:E:407:VAL:HG13	1.82	0.62
1:E:429:LEU:HA	1:E:432:VAL:HG12	1.81	0.62
2:D:140:PRO:HG2	2:D:379:LEU:HG	1.81	0.62
3:K:40:LYS:NZ	4:L:39:LYS:O	2.33	0.62
1:E:279:CYS:HB2	1:E:326:ARG:HG3	1.82	0.61
3:K:219:GLU:O	3:K:223:GLN:HG2	2.00	0.61
1:A:22:GLY:O	1:A:82:VAL:N	2.33	0.61
3:G:124:ARG:NH1	3:G:201:CYS:SG	2.73	0.61
3:I:107:HIS:O	3:I:111:LYS:HD2	2.00	0.61
1:C:23:TYR:HB2	1:C:79:ASN:HA	1.81	0.61
1:E:398:LEU:O	1:E:403:ARG:NH1	2.31	0.61
4:J:83:ILE:O	4:J:87:ASN:N	2.33	0.61
2:F:328:GLN:HG3	2:F:330:PRO:HD3	1.82	0.60
2:B:15:LEU:O	3:K:208:ARG:NH2	2.33	0.60
2:F:104:ARG:NH1	2:F:117:PRO:O	2.25	0.60
4:J:84:HIS:O	4:J:88:ALA:N	2.24	0.60
1:C:213:VAL:HG22	1:C:331:TYR:HB3	1.82	0.60
4:J:88:ALA:O	4:J:92:LYS:N	2.30	0.60
6:N:58:ALA:O	6:N:62:PHE:N	2.35	0.60
2:D:400:LEU:HD11	2:D:458:ALA:HB1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:273:SER:O	7:O:277:SER:N	2.30	0.60
1:C:290:LEU:HD21	2:D:135:SER:HA	1.84	0.59
2:D:206:ALA:HA	2:D:234:ARG:HG2	1.83	0.59
1:E:375:SER:H	5:M:195:LEU:HD11	1.66	0.59
2:F:254:ARG:NH1	2:F:308:ASP:OD1	2.34	0.59
2:B:127:ILE:HG21	2:B:255:ILE:HD13	1.84	0.59
1:A:266:SER:HB2	1:A:308:VAL:HG21	1.84	0.59
1:E:300:LEU:HD21	1:E:304:ARG:HB2	1.85	0.59
1:A:449:PRO:HG3	1:A:524:ALA:HA	1.83	0.58
2:D:442:ALA:O	2:D:449:ARG:NH1	2.36	0.58
1:E:143:ILE:HG21	1:E:149:LEU:HD23	1.85	0.58
2:B:46:VAL:HG21	2:B:86:VAL:HG12	1.86	0.58
2:B:127:ILE:HB	2:B:254:ARG:HG2	1.85	0.58
2:B:384:ILE:HG21	2:B:394:SER:HB3	1.85	0.58
1:A:46:VAL:HG23	1:A:84:ARG:HA	1.86	0.58
3:G:108:ASN:OD1	3:G:109:SER:N	2.36	0.58
3:I:191:VAL:HG12	3:I:202:GLU:HA	1.86	0.58
1:C:561:GLY:HA2	1:C:566:GLY:HA3	1.86	0.58
1:C:277:VAL:HG11	1:C:333:GLY:HA3	1.86	0.57
1:A:23:TYR:HB2	1:A:79:ASN:HA	1.86	0.57
2:B:79:ILE:HG23	2:B:84:THR:HG21	1.87	0.57
2:D:168:ALA:H	2:D:171:LEU:HD12	1.68	0.57
3:I:114:LEU:HD21	3:I:142:VAL:HG22	1.86	0.57
2:B:384:ILE:HG23	2:B:393:HIS:HB3	1.85	0.57
1:C:250:ILE:HG22	1:C:436:TRP:HB2	1.87	0.56
1:A:195:GLU:HA	1:A:204:SER:HA	1.87	0.56
2:B:46:VAL:HG23	2:B:88:PHE:HA	1.87	0.56
2:D:158:ALA:HB2	2:D:383:ALA:HB2	1.86	0.56
3:K:124:ARG:HH11	3:K:201:CYS:HB3	1.68	0.56
2:B:306:TYR:HB2	2:B:346:LEU:HD11	1.87	0.56
2:D:102:LEU:O	3:G:78:ARG:NH1	2.39	0.56
1:E:581:LEU:HD13	1:E:611:LEU:HA	1.86	0.56
2:D:143:MET:HB2	2:D:383:ALA:HB1	1.88	0.55
2:F:169:ALA:O	2:F:359:ARG:NH1	2.38	0.55
2:B:367:TYR:O	2:B:369:PRO:HD3	2.07	0.55
1:A:101:ILE:HG23	1:A:109:LEU:HB2	1.88	0.55
1:A:526:ASN:O	1:A:528:PHE:N	2.40	0.55
1:E:598:PRO:HA	1:E:601:VAL:HG12	1.89	0.55
2:D:253:PRO:HB2	2:D:312:ILE:HD11	1.88	0.54
2:D:295:VAL:HG22	5:M:203:LEU:HD21	1.88	0.54
1:C:581:LEU:HD13	1:C:611:LEU:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:276:THR:HA	2:D:331:ILE:HG12	1.87	0.54
4:H:53:VAL:O	4:H:58:GLN:NE2	2.39	0.54
1:A:306:GLU:HG2	1:A:310:LYS:HD3	1.90	0.54
2:F:56:ARG:NH2	2:F:75:GLY:O	2.41	0.54
2:F:128:SER:HA	2:F:315:ARG:NH1	2.23	0.54
1:A:304:ARG:CZ	1:A:305:GLU:H	2.19	0.54
2:F:297:GLY:N	2:F:301:TYR:O	2.39	0.54
4:H:46:ILE:O	4:H:50:ARG:HG2	2.07	0.54
3:G:116:GLY:HA3	4:H:108:VAL:HG21	1.90	0.54
1:E:26:LYS:HB3	1:E:33:ILE:HB	1.88	0.54
1:A:250:ILE:HD11	1:A:436:TRP:HE3	1.72	0.54
1:C:301:PRO:HG2	1:C:304:ARG:HB2	1.89	0.53
2:B:286:ARG:HE	2:B:301:TYR:HA	1.71	0.53
3:K:89:VAL:O	3:K:92:MET:HG3	2.07	0.53
1:A:478:ILE:HG23	1:A:548:ILE:HG13	1.89	0.53
2:B:27:VAL:HG22	2:B:32:VAL:HG12	1.90	0.53
3:G:125:LEU:HD11	3:G:201:CYS:HB2	1.90	0.53
2:B:388:MET:HG2	2:B:389:THR:HG22	1.91	0.53
1:E:109:LEU:HD23	2:F:134:PRO:HD2	1.90	0.53
1:C:354:THR:OG1	1:C:412:ALA:O	2.27	0.53
2:F:207:ILE:HB	2:F:235:VAL:HG22	1.90	0.53
2:F:209:PHE:HB3	2:F:237:LEU:HD23	1.91	0.52
1:E:151:GLY:HA2	1:E:170:LEU:HD23	1.91	0.52
2:D:309:LEU:HA	2:D:312:ILE:HG22	1.92	0.52
6:N:17:MET:HA	6:N:45:ILE:HA	1.92	0.52
1:A:289:VAL:HG22	1:A:293:PHE:CE2	2.45	0.52
2:D:171:LEU:HD13	2:D:357:ILE:HG22	1.92	0.52
1:E:225:ALA:HA	1:E:394:LYS:HD3	1.92	0.52
2:F:117:PRO:HB2	3:I:86:ASP:OD2	2.10	0.52
4:J:97:VAL:O	4:J:101:LEU:HD23	2.09	0.52
2:D:22:ARG:NH2	2:D:82:LYS:O	2.41	0.51
2:F:356:TYR:HD2	2:F:371:ASN:HB3	1.76	0.51
3:I:220:ILE:HG12	4:J:100:MET:HG2	1.92	0.51
1:A:108:PRO:HD3	1:A:129:ALA:HA	1.93	0.51
1:A:228:PRO:HA	1:A:243:VAL:HA	1.92	0.51
1:A:265:LEU:HA	1:A:269:SER:HB3	1.92	0.51
1:E:251:PRO:HD2	1:E:437:GLY:HA2	1.91	0.51
2:B:164:PRO:HG3	2:B:351:THR:HG21	1.92	0.51
1:C:154:LEU:HD23	1:C:169:ALA:HB2	1.92	0.51
8:P:291:ILE:HA	8:P:296:PRO:HD3	1.92	0.51
4:J:85:HIS:HA	4:J:88:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ILE:HA	2:B:250:ILE:HD13	1.92	0.51
1:E:248:CYS:SG	1:E:249:ALA:N	2.83	0.51
2:D:161:GLN:HG3	2:D:162:LYS:N	2.25	0.50
2:F:112:PRO:HG2	2:F:118:PRO:HA	1.91	0.50
2:D:15:LEU:HD23	2:D:15:LEU:H	1.75	0.50
1:A:286:MET:HA	1:A:289:VAL:HG12	1.92	0.50
1:E:231:THR:N	1:E:237:ASP:OD2	2.44	0.50
1:E:213:VAL:HA	1:E:335:THR:HG21	1.94	0.50
2:F:23:THR:HG22	3:I:198:LYS:HB3	1.93	0.50
7:O:274:LEU:O	7:O:279:LEU:N	2.38	0.50
2:B:360:GLN:HG2	2:B:361:LEU:HD12	1.94	0.50
1:C:89:LEU:HD23	1:C:213:VAL:HG11	1.95	0.49
4:L:96:ASP:OD1	4:L:97:VAL:N	2.45	0.49
2:D:161:GLN:NE2	2:D:379:LEU:HB2	2.28	0.49
2:F:241:LEU:N	2:F:244:ASP:OD2	2.46	0.49
3:K:208:ARG:HA	3:K:211:VAL:HG12	1.93	0.49
2:B:208:VAL:HB	2:B:273:VAL:HG12	1.94	0.49
2:B:343:THR:HB	2:B:344:PRO:HD3	1.93	0.49
1:C:170:LEU:HD21	1:C:194:LEU:HD22	1.93	0.49
3:I:137:ASP:OD1	3:I:137:ASP:N	2.44	0.49
1:C:108:PRO:HD3	1:C:129:ALA:HA	1.93	0.49
1:C:289:VAL:HG13	1:C:293:PHE:CD2	2.47	0.49
2:B:165:LEU:HD12	2:B:355:ILE:HB	1.95	0.49
2:F:459:TRP:HE1	2:F:478:LEU:HD13	1.77	0.49
2:D:45:ILE:HD11	2:D:93:LEU:HG	1.95	0.49
1:E:584:ARG:HH12	1:E:607:LEU:HA	1.76	0.49
2:B:246:THR:O	2:B:250:ILE:HD12	2.12	0.48
1:C:508:ASP:O	1:C:512:LEU:HD23	2.13	0.48
2:B:20:GLU:HA	2:B:87:GLN:HA	1.94	0.48
2:B:431:GLU:OE2	2:B:464:ILE:HG21	2.13	0.48
2:D:60:VAL:HG22	2:D:70:VAL:HG22	1.95	0.48
2:D:27:VAL:HG22	2:D:32:VAL:HG12	1.95	0.48
2:F:400:LEU:HD23	2:F:436:PHE:HE1	1.78	0.48
3:K:100:VAL:HG11	3:K:209:LEU:HD12	1.94	0.48
1:C:131:ASP:OD1	1:C:134:THR:N	2.44	0.48
2:D:306:TYR:HD2	2:D:346:LEU:HD22	1.79	0.48
2:F:73:PHE:HA	2:F:247:ILE:HG21	1.96	0.48
3:K:24:LYS:O	3:K:28:ILE:HD12	2.14	0.48
2:F:416:VAL:HG23	2:F:417:VAL:HG23	1.95	0.48
3:G:216:LYS:O	3:G:220:ILE:HG12	2.14	0.48
1:E:357:TRP:CG	1:E:357:TRP:O	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:LEU:HD23	1:E:300:LEU:H	1.79	0.48
3:I:109:SER:HA	3:I:112:LYS:NZ	2.28	0.48
1:A:137:GLU:O	1:A:158:VAL:HG13	2.14	0.47
2:B:104:ARG:NH1	2:B:117:PRO:O	2.40	0.47
1:E:558:VAL:HG22	1:E:568:LYS:HA	1.95	0.47
2:F:164:PRO:HD3	2:F:351:THR:OG1	2.14	0.47
1:C:380:TYR:O	1:C:384:ARG:HG2	2.14	0.47
2:D:112:PRO:HG3	2:D:118:PRO:HA	1.95	0.47
2:D:414:LYS:HA	2:D:417:VAL:HG22	1.96	0.47
2:D:149:SER:HB2	2:D:449:ARG:HD2	1.95	0.47
2:F:95:THR:HG21	2:F:255:ILE:HG23	1.97	0.47
3:I:204:THR:HG23	3:I:207:ALA:H	1.80	0.47
2:B:145:GLN:HB2	2:B:187:VAL:HG22	1.96	0.47
1:E:273:THR:HB	1:E:347:VAL:HG23	1.97	0.47
4:J:38:ALA:O	4:J:41:GLU:HG3	2.14	0.47
3:I:85:GLN:O	3:I:88:LEU:HG	2.13	0.47
1:E:493:ASN:HA	1:E:496:VAL:HG12	1.97	0.47
3:K:193:ALA:HB2	3:K:200:VAL:HG12	1.96	0.47
1:C:331:TYR:HA	1:C:334:ILE:HG22	1.96	0.47
2:F:144:ILE:HD12	2:F:157:ILE:HG13	1.96	0.47
1:E:167:HIS:H	1:E:343:MET:CE	2.27	0.47
2:D:475:GLY:HA2	2:D:478:LEU:HD12	1.98	0.47
1:C:101:ILE:HG22	1:C:109:LEU:HD12	1.97	0.46
1:E:315:VAL:HG12	1:E:315:VAL:O	2.15	0.46
3:G:99:GLU:O	3:G:103:VAL:HG23	2.15	0.46
2:D:373:LEU:HB3	2:D:374:PRO:HD3	1.97	0.46
2:F:335:PRO:HG2	2:F:341:HIS:CD2	2.49	0.46
1:E:30:PRO:HA	1:E:73:THR:HG21	1.97	0.46
1:E:279:CYS:O	1:E:353:SER:OG	2.33	0.46
1:A:397:CYS:SG	1:A:403:ARG:HD3	2.56	0.46
2:D:272:LEU:HD21	2:D:274:ILE:HD11	1.97	0.46
2:D:345:ASP:O	2:D:349:TYR:HD1	1.98	0.46
1:E:292:ASP:OD1	1:E:293:PHE:N	2.48	0.46
1:A:569:ILE:HD11	1:A:573:LEU:HD23	1.97	0.46
1:A:246:GLY:O	1:A:408:THR:OG1	2.32	0.46
1:C:294:PRO:HA	1:C:309:MET:HG2	1.97	0.46
1:C:22:GLY:O	1:C:82:VAL:N	2.33	0.46
1:C:492:LEU:HA	1:C:495:ILE:HD13	1.97	0.46
1:E:347:VAL:O	1:E:407:VAL:HA	2.16	0.46
2:F:105:ILE:HG23	2:F:237:LEU:HB2	1.97	0.46
1:A:194:LEU:O	1:A:205:PHE:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:124:ARG:NH1	3:K:201:CYS:HB3	2.31	0.46
1:E:211:TRP:CZ2	1:E:218:PRO:HD3	2.51	0.45
2:F:48:ILE:HD13	2:F:72:VAL:HG12	1.98	0.45
1:A:74:ALA:HA	2:B:42:TYR:HD2	1.80	0.45
2:B:272:LEU:HD12	2:B:327:THR:O	2.16	0.45
2:D:163:ILE:HD13	2:D:353:GLY:HA3	1.97	0.45
2:D:200:GLY:O	2:D:204:ASN:N	2.47	0.45
1:E:131:ASP:OD2	1:E:134:THR:N	2.47	0.45
3:G:60:LYS:O	3:G:63:GLU:HG2	2.16	0.45
4:J:87:ASN:O	4:J:91:GLU:N	2.49	0.45
1:C:158:VAL:HG21	1:C:207:MET:HE3	1.97	0.45
1:E:415:PRO:HB3	1:E:425:THR:HG21	1.99	0.45
2:F:459:TRP:NE1	2:F:478:LEU:HB2	2.29	0.45
3:G:51:ILE:HD11	4:H:53:VAL:HG11	1.99	0.45
3:G:212:VAL:HG12	4:H:101:LEU:HD13	1.99	0.45
1:C:197:GLU:HA	1:C:202:LYS:HA	1.98	0.45
1:E:475:PHE:HA	1:E:478:ILE:HG12	1.98	0.45
2:F:144:ILE:HD11	2:F:159:ARG:HA	1.98	0.45
1:C:471:PHE:HE2	1:C:541:VAL:HG11	1.81	0.45
3:K:134:CYS:HB2	3:K:178:HIS:HB3	1.99	0.45
1:C:360:ALA:O	1:C:364:ILE:HG12	2.17	0.45
1:C:514:THR:HG21	1:C:551:TYR:HB2	1.98	0.45
1:E:323:VAL:HG13	1:E:326:ARG:HH22	1.82	0.45
3:K:182:HIS:HB2	3:K:185:SER:HB2	1.99	0.45
5:M:66:SER:O	5:M:70:ILE:HG12	2.17	0.45
2:B:309:LEU:HD12	2:B:346:LEU:HD22	1.99	0.44
2:D:407:GLY:C	2:D:433:LEU:HD11	2.37	0.44
3:I:47:GLU:O	3:I:50:LYS:HG3	2.18	0.44
2:B:129:GLY:H	2:B:315:ARG:HH12	1.65	0.44
1:C:413:VAL:HG12	1:C:414:SER:H	1.82	0.44
1:E:89:LEU:O	1:E:213:VAL:HG23	2.17	0.44
1:E:340:PHE:HD1	1:E:343:MET:SD	2.40	0.44
3:K:85:GLN:O	3:K:88:LEU:HG	2.17	0.44
2:B:305:MET:HE1	2:B:346:LEU:HD13	1.99	0.44
2:D:14:THR:HG22	4:H:107:THR:HG23	1.99	0.44
7:O:35:PRO:HD2	7:O:322:PRO:HB3	2.00	0.44
1:A:230:LEU:HB3	1:A:270:ASN:OD1	2.18	0.44
1:A:552:ASN:O	1:A:555:ASN:N	2.50	0.44
2:B:261:GLU:HA	2:B:326:ILE:HD11	2.00	0.44
3:G:189:GLY:HA3	3:G:204:THR:HA	2.00	0.44
1:E:226:ASP:OD1	1:E:226:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:SER:HA	2:F:315:ARG:HH12	1.81	0.44
3:K:40:LYS:HG2	4:L:42:ALA:HB3	2.00	0.44
2:B:247:ILE:O	2:B:251:ILE:HG23	2.18	0.43
2:F:96:PRO:HB3	2:F:124:TYR:CE1	2.53	0.43
4:J:93:ILE:O	4:J:97:VAL:HG23	2.18	0.43
3:K:96:ALA:O	3:K:100:VAL:HG13	2.18	0.43
3:K:224:LEU:HG	4:L:93:ILE:HD11	2.00	0.43
1:A:78:VAL:HG12	1:A:79:ASN:OD1	2.19	0.43
1:A:175:MET:O	1:A:198:PHE:HB2	2.18	0.43
1:A:538:TYR:O	1:A:542:TRP:HD1	2.01	0.43
2:B:145:GLN:NE2	2:B:450:ASN:HA	2.33	0.43
2:B:209:PHE:HD2	2:B:237:LEU:HD13	1.84	0.43
2:B:360:GLN:O	2:B:364:ARG:HG3	2.18	0.43
1:C:492:LEU:HD21	1:C:512:LEU:HD21	2.01	0.43
2:D:79:ILE:HG23	2:D:84:THR:HG21	2.00	0.43
2:F:15:LEU:HD11	3:I:208:ARG:HG3	2.01	0.43
2:B:171:LEU:HD13	2:B:357:ILE:HG22	1.99	0.43
2:F:157:ILE:HD13	2:F:163:ILE:HG22	2.01	0.43
3:K:32:ALA:HB1	4:L:31:LYS:HA	2.00	0.43
2:B:344:PRO:HA	2:B:347:THR:HG22	2.01	0.43
1:C:413:VAL:HG12	1:C:414:SER:N	2.34	0.43
1:A:531:TYR:CE1	1:A:590:PHE:HA	2.54	0.43
1:C:119:VAL:HG21	2:D:319:ILE:HD11	2.01	0.43
1:C:162:SER:OG	1:C:310:LYS:NZ	2.31	0.43
1:C:539:LYS:O	1:C:543:MET:HG3	2.19	0.43
1:A:211:TRP:CZ2	1:A:218:PRO:HD3	2.54	0.43
1:A:308:VAL:HG22	1:A:312:THR:OG1	2.19	0.43
1:C:415:PRO:O	1:C:417:GLY:N	2.48	0.43
2:F:47:ASN:OD1	2:F:47:ASN:N	2.48	0.43
5:M:95:VAL:O	6:N:12:SER:N	2.52	0.43
1:A:158:VAL:HG21	1:A:207:MET:HE3	2.00	0.42
1:C:614:GLY:C	1:C:616:ARG:H	2.22	0.42
3:I:97:SER:O	3:I:100:VAL:HG12	2.19	0.42
3:K:193:ALA:HA	3:K:199:ILE:O	2.19	0.42
1:C:272:ASP:HB2	1:C:345:TYR:HB3	2.02	0.42
2:D:117:PRO:HG2	3:G:82:LEU:HG	2.01	0.42
2:D:460:THR:HA	2:D:463:ARG:HE	1.83	0.42
2:B:60:VAL:HG22	2:B:70:VAL:HG22	2.01	0.42
1:A:53:LEU:HB3	1:A:69:VAL:HG11	2.02	0.42
2:D:367:TYR:O	2:D:369:PRO:HD3	2.20	0.42
1:E:109:LEU:CD2	2:F:134:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:215:LYS:HD2	3:I:215:LYS:C	2.40	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.86	0.42
2:D:456:ASP:O	2:D:460:THR:HG23	2.19	0.42
2:F:164:PRO:HG2	2:F:166:PHE:HE1	1.84	0.42
2:F:319:ILE:HG23	2:F:322:ARG:HB2	2.01	0.42
3:I:222:LYS:C	3:I:222:LYS:HD3	2.40	0.42
1:A:93:LEU:HD12	1:A:339:TYR:CD2	2.54	0.42
6:N:113:LEU:H	6:N:113:LEU:HD12	1.84	0.42
2:B:373:LEU:HB3	2:B:374:PRO:HD3	2.02	0.42
1:C:74:ALA:HA	2:D:42:TYR:HD1	1.83	0.42
2:B:319:ILE:HG22	2:B:322:ARG:H	1.84	0.42
1:E:158:VAL:HG13	1:E:166:HIS:HB3	2.00	0.42
1:E:584:ARG:NH2	1:E:607:LEU:HG	2.35	0.42
1:A:46:VAL:HG11	1:A:67:ILE:HD13	2.01	0.42
1:A:245:GLY:H	1:A:408:THR:HB	1.85	0.42
1:E:271:SER:O	1:E:311:ARG:NH2	2.53	0.41
3:I:75:ASN:O	3:I:79:ILE:HG12	2.20	0.41
3:K:88:LEU:HD13	4:L:90:ALA:HB2	2.02	0.41
7:O:29:LYS:NZ	7:O:36:LEU:O	2.50	0.41
2:B:163:ILE:HD12	2:B:353:GLY:HA3	2.02	0.41
2:D:407:GLY:O	2:D:433:LEU:HD11	2.20	0.41
3:I:131:LEU:HD12	3:I:195:ARG:HE	1.84	0.41
8:P:247:TYR:O	8:P:251:THR:N	2.53	0.41
1:A:442:LEU:HB3	1:A:447:HIS:HB2	2.02	0.41
2:B:34:LEU:HD21	2:B:86:VAL:HG11	2.03	0.41
1:E:250:ILE:HD11	1:E:436:TRP:HE3	1.86	0.41
1:A:267:LYS:HE3	1:A:268:TYR:CZ	2.55	0.41
2:B:128:SER:HA	2:B:315:ARG:HH22	1.86	0.41
1:C:266:SER:HA	1:C:274:VAL:HG21	2.01	0.41
1:E:297:THR:OG1	1:E:306:GLU:O	2.39	0.41
1:E:331:TYR:HA	1:E:334:ILE:HG22	2.01	0.41
1:E:513:GLU:C	1:E:515:ALA:H	2.24	0.41
2:F:120:LEU:HG	3:I:221:ARG:HD2	2.02	0.41
2:B:246:THR:O	2:B:249:ARG:N	2.54	0.41
2:D:205:PHE:O	2:D:271:VAL:HA	2.21	0.41
2:D:357:ILE:HG23	2:D:369:PRO:HB2	2.03	0.41
1:E:234:ARG:O	1:E:238:ALA:HB3	2.21	0.41
1:A:449:PRO:HD3	1:A:525:GLN:H	1.85	0.41
1:A:574:ILE:HA	1:A:577:ARG:HG2	2.03	0.41
2:B:366:ILE:HG23	2:B:442:ALA:HB2	2.01	0.41
1:E:121:ILE:HG12	2:F:131:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:MET:O	1:E:345:TYR:OH	2.26	0.41
1:E:585:LEU:HD11	1:E:611:LEU:HD22	2.02	0.41
2:F:168:ALA:HB3	2:F:359:ARG:HH11	1.86	0.41
2:F:367:TYR:CE2	2:F:445:ALA:HA	2.56	0.41
1:E:142:LYS:HA	1:E:142:LYS:HE2	2.02	0.41
1:E:340:PHE:O	1:E:343:MET:HB2	2.21	0.41
1:A:189:LEU:HD23	1:A:208:LEU:HD12	2.03	0.41
2:B:76:THR:HB	2:B:79:ILE:HD12	2.02	0.41
1:E:138:PHE:HB3	1:E:185:GLY:O	2.21	0.41
2:B:396:VAL:HG21	2:B:455:LEU:HD22	2.03	0.41
1:C:315:VAL:HG12	1:C:315:VAL:O	2.21	0.41
2:F:161:GLN:CD	2:F:379:LEU:HB2	2.42	0.41
2:F:347:THR:O	2:F:351:THR:N	2.52	0.41
5:M:51:ILE:HA	5:M:54:THR:HG22	2.03	0.41
2:D:373:LEU:HD12	2:D:373:LEU:HA	1.89	0.40
1:C:45:LEU:O	1:C:85:THR:OG1	2.29	0.40
2:D:146:THR:HG21	2:D:157:ILE:HD12	2.03	0.40
1:E:252:GLY:HA2	1:E:438:LEU:HD12	2.03	0.40
2:B:393:HIS:CE1	2:B:451:ILE:HD11	2.56	0.40
1:E:195:GLU:HA	1:E:203:LYS:O	2.21	0.40
1:E:228:PRO:HG3	1:E:467:PHE:CE2	2.57	0.40
3:K:100:VAL:HG12	4:L:102:LEU:HD11	2.03	0.40
1:A:250:ILE:HD11	1:A:436:TRP:CE3	2.52	0.40
1:A:297:THR:OG1	1:A:306:GLU:O	2.31	0.40
2:B:335:PRO:HD2	2:B:341:HIS:CG	2.57	0.40
1:C:354:THR:HA	1:C:357:TRP:HB3	2.02	0.40
1:C:359:GLU:OE1	1:C:362:ARG:NH1	2.54	0.40
2:D:143:MET:SD	2:D:156:SER:OG	2.69	0.40
2:D:261:GLU:HA	2:D:326:ILE:HD11	2.03	0.40
5:M:131:GLN:O	5:M:135:CYS:N	2.50	0.40
1:A:491:ASP:HA	1:A:494:GLU:OE1	2.22	0.40
2:D:150:THR:HG21	2:D:441:VAL:HG13	2.03	0.40
3:G:139:HIS:HE1	3:G:178:HIS:ND1	2.19	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	A	585/623 (94%)	565 (97%)	19 (3%)	1 (0%)	47 79
1	C	601/623 (96%)	563 (94%)	38 (6%)	0	100 100
1	E	601/623 (96%)	562 (94%)	38 (6%)	1 (0%)	47 79
2	B	456/488 (93%)	423 (93%)	32 (7%)	1 (0%)	47 79
2	D	463/488 (95%)	435 (94%)	28 (6%)	0	100 100
2	F	459/488 (94%)	433 (94%)	26 (6%)	0	100 100
3	G	200/230 (87%)	193 (96%)	7 (4%)	0	100 100
3	I	203/230 (88%)	195 (96%)	8 (4%)	0	100 100
3	K	213/230 (93%)	203 (95%)	10 (5%)	0	100 100
4	H	95/110 (86%)	94 (99%)	1 (1%)	0	100 100
4	J	94/110 (86%)	91 (97%)	3 (3%)	0	100 100
4	L	99/110 (90%)	99 (100%)	0	0	100 100
5	M	211/259 (82%)	196 (93%)	15 (7%)	0	100 100
6	N	105/130 (81%)	76 (72%)	25 (24%)	4 (4%)	3 28
7	O	303/375 (81%)	283 (93%)	20 (7%)	0	100 100
8	P	277/452 (61%)	258 (93%)	19 (7%)	0	100 100
9	a	705/823 (86%)	661 (94%)	43 (6%)	1 (0%)	51 84
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%)	146 (95%)	7 (5%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	7527/8471 (89%)	7125 (95%)	394 (5%)	8 (0%)	54	84

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	ALA
1	E	448	PHE
6	N	32	VAL
6	N	21	GLU
2	B	389	THR
6	N	101	LYS
6	N	35	VAL
9	a	59	SER

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/517 (63%)	326 (99%)	2 (1%)	86	91
1	C	357/517 (69%)	354 (99%)	3 (1%)	81	89
1	E	387/517 (75%)	386 (100%)	1 (0%)	92	95
2	B	272/413 (66%)	270 (99%)	2 (1%)	84	90
2	D	275/413 (67%)	270 (98%)	5 (2%)	59	77
2	F	279/413 (68%)	279 (100%)	0	100	100
3	G	87/206 (42%)	86 (99%)	1 (1%)	73	84
3	I	108/206 (52%)	106 (98%)	2 (2%)	57	75
3	K	96/206 (47%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	21/87 (24%)	21 (100%)	0	100	100
4	J	14/87 (16%)	14 (100%)	0	100	100
4	L	25/87 (29%)	25 (100%)	0	100	100
5	M	15/225 (7%)	15 (100%)	0	100	100
6	N	6/111 (5%)	6 (100%)	0	100	100
7	O	13/336 (4%)	13 (100%)	0	100	100
8	P	17/407 (4%)	17 (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
14	n	5/115 (4%)	5 (100%)	0	100	100
All	All	2402/6897 (35%)	2386 (99%)	16 (1%)	84	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ARG
1	A	403	ARG
2	B	372	VAL
2	B	375	SER
1	C	107	ARG
1	C	347	VAL
1	C	404	THR
2	D	154	MET
2	D	376	LEU
2	D	397	SER
2	D	401	TYR

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Mol	Chain	Res	Type
2	D	473	ILE
1	E	181	VAL
3	G	139	HIS
3	I	50	LYS
3	I	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	166	HIS
2	D	161	GLN
3	G	139	HIS
3	G	178	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

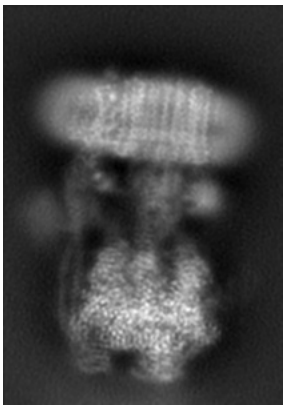
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26827. These allow visual inspection of the internal detail of the map and identification of artifacts.

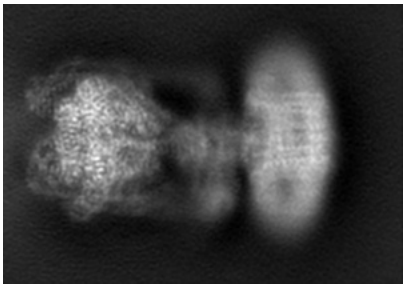
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

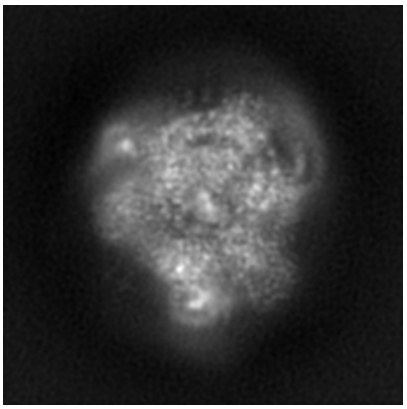
6.1.1 Primary map



X

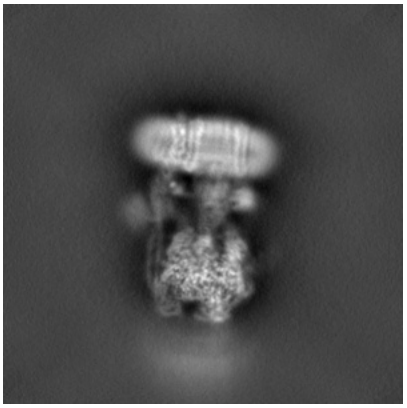


Y

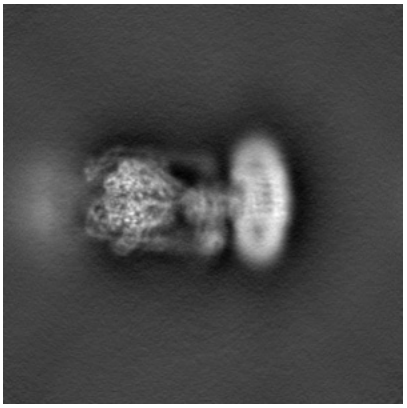


Z

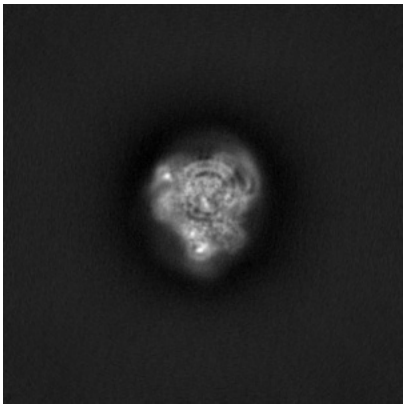
6.1.2 Raw map



X



Y

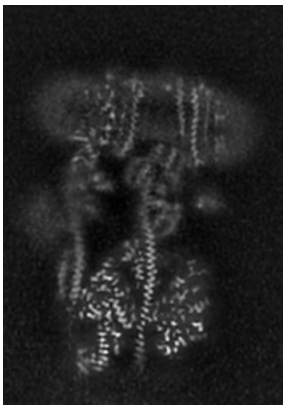


Z

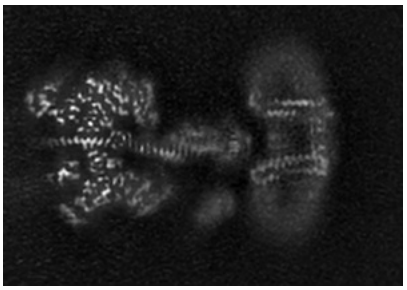
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

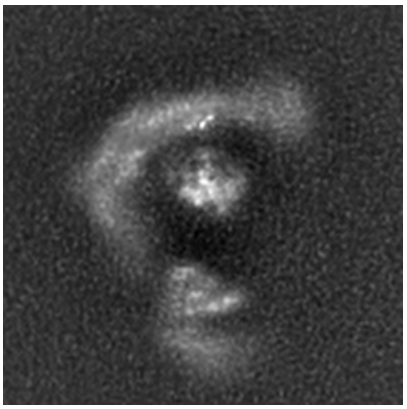
6.2.1 Primary map



X Index: 70



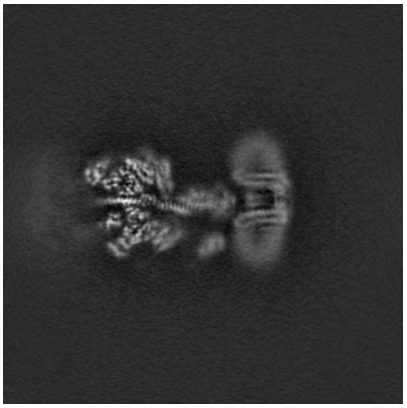
Y Index: 70



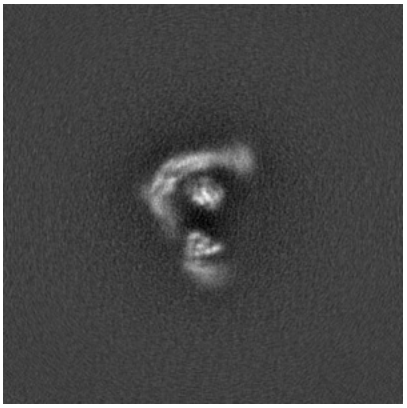
Z Index: 100

6.2.2 Raw map

X Index: 150



Y Index: 150

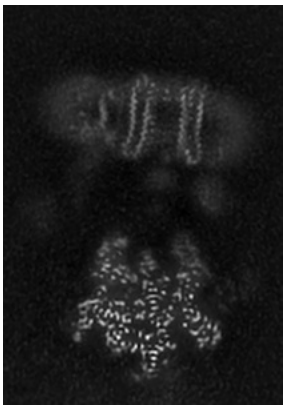


Z Index: 150

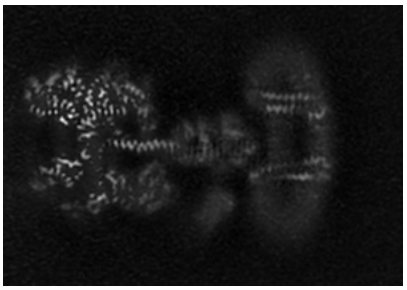
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

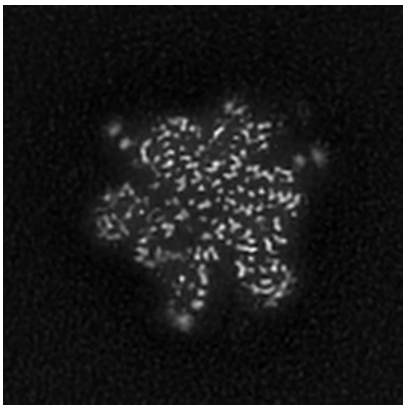
6.3.1 Primary map



X Index: 86



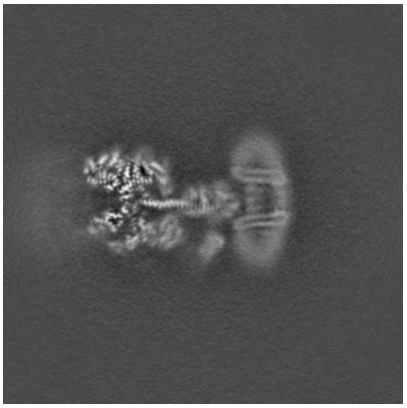
Y Index: 74



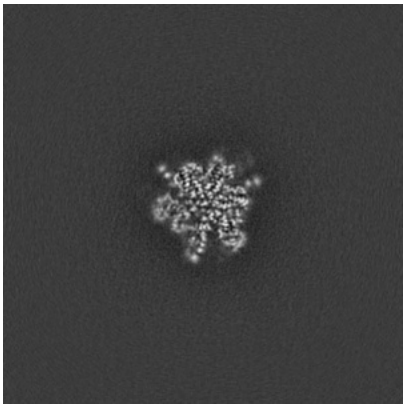
Z Index: 44

6.3.2 Raw map

X Index: 151



Y Index: 154

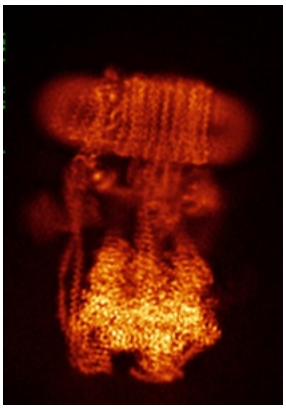


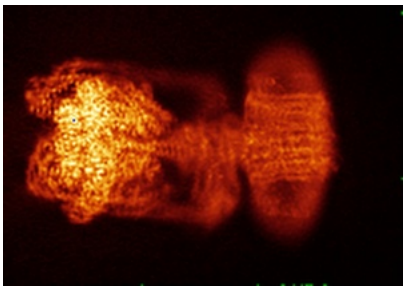
Z Index: 94

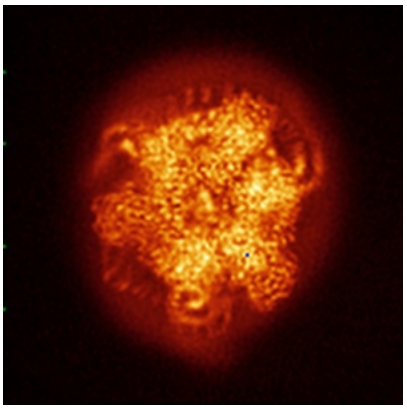
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

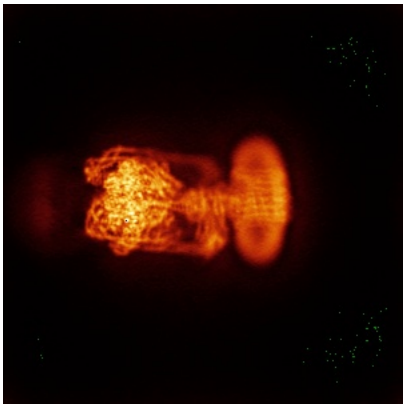

X

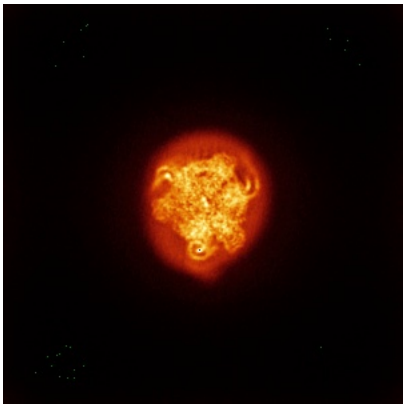

Y


Z

6.4.2 Raw map


X


Y


Z

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

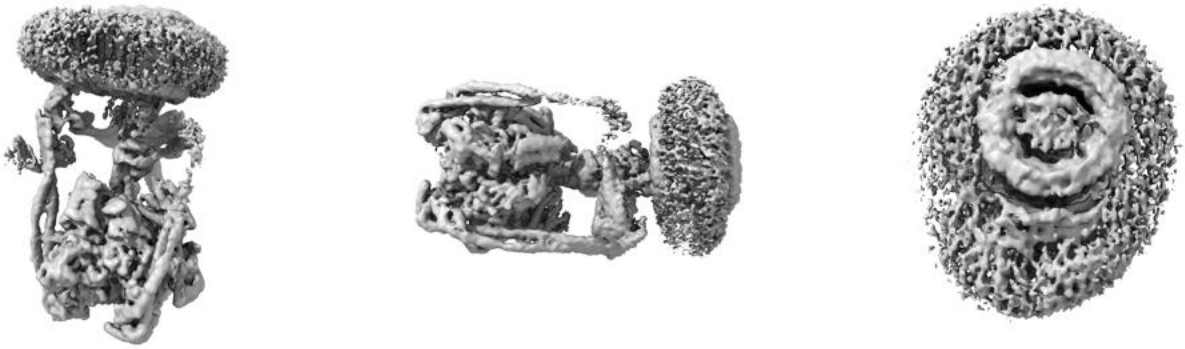
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

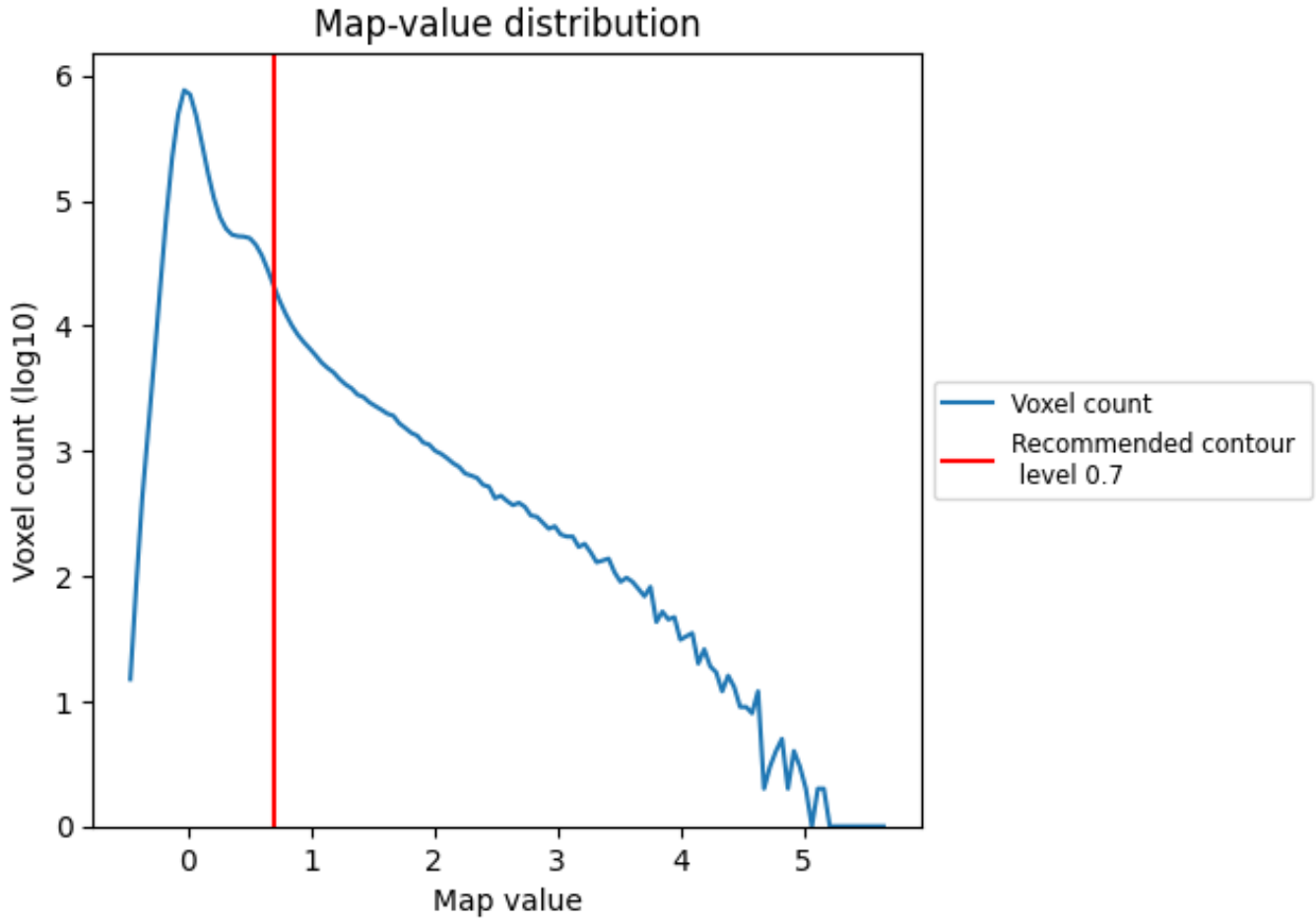
6.6 Mask visualisation (i)

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

7 Map analysis

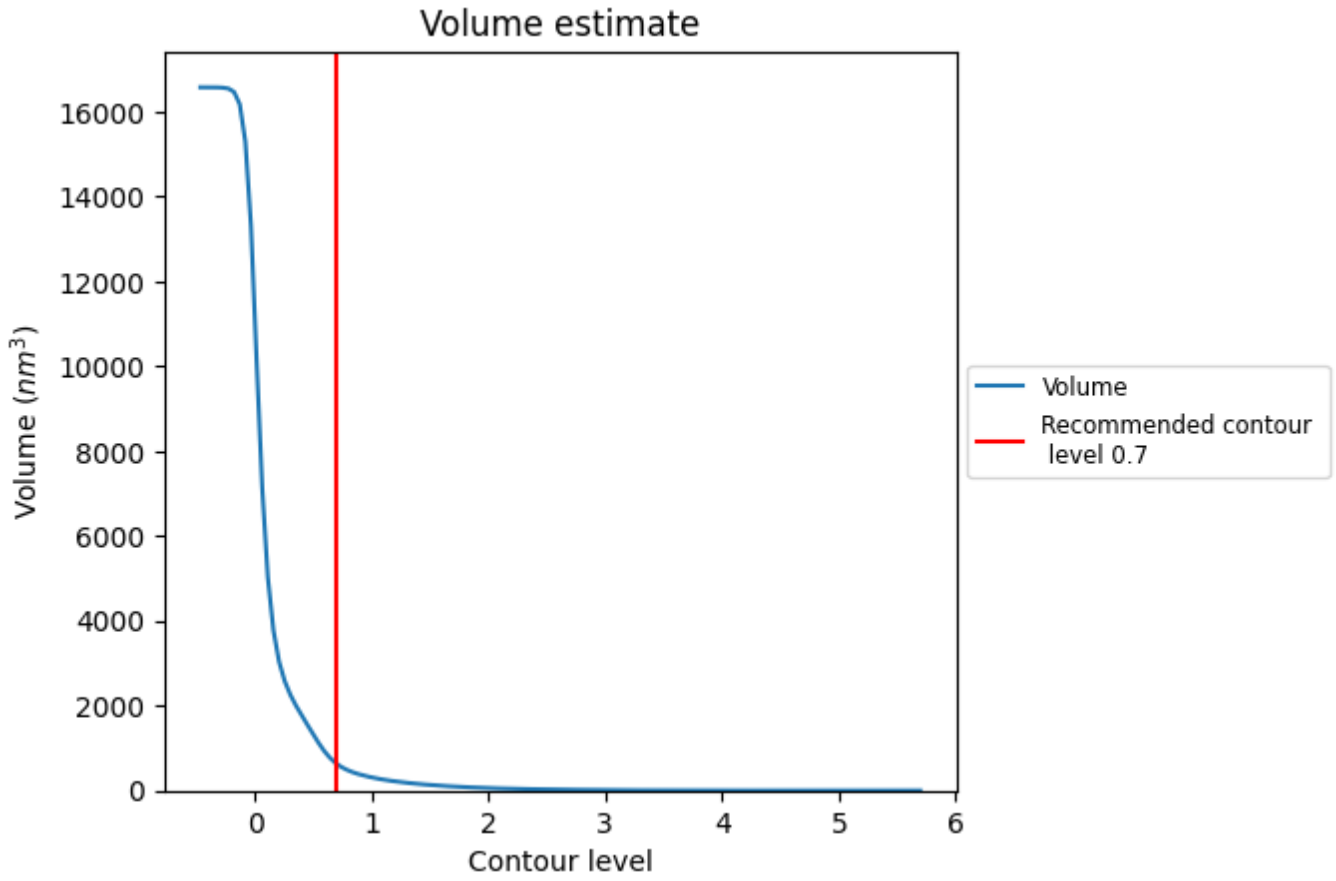
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 637 nm^3; this corresponds to an approximate mass of 576 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.

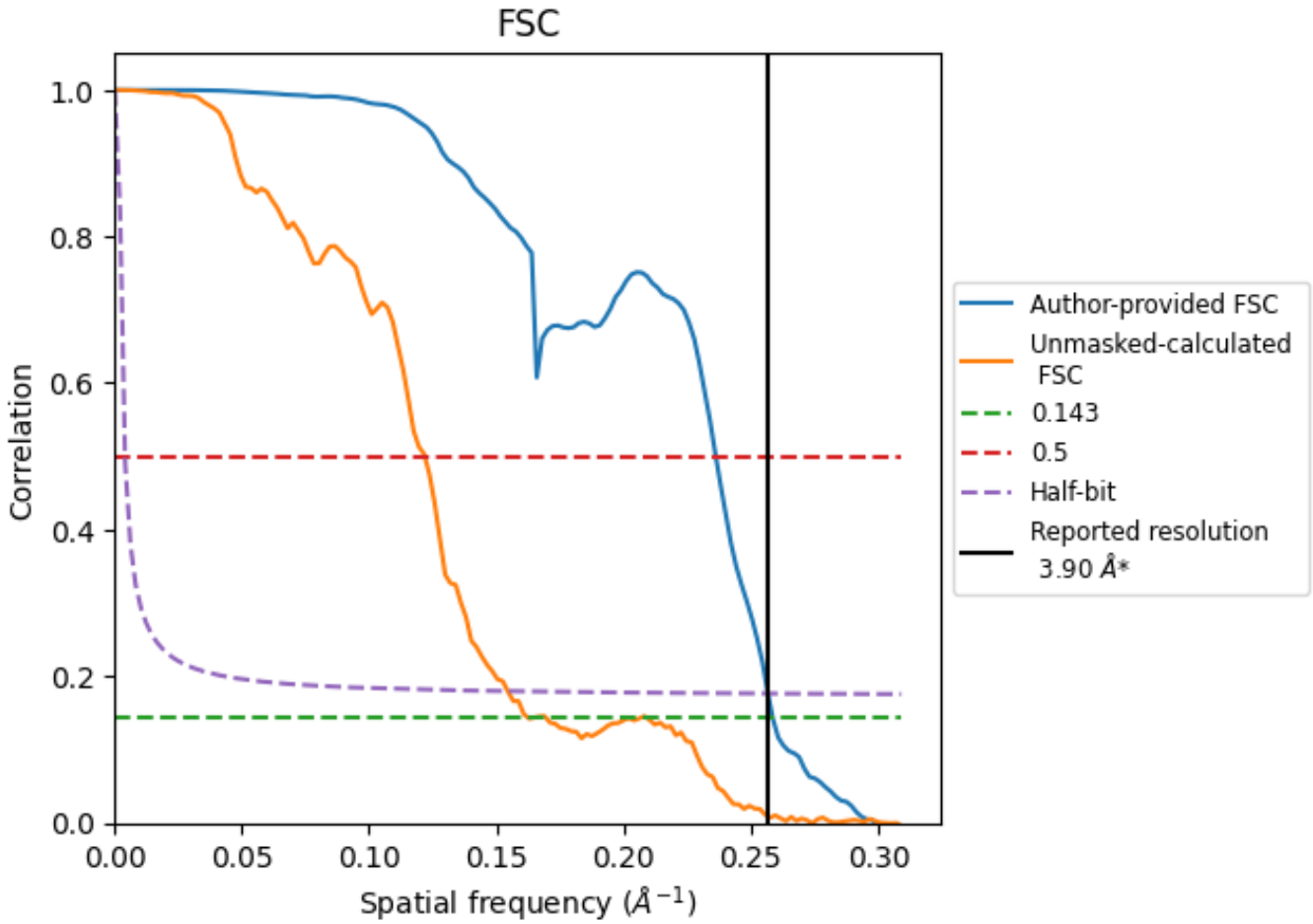
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

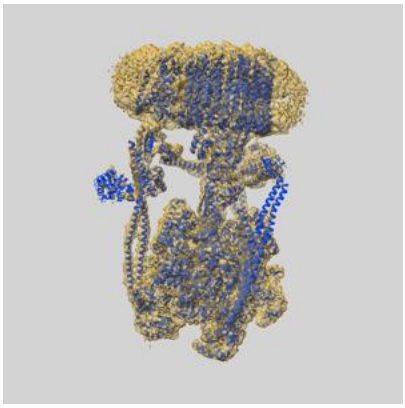
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.87	4.23	3.89
Unmasked-calculated*	6.15	8.20	6.47

*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 6.15 differs from the reported value 3.9 by more than 10 %

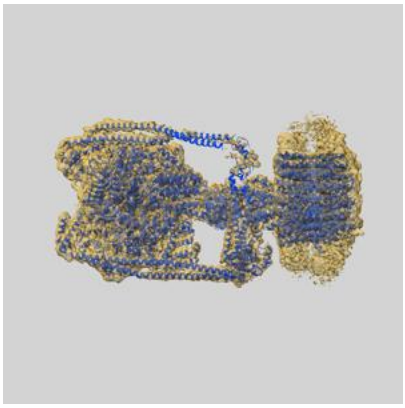
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26827 and PDB model 7UWB. Per-residue inclusion information can be found in section 3 on page 8.

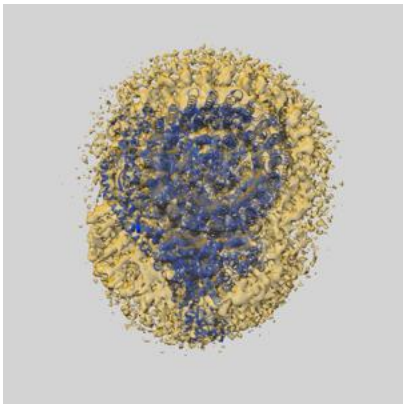
9.1 Map-model overlay



X



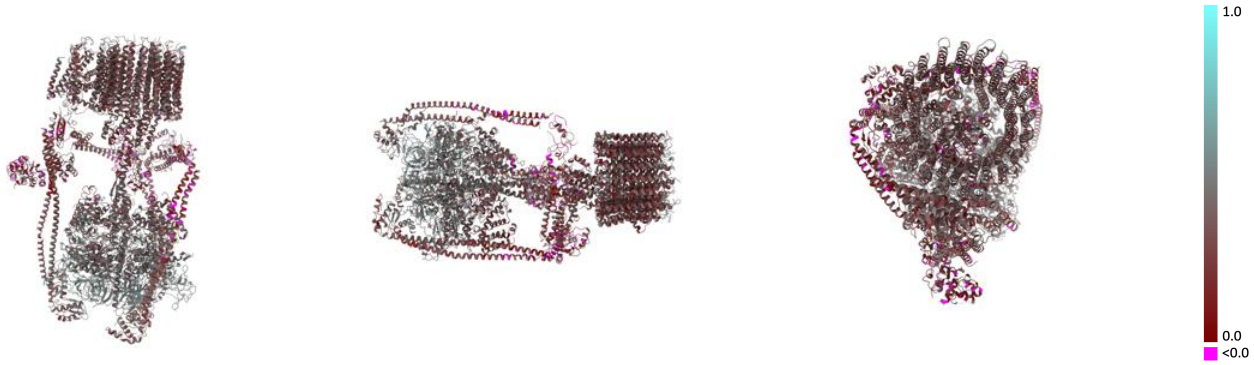
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

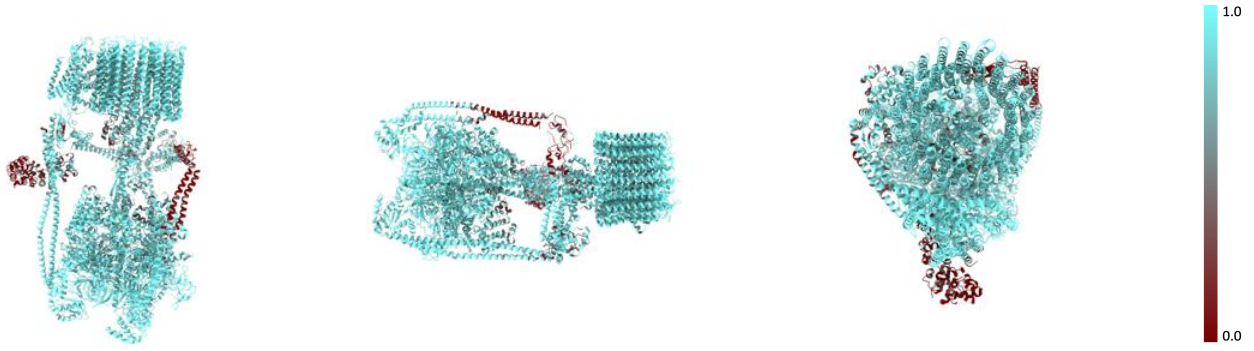
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

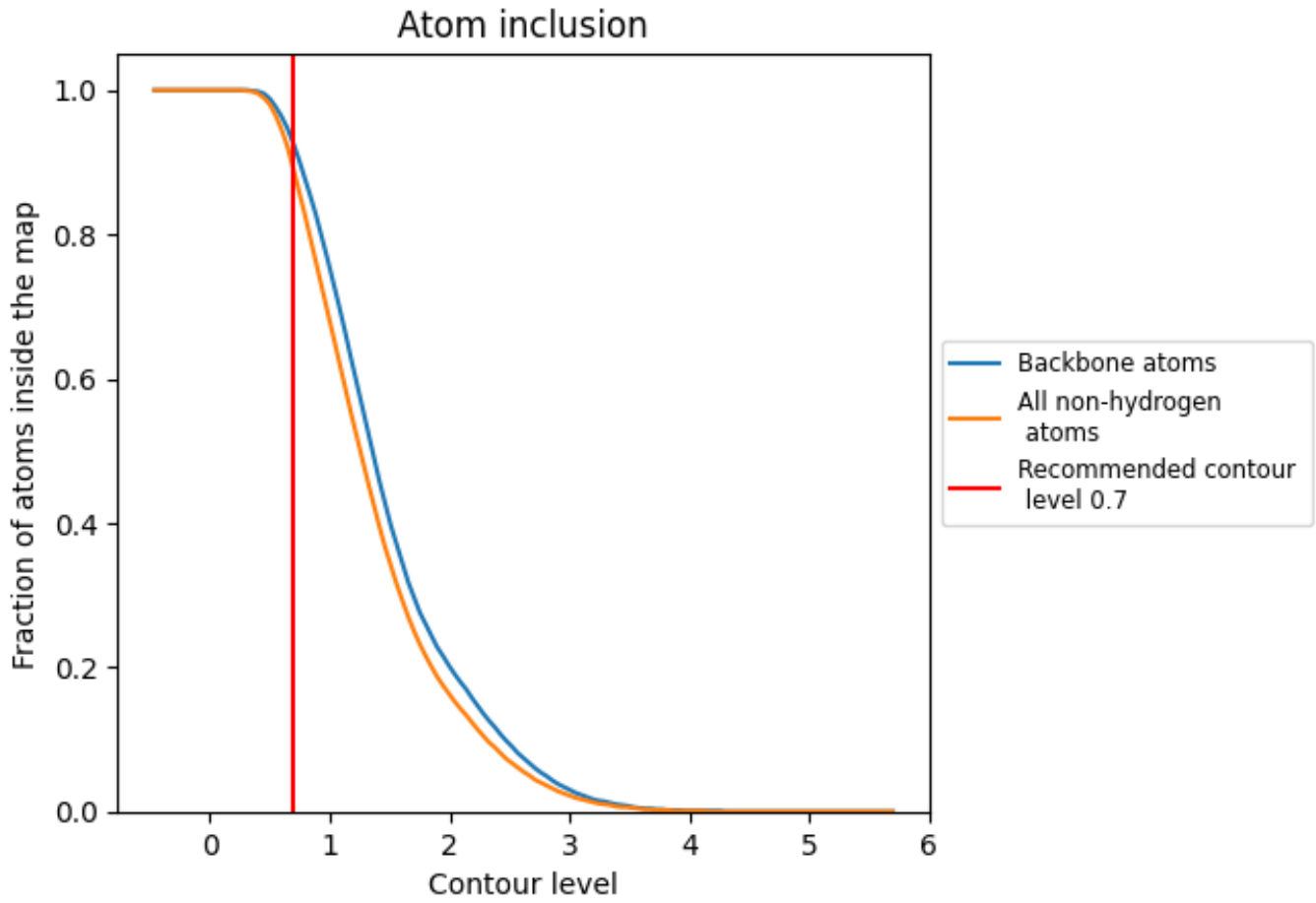
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8880	0.3780
A	0.8980	0.4020
B	0.9510	0.4550
C	0.9500	0.4480
D	0.9580	0.4630
E	0.9590	0.4560
F	0.9320	0.4370
G	0.7960	0.3520
H	0.6110	0.2900
I	0.9050	0.3420
J	0.9030	0.2760
K	0.9360	0.3620
L	0.9240	0.3240
M	0.9450	0.3660
N	0.8640	0.2910
O	0.6500	0.2350
P	0.2670	0.2140
a	0.8960	0.3000
b	0.7940	0.3530
c	0.9340	0.3240
d	0.7780	0.3010
e	0.9660	0.3640
g	0.9460	0.3300
h	0.9340	0.3380
i	0.9320	0.3380
j	0.9540	0.3510
k	0.9380	0.3310
l	0.9320	0.3530
m	0.9450	0.3600
n	0.9150	0.3450
o	0.9200	0.3430
r	0.8920	0.3660