



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 08:39 AM EDT

PDB ID : 9ODU / pdb\_00009odu  
EMDB ID : EMD-70377  
Title : Yeast V-ATPase bound to Rtc5p, rotary state 2  
Authors : Wilkens, S.; Khan, M.M.  
Deposited on : 2025-04-27  
Resolution : 3.90 Å (reported)  
Based on initial models : 9moy, 9nn1, 7fdb

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

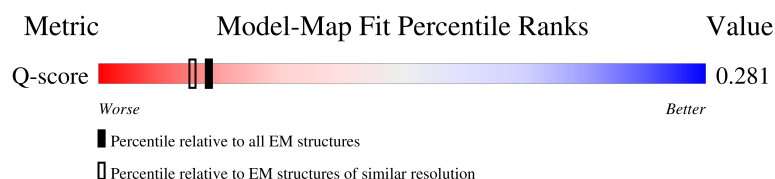
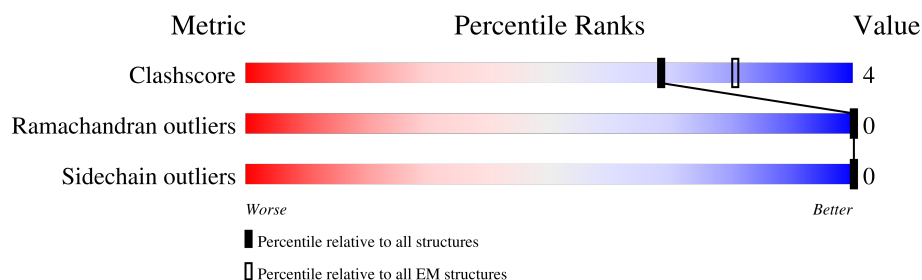
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 ( 3.40 - 4.40 )

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  $\geq 3$ , 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	A	617	
1	C	617	
1	E	617	
2	G	233	

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Mol	Chain	Length	Quality of chain
2	I	233	
2	K	233	
3	H	114	
3	J	114	
3	L	114	
4	M	256	
5	N	118	
6	O	392	
7	R	567	
8	S	345	
9	T	213	
10	U	164	
11	V	160	
11	W	160	
11	X	160	
11	Y	160	
11	Z	160	
11	a	160	
11	b	160	
11	c	160	
12	d	73	
13	e	265	
14	f	85	
15	P	478	
16	Q	840	

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Mol	Chain	Length	Quality of chain
17	B	517	<div><div></div><div>81%10%9%</div></div>
17	D	517	<div><div></div><div>79%12%9%</div></div>
17	F	517	<div><div></div><div>83%9%9%</div></div>

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 139120 atoms, of which 70053 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 H(+)-transporting two-sector ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	594	Total	C	H	N	O	S	0	0
			9113	2909	4526	761	897	20		
1	C	594	Total	C	H	N	O	S	0	0
			9113	2909	4526	761	897	20		
1	E	594	Total	C	H	N	O	S	0	0
			9113	2909	4526	761	897	20		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	225	Total	C	H	N	O	S	0	0
			3676	1131	1874	309	357	5		
2	I	225	Total	C	H	N	O	S	0	0
			3676	1131	1874	309	357	5		
2	K	225	Total	C	H	N	O	S	0	0
			3676	1131	1874	309	357	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	H	111	Total	C	H	N	O		0	0
			1793	546	922	153	172			
3	J	111	Total	C	H	N	O		0	0
			1793	546	922	153	172			
3	L	111	Total	C	H	N	O		0	0
			1793	546	922	153	172			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	M	221	Total	C	H	N	O	S	0	0
			3604	1112	1825	322	340	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	N	115	Total	C	H	N	O		0	0
			1857	589	929	157	182			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	O	392	Total	C	H	N	O	S	0	0
			6276	2005	3155	516	595	5		

- Molecule 7 is a protein called Restriction of telomere capping protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	R	556	Total	C	H	N	O	S	0	0
			8886	2825	4444	748	846	23		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	S	344	Total	C	H	N	O	S	0	0
			5471	1774	2678	453	553	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	T	200	Total	C	H	N	O	S	0	0
			3055	995	1563	231	259	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	U	157	Total	C	H	N	O	S	0	0
			2334	753	1195	179	195	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	V	159	Total	C	H	N	O	S	0	0
			2354	751	1214	182	199	8		
11	W	159	Total	C	H	N	O	S	0	0
			2354	751	1214	182	199	8		

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Mol	Chain	Residues	Atoms						AltConf	Trace
11	X	159	Total	C	H	N	O	S	0	0
			2354	751	1214	182	199	8		
11	Y	160	Total	C	H	N	O	S	0	0
			2365	754	1219	183	200	9		
11	Z	159	Total	C	H	N	O	S	0	0
			2354	751	1214	182	199	8		
11	a	159	Total	C	H	N	O	S	0	0
			2354	751	1214	182	199	8		
11	b	160	Total	C	H	N	O	S	0	0
			2365	754	1219	183	200	9		
11	c	159	Total	C	H	N	O	S	0	0
			2354	751	1214	182	199	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	d	69	Total	C	H	N	O	S	0	0
			1134	369	581	91	86	7		

- Molecule 13 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	e	52	Total	C	H	N	O	S	0	0
			836	268	433	59	74	2		

- Molecule 14 is a protein called Yeast V-ATPase subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	f	76	Total	C	H	N	O	S	0	0
			1160	386	577	94	100	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	459	Total	C	H	N	O	S	0	0
			7499	2358	3808	620	701	12		

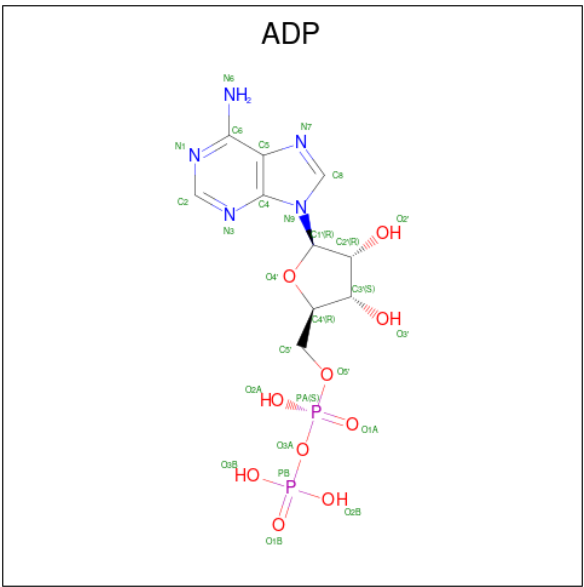
- Molecule 16 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	747	Total	C	H	N	O	S	0	0
			12113	3960	6044	986	1088	35		

- Molecule 17 is a protein called V-type proton ATPase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	B	471	Total	C	H	N	O	S	0	0
			7408	2347	3702	634	713	12		
17	D	471	Total	C	H	N	O	S	0	0
			7408	2347	3702	634	713	12		
17	F	473	Total	C	H	N	O	S	0	0
			7440	2355	3717	639	717	12		

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



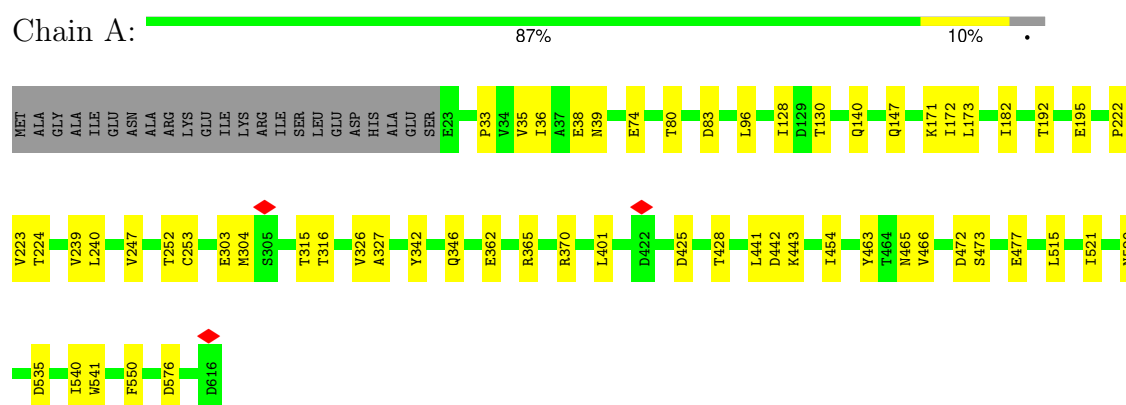
Mol	Chain	Residues	Atoms						AltConf
18	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	



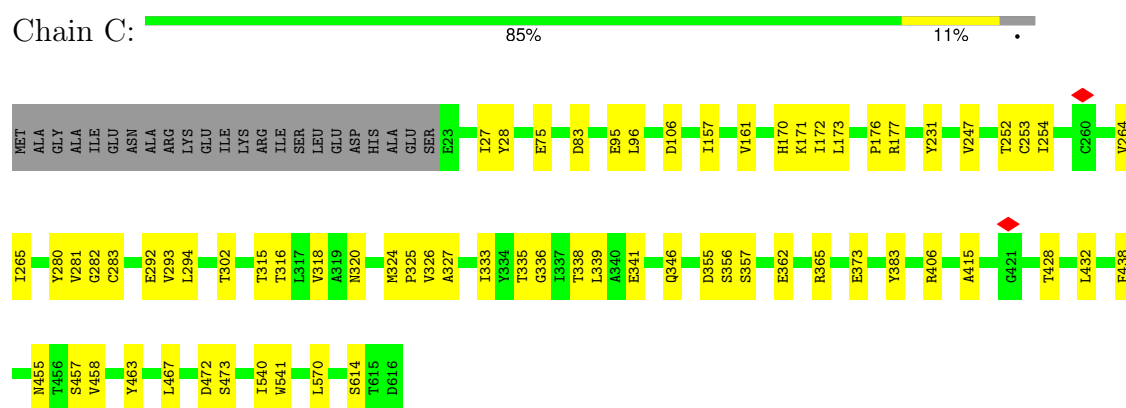
### 3 Residue-property plots

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.

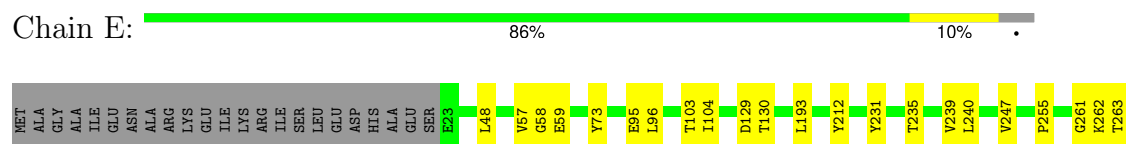
- Molecule 1: H(+)-transporting two-sector ATPase



- Molecule 1: H(+)-transporting two-sector ATPase

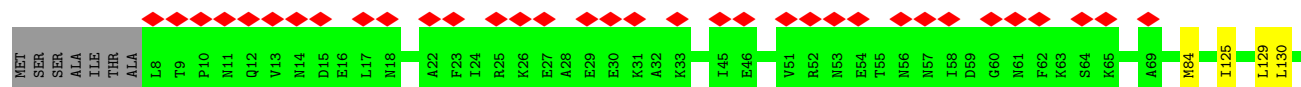
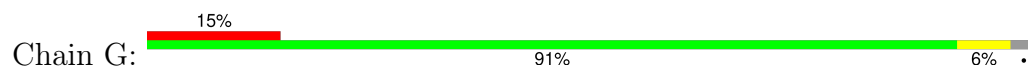


- Molecule 1: H(+)-transporting two-sector ATPase

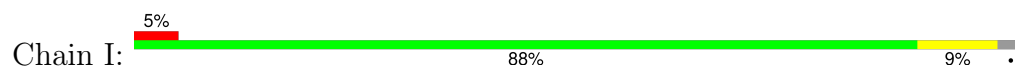




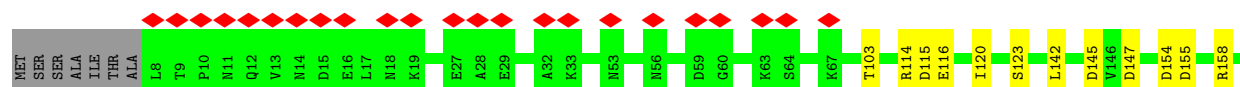
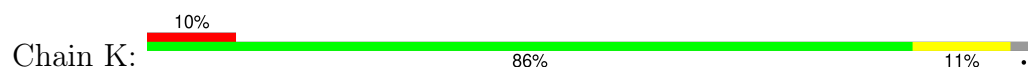
• Molecule 2: V-type proton ATPase subunit E



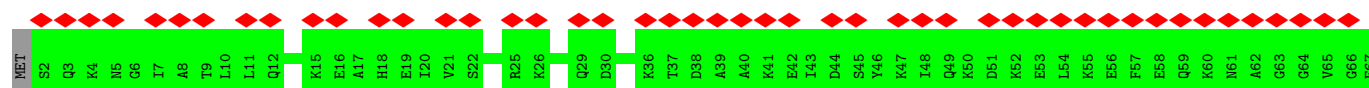
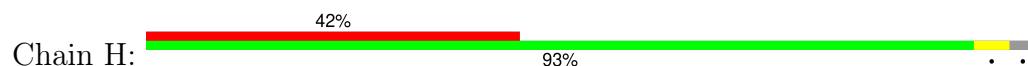
• Molecule 2: V-type proton ATPase subunit E



• Molecule 2: V-type proton ATPase subunit E



• Molecule 3: V-type proton ATPase subunit G




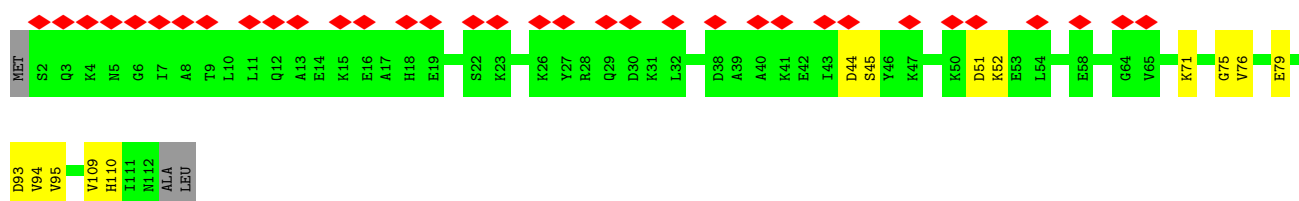
- Molecule 3: V-type proton ATPase subunit G

Chain J:  92% 5%




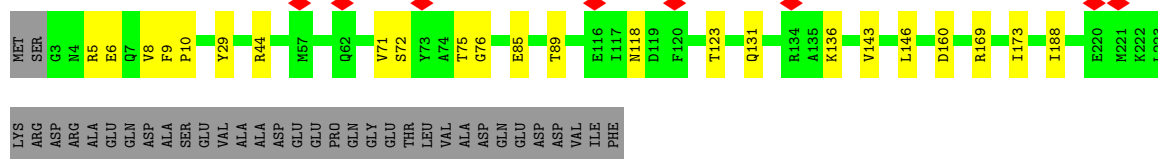
- Molecule 3: V-type proton ATPase subunit G

Chain L:  30% 86% 11%




- Molecule 4: V-type proton ATPase subunit D

Chain M:  77% 9% 14%

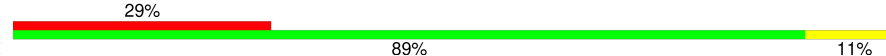


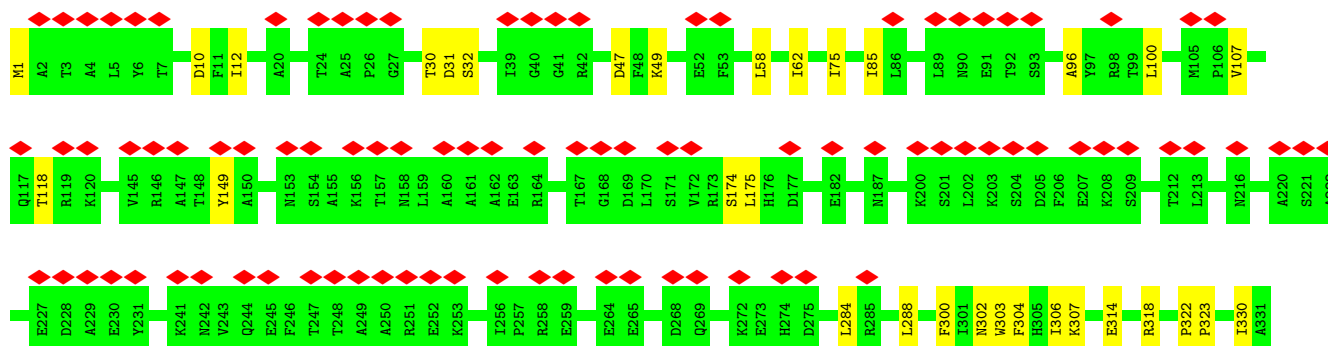
- Molecule 5: V-type proton ATPase subunit F

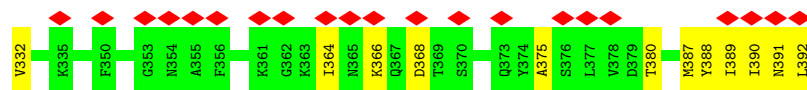
Chain N:  19% 83% 14%



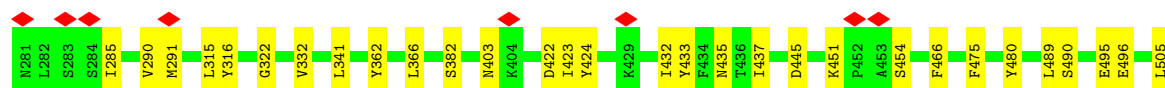
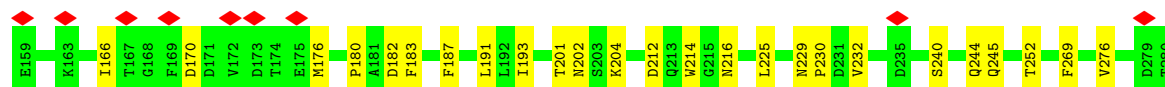
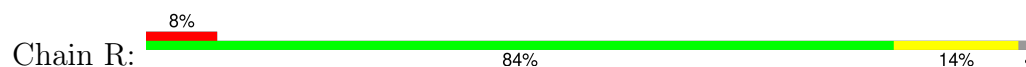
- Molecule 6: V-type proton ATPase subunit C

Chain O:  29% 89% 11%

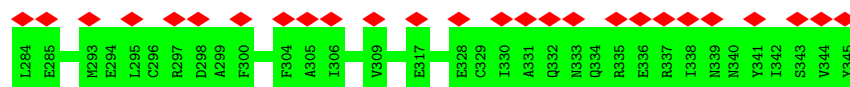
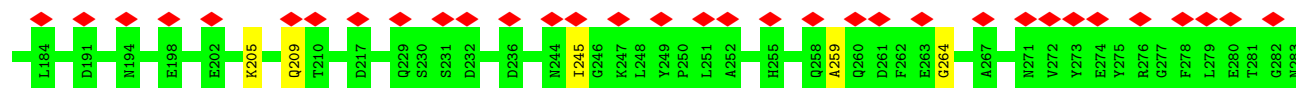
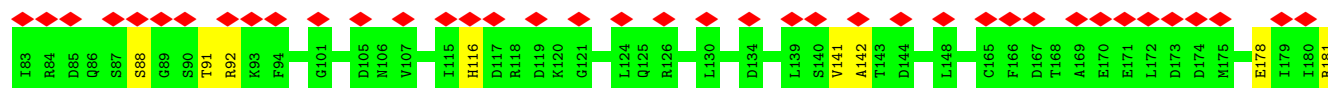
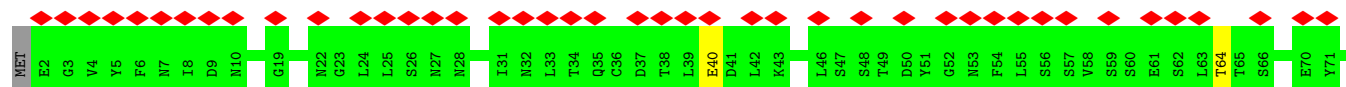
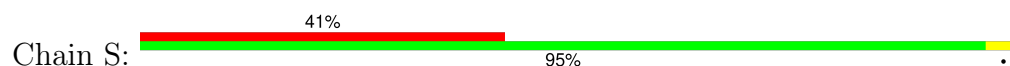




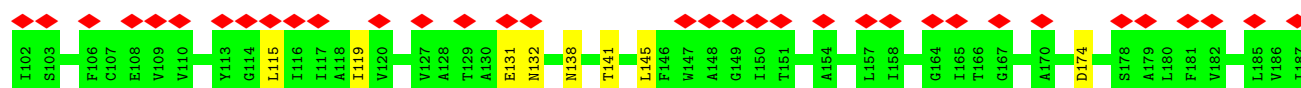
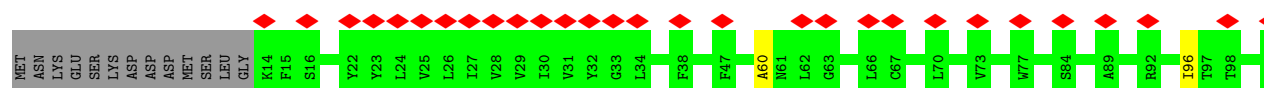
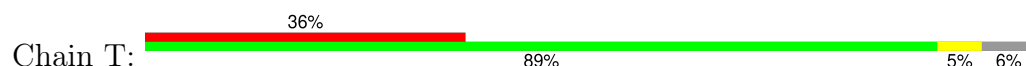
• Molecule 7: Restriction of telomere capping protein 5

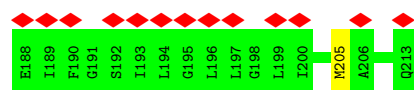


• Molecule 8: V-type proton ATPase subunit d

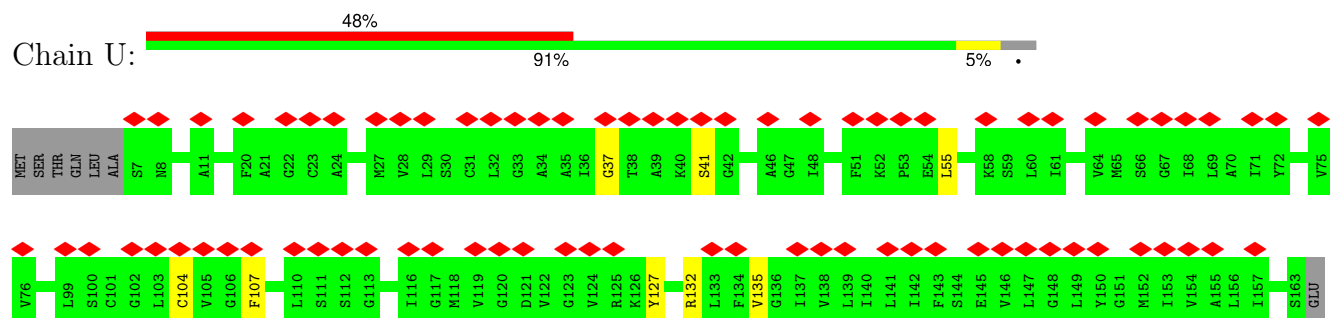


• Molecule 9: V-type proton ATPase subunit c''

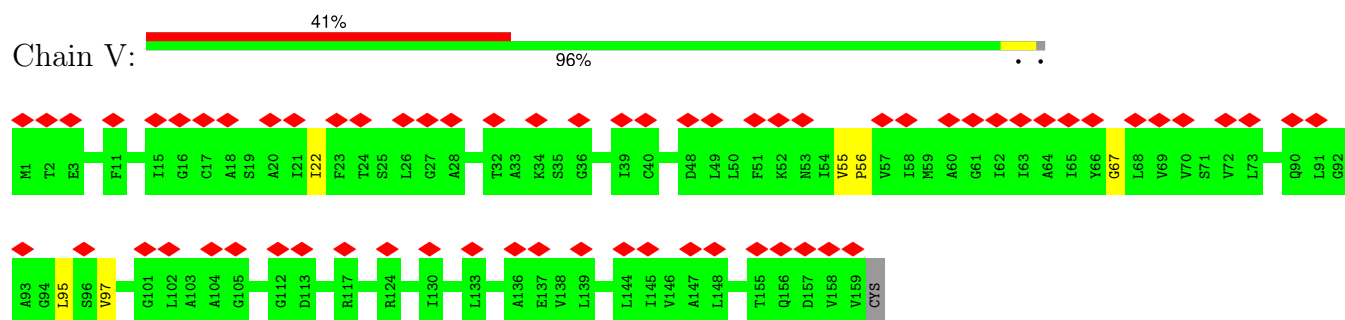




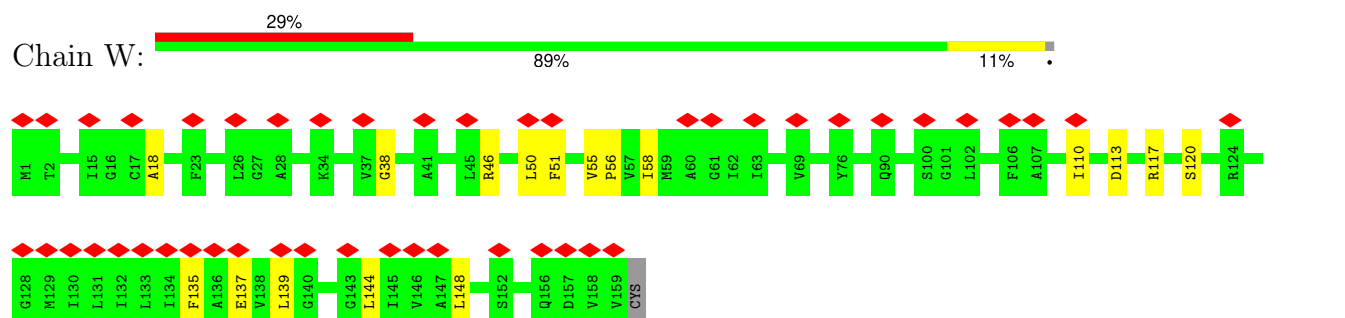
- Molecule 10: V-type proton ATPase subunit c'



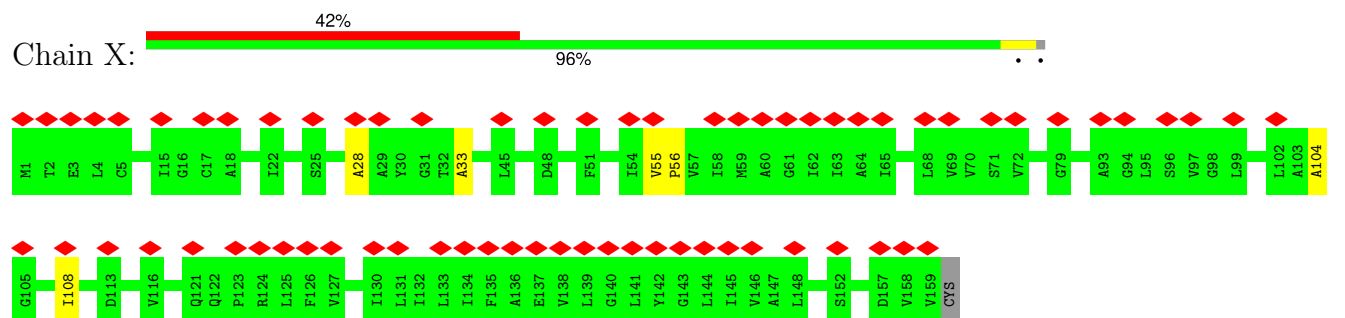
- Molecule 11: V-type proton ATPase subunit c



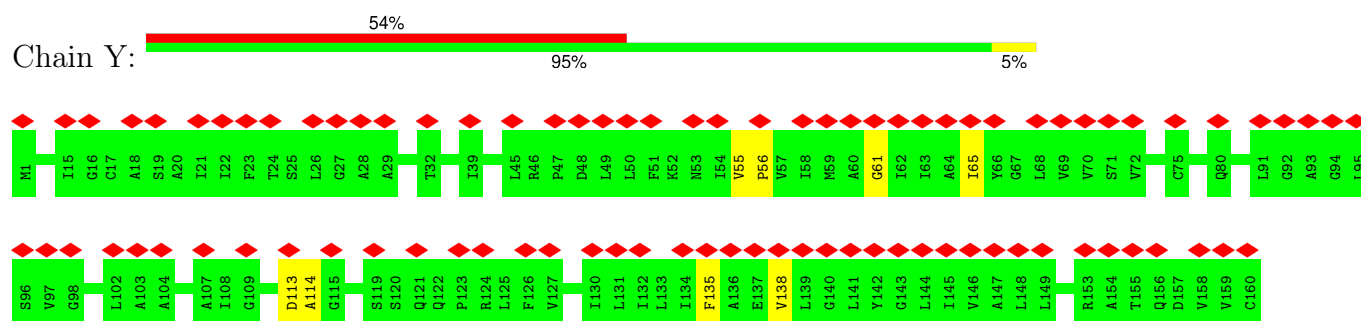
- Molecule 11: V-type proton ATPase subunit c



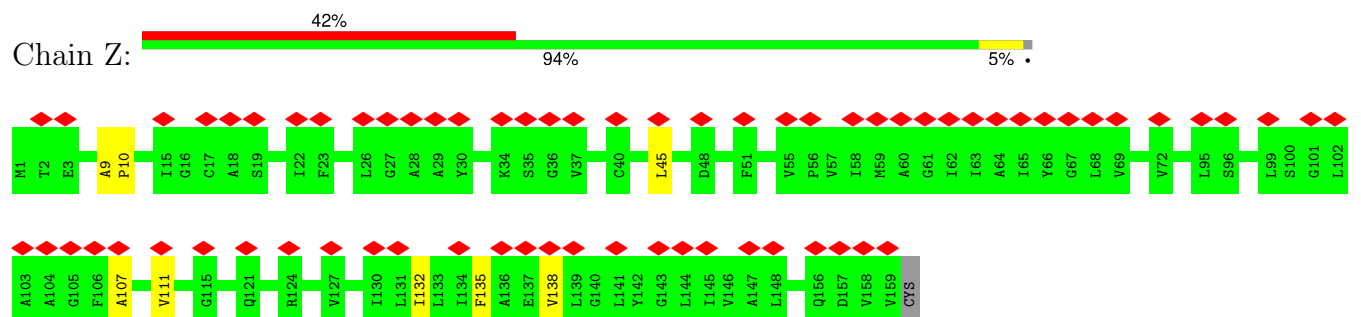
- Molecule 11: V-type proton ATPase subunit c



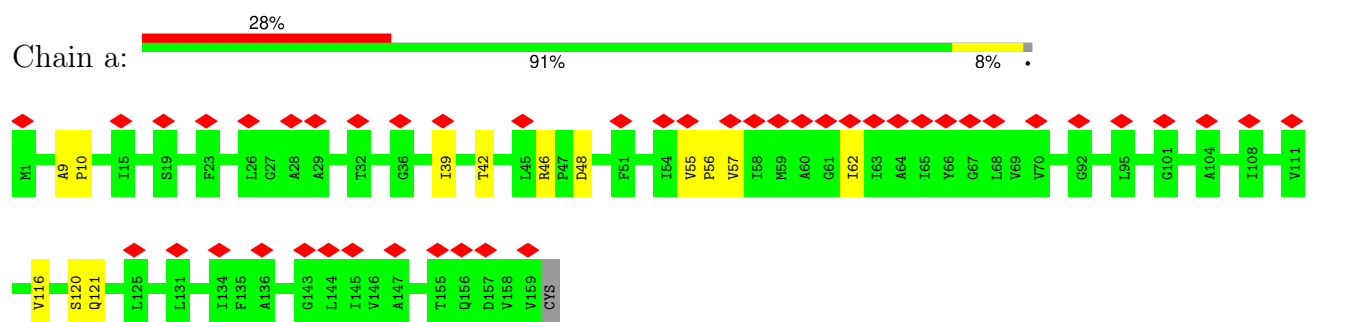
- Molecule 11: V-type proton ATPase subunit c



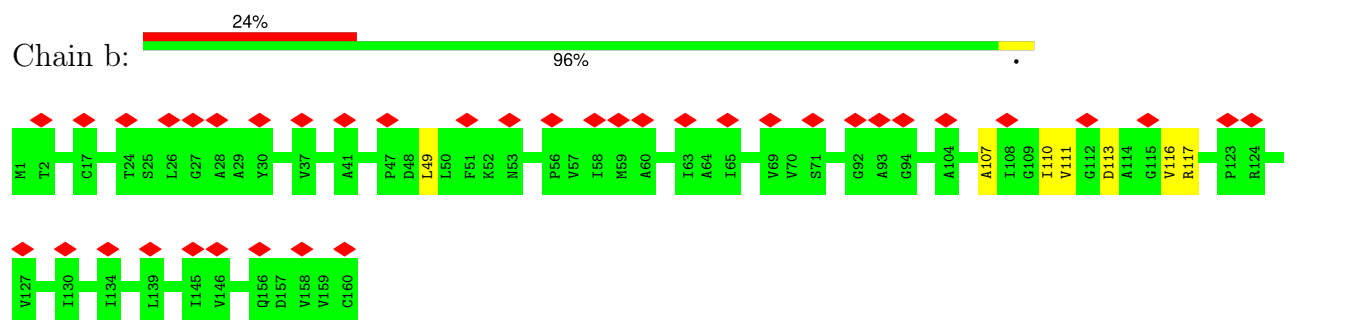
• Molecule 11: V-type proton ATPase subunit c



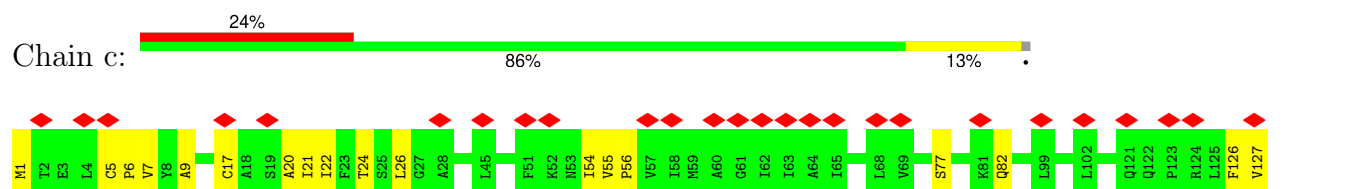
• Molecule 11: V-type proton ATPase subunit c



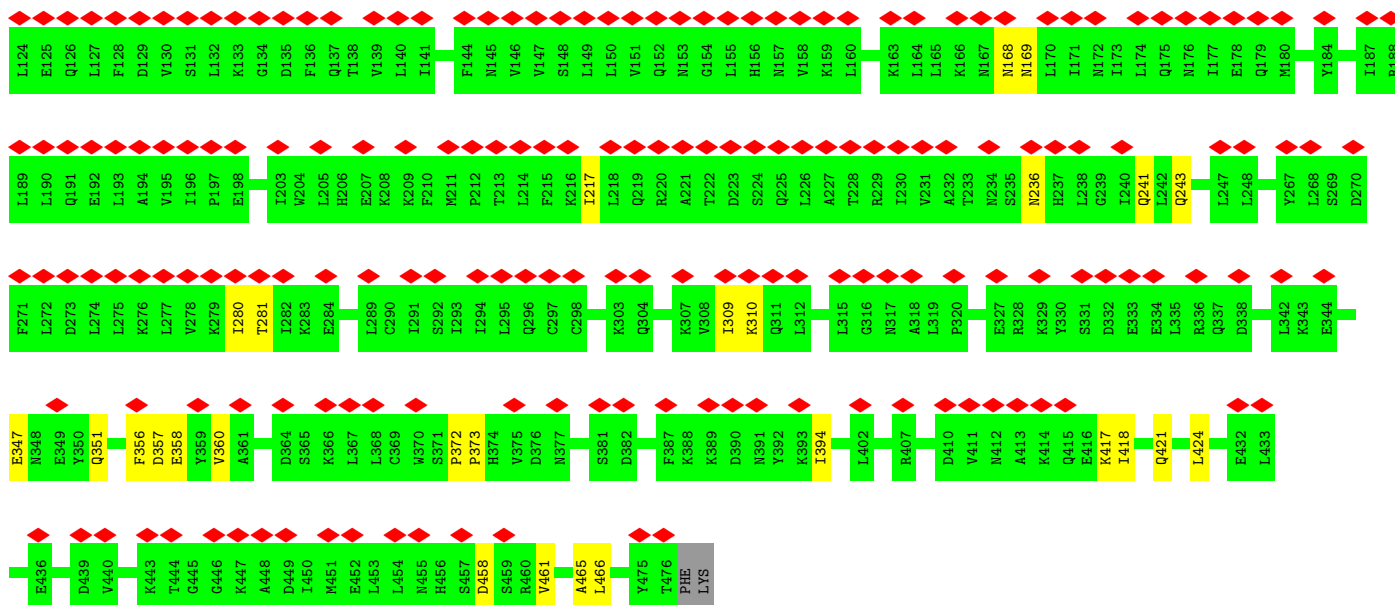
• Molecule 11: V-type proton ATPase subunit c



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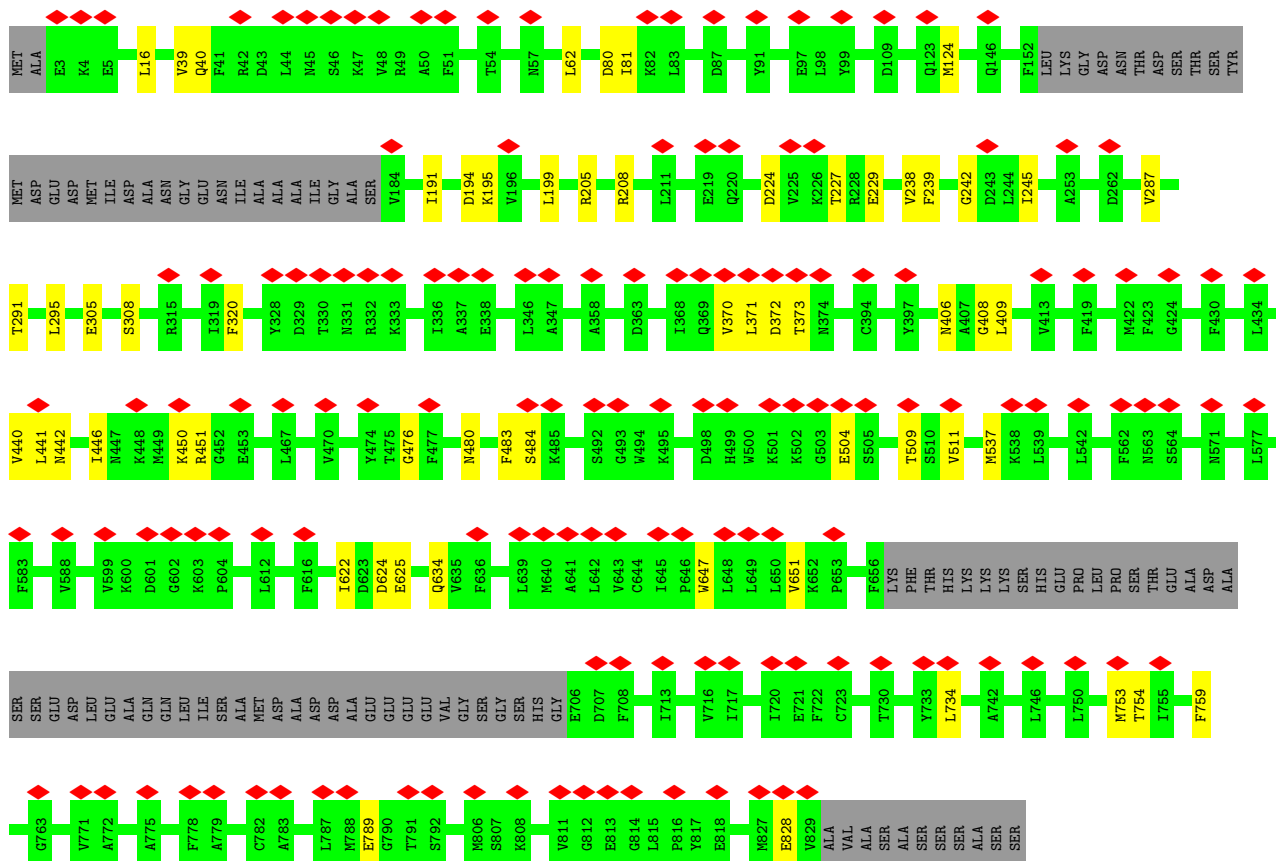







• Molecule 16: V-type proton ATPase subunit a, vacuolar isoform

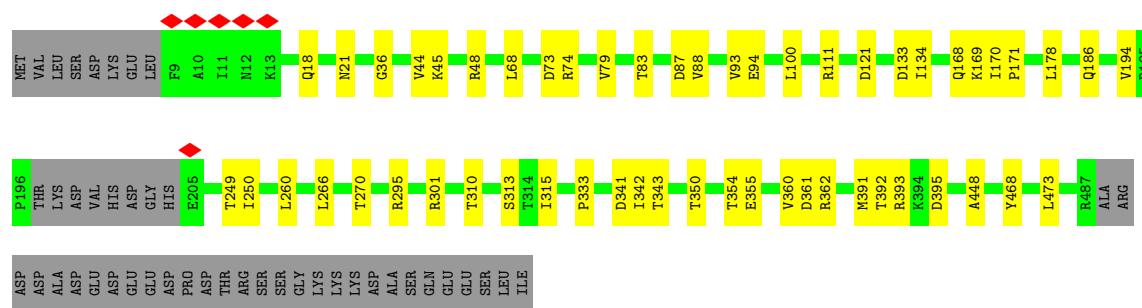
Chain Q: 18% 82% 7% 11%




• Molecule 17: V-type proton ATPase subunit B

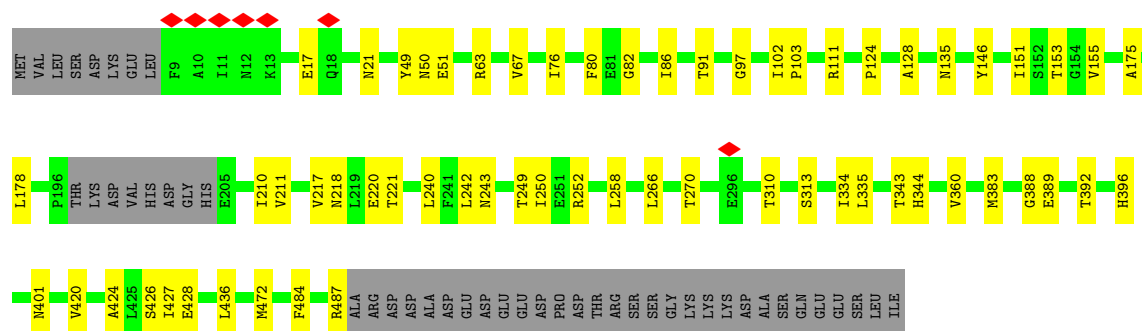


Chain B: 




• Molecule 17: V-type proton ATPase subunit B

Chain D: 



• Molecule 17: V-type proton ATPase subunit B

Chain F: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.25	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	532.8, 532.8, 532.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.665, 1.665, 1.665	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.16	0/4686	0.28	0/6351
1	C	0.16	0/4686	0.29	0/6351
1	E	0.17	0/4686	0.30	0/6351
2	G	0.11	0/1817	0.24	0/2436
2	I	0.13	0/1817	0.25	0/2436
2	K	0.13	0/1817	0.26	0/2436
3	H	0.10	0/876	0.22	0/1164
3	J	0.12	0/876	0.22	0/1164
3	L	0.13	0/876	0.28	0/1164
4	M	0.13	0/1798	0.26	0/2411
5	N	0.12	0/944	0.25	0/1277
6	O	0.10	0/3184	0.29	0/4314
7	R	0.12	0/4531	0.28	0/6116
8	S	0.10	0/2852	0.27	0/3870
9	T	0.09	0/1523	0.23	0/2068
10	U	0.10	0/1162	0.23	0/1575
11	V	0.08	0/1158	0.23	0/1574
11	W	0.09	0/1158	0.25	0/1574
11	X	0.09	0/1158	0.24	0/1574
11	Y	0.08	0/1164	0.22	0/1582
11	Z	0.09	0/1158	0.26	0/1574
11	a	0.08	0/1158	0.23	0/1574
11	b	0.08	0/1164	0.22	0/1582
11	c	0.08	0/1158	0.24	0/1574
12	d	0.19	0/569	0.40	0/776
13	e	0.12	0/409	0.26	0/557
14	f	0.11	0/600	0.25	0/822
15	P	0.09	0/3744	0.26	0/5060
16	Q	0.11	0/6221	0.28	0/8421
17	B	0.18	0/3776	0.31	0/5114
17	D	0.17	0/3776	0.31	0/5114
17	F	0.17	0/3792	0.30	0/5134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.13	0/70294	0.28	0/95090

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4587	4526	4525	34	0
1	C	4587	4526	4525	39	0
1	E	4587	4526	4525	42	0
2	G	1802	1874	1873	8	0
2	I	1802	1874	1873	16	0
2	K	1802	1874	1873	14	0
3	H	871	922	921	3	0
3	J	871	922	921	5	0
3	L	871	922	921	8	0
4	M	1779	1825	1824	17	0
5	N	928	929	926	13	0
6	O	3121	3155	3155	34	0
7	R	4442	4444	4440	48	0
8	S	2793	2678	2677	10	0
9	T	1492	1563	1562	6	0
10	U	1139	1195	1194	6	0
11	V	1140	1214	1214	6	0
11	W	1140	1214	1214	12	0
11	X	1140	1214	1214	4	0
11	Y	1146	1219	1219	4	0
11	Z	1140	1214	1214	5	0
11	a	1140	1214	1214	11	0
11	b	1146	1219	1219	4	0
11	c	1140	1214	1214	13	0
12	d	553	581	581	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	e	403	433	432	2	0
14	f	583	577	576	8	0
15	P	3691	3808	3807	20	0
16	Q	6069	6044	6041	46	0
17	B	3706	3702	3700	34	0
17	D	3706	3702	3700	40	0
17	F	3723	3717	3715	27	0
18	E	27	12	12	7	0
All	All	69067	70053	70021	508	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 4.

All (508) 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)
4:M:89:THR:OG1	4:M:118:ASN:OD1	1.91	0.87
2:I:51:VAL:O	2:I:55:THR:OG1	1.97	0.82
17:B:266:LEU:O	17:B:270:THR:OG1	2.00	0.80
4:M:44:ARG:NH1	5:N:116:PHE:O	2.18	0.76
12:d:64:ARG:NH1	16:Q:504:GLU:O	2.18	0.76
1:E:286:ARG:NH1	1:E:289:GLU:OE2	2.22	0.73
12:d:24:MET:SD	12:d:25:ALA:N	2.62	0.73
18:E:701:ADP:O1A	17:F:381:ARG:NH1	2.21	0.73
6:O:303:TRP:O	6:O:307:LYS:NZ	2.21	0.73
11:W:46:ARG:NH1	11:W:120:SER:O	2.22	0.72
2:I:143:GLU:OE1	2:I:143:GLU:N	2.23	0.72
17:F:190:GLN:NE2	17:F:451:ASP:OD1	2.23	0.72
1:C:280:TYR:OH	1:C:355:ASP:OD2	2.07	0.71
7:R:480:TYR:OH	7:R:496:GLU:OE1	2.06	0.71
1:A:74:GLU:N	1:A:74:GLU:OE1	2.24	0.70
5:N:34:GLU:OE2	5:N:61:ARG:NH1	2.25	0.70
3:L:51:ASP:OD1	3:L:52:LYS:N	2.25	0.69
1:A:529:ASN:N	1:A:535:ASP:OD2	2.25	0.69
17:D:102:ILE:HD12	17:D:258:LEU:HD22	1.76	0.68
2:K:158:ARG:NE	2:K:162:GLU:OE2	2.26	0.67
17:F:486:ASP:OD1	17:F:487:ARG:N	2.28	0.67
4:M:169:ARG:NH1	7:R:547:GLU:OE1	2.27	0.67
16:Q:224:ASP:OD1	16:Q:229:GLU:N	2.28	0.66
17:F:266:LEU:O	17:F:270:THR:OG1	2.13	0.66
1:E:239:VAL:HG13	1:E:240:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:ASN:OD1	1:E:466:VAL:N	2.28	0.66
16:Q:205:ARG:O	16:Q:208:ARG:NH1	2.28	0.66
10:U:107:PHE:HB2	11:V:22:ILE:HD12	1.79	0.65
17:B:73:ASP:OD1	17:B:74:ARG:N	2.29	0.65
4:M:131:GLN:OE1	4:M:131:GLN:N	2.29	0.65
6:O:314:GLU:OE2	6:O:388:TYR:OH	2.10	0.65
17:B:133:ASP:OD1	17:B:134:ILE:N	2.31	0.64
17:D:266:LEU:O	17:D:270:THR:OG1	2.12	0.64
1:E:262:LYS:N	18:E:701:ADP:O1B	2.30	0.64
17:D:63:ARG:NH1	17:D:82:GLY:O	2.30	0.64
17:F:257:ARG:NH2	17:F:311:ASP:OD1	2.31	0.64
13:e:242:SER:HG	13:e:243:TRP:CD1	2.16	0.63
17:B:310:THR:O	17:B:313:SER:OG	2.11	0.63
7:R:212:ASP:OD1	7:R:216:ASN:ND2	2.32	0.63
7:R:230:PRO:O	7:R:382:SER:OG	2.16	0.63
3:L:93:ASP:OD1	3:L:94:VAL:N	2.32	0.62
7:R:507:GLN:O	17:F:487:ARG:NH2	2.32	0.62
17:B:87:ASP:OD1	17:B:88:VAL:N	2.32	0.62
17:F:412:ASP:OD1	17:F:413:ALA:N	2.33	0.62
1:E:405:ASP:OD1	1:E:406:ARG:N	2.33	0.62
17:B:341:ASP:OD1	17:B:342:ILE:N	2.33	0.62
1:C:463:TYR:O	1:C:467:LEU:HD23	2.00	0.61
11:b:107:ALA:O	11:b:111:VAL:HG22	2.01	0.61
11:c:1:MET:HE1	11:c:7:VAL:HG12	1.82	0.61
17:D:178:LEU:HD23	17:D:360:VAL:HG12	1.81	0.61
11:a:46:ARG:NH1	11:a:48:ASP:OD2	2.33	0.61
14:f:18:ALA:O	14:f:22:VAL:HG13	2.01	0.61
5:N:20:LEU:HD21	5:N:68:LEU:HD13	1.83	0.61
17:F:346:ILE:HB	17:F:347:PRO:HD3	1.82	0.61
3:L:71:LYS:O	3:L:75:GLY:N	2.35	0.60
12:d:18:SER:O	12:d:22:TRP:N	2.33	0.60
15:P:357:ASP:OD1	15:P:358:GLU:N	2.34	0.60
15:P:236:ASN:O	15:P:241:GLN:NE2	2.35	0.59
17:B:186:GLN:NE2	17:B:448:ALA:O	2.36	0.59
16:Q:509:THR:HG23	16:Q:511:VAL:HG13	1.85	0.59
2:I:113:ASN:ND2	2:I:116:GLU:OE1	2.36	0.59
16:Q:372:ASP:OD1	16:Q:373:THR:N	2.36	0.59
2:I:19:LYS:NZ	16:Q:208:ARG:O	2.35	0.58
7:R:40:THR:OG1	7:R:43:GLU:OE1	2.19	0.58
3:H:98:LEU:O	3:H:101:THR:OG1	2.19	0.58
2:K:185:SER:N	2:K:204:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:567:MET:O	17:D:401:ASN:ND2	2.37	0.58
7:R:95:MET:SD	7:R:96:LYS:N	2.77	0.58
17:F:471:GLU:N	17:F:471:GLU:OE1	2.36	0.58
17:B:170:ILE:HG23	17:B:170:ILE:O	2.04	0.57
2:I:141:ALA:HB2	2:I:188:VAL:HG12	1.85	0.57
5:N:68:LEU:HD21	5:N:94:ILE:HG21	1.87	0.57
1:E:263:THR:OG1	18:E:701:ADP:O2B	2.17	0.57
1:A:80:THR:OG1	1:A:83:ASP:OD2	2.23	0.57
2:G:192:ASN:OD1	2:G:195:ASP:N	2.37	0.56
8:S:178:GLU:OE1	8:S:181:ARG:NH1	2.38	0.56
1:E:48:LEU:HD11	1:E:57:VAL:HG13	1.86	0.56
11:Y:61:GLY:O	11:Y:65:ILE:HD12	2.05	0.56
17:B:171:PRO:CD	17:B:354:THR:HG21	2.35	0.56
7:R:403:ASN:OD1	7:R:435:ASN:ND2	2.38	0.56
16:Q:483:PHE:O	16:Q:484:SER:OG	2.17	0.56
6:O:1:MET:SD	6:O:12:ILE:HG22	2.46	0.56
1:C:171:LYS:N	1:C:346:GLN:OE1	2.38	0.56
16:Q:446:ILE:HD12	16:Q:451:ARG:NH1	2.19	0.56
16:Q:242:GLY:H	16:Q:245:ILE:HD11	1.71	0.56
7:R:91:ASN:O	7:R:95:MET:N	2.38	0.56
4:M:146:LEU:HD12	5:N:94:ILE:HD12	1.88	0.55
1:E:309:GLU:N	1:E:309:GLU:OE1	2.39	0.55
7:R:187:PHE:O	7:R:191:LEU:HD23	2.06	0.55
6:O:10:ASP:OD1	6:O:391:ASN:ND2	2.38	0.55
2:I:147:ASP:OD1	2:I:147:ASP:N	2.39	0.55
1:C:428:THR:O	1:C:432:LEU:HD23	2.07	0.55
2:I:154:ASP:N	2:I:154:ASP:OD1	2.38	0.55
7:R:225:LEU:HG	7:R:232:VAL:HG21	1.88	0.55
17:D:218:ASN:OD1	17:D:220:GLU:N	2.40	0.55
7:R:285:ILE:HG22	7:R:285:ILE:O	2.07	0.55
16:Q:789:GLU:N	16:Q:789:GLU:OE1	2.40	0.55
2:K:154:ASP:OD1	2:K:155:ASP:N	2.39	0.55
1:E:483:ASP:OD1	1:E:483:ASP:N	2.40	0.54
2:G:125:ILE:HG12	2:G:188:VAL:HG21	1.88	0.54
11:a:39:ILE:HG13	11:a:116:VAL:HG21	1.89	0.54
1:E:48:LEU:HD12	1:E:58:GLY:O	2.08	0.54
11:c:22:ILE:O	11:c:26:LEU:HD23	2.08	0.54
12:d:26:PRO:HB2	12:d:30:GLN:HA	1.90	0.54
16:Q:227:THR:HG22	16:Q:227:THR:O	2.07	0.54
17:D:334:ILE:C	17:D:335:LEU:HD12	2.32	0.54
1:E:368:SER:OG	1:E:373:GLU:OE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ILE:HD11	1:A:550:PHE:HB3	1.90	0.54
1:E:264:VAL:HG21	18:E:701:ADP:C8	2.43	0.54
17:D:17:GLU:O	17:D:21:ASN:ND2	2.41	0.54
17:F:416:MET:O	17:F:420:VAL:HG22	2.08	0.54
17:B:171:PRO:HD3	17:B:354:THR:HG21	1.90	0.53
1:A:477:GLU:OE1	1:A:477:GLU:N	2.40	0.53
1:C:355:ASP:O	1:C:415:ALA:HB3	2.09	0.53
6:O:31:ASP:OD1	6:O:32:SER:N	2.41	0.53
7:R:182:ASP:OD1	7:R:183:PHE:N	2.40	0.53
4:M:9:PHE:HE2	17:D:344:HIS:HD1	1.56	0.53
2:I:126:VAL:HG21	2:I:159:GLU:OE1	2.09	0.53
14:f:6:SER:OG	14:f:72:GLN:O	2.24	0.53
1:C:472:ASP:OD1	1:C:473:SER:N	2.42	0.53
6:O:75:ILE:HD11	6:O:306:ILE:HD11	1.90	0.53
7:R:201:THR:O	7:R:202:ASN:OD1	2.26	0.53
1:A:172:ILE:C	1:A:173:LEU:HD12	2.34	0.53
6:O:314:GLU:O	6:O:318:ARG:N	2.39	0.53
16:Q:446:ILE:HG23	16:Q:451:ARG:NH2	2.24	0.53
4:M:160:ASP:OD2	5:N:111:ARG:NH1	2.42	0.52
5:N:51:THR:HG22	5:N:77:ILE:HG22	1.91	0.52
16:Q:287:VAL:O	16:Q:291:THR:HG23	2.09	0.52
17:F:36:GLY:O	17:F:83:THR:HG21	2.08	0.52
3:L:44:ASP:OD1	3:L:45:SER:N	2.43	0.52
11:W:137:GLU:N	11:W:137:GLU:OE1	2.42	0.52
17:D:240:LEU:HD21	17:D:242:LEU:HD21	1.90	0.52
1:E:193:LEU:HD12	1:E:212:TYR:HB3	1.92	0.52
4:M:143:VAL:HG21	5:N:25:ILE:HD11	1.92	0.52
11:Y:135:PHE:O	11:Y:138:VAL:HG22	2.10	0.52
8:S:88:SER:N	8:S:91:THR:OG1	2.42	0.52
1:A:252:THR:HG22	1:A:253:CYS:N	2.25	0.52
1:A:576:ASP:OD1	1:A:576:ASP:N	2.42	0.52
15:P:424:LEU:HD23	15:P:465:ALA:HA	1.91	0.52
1:A:171:LYS:N	1:A:346:GLN:OE1	2.44	0.51
1:C:106:ASP:OD1	1:C:320:ASN:ND2	2.35	0.51
6:O:75:ILE:HD11	6:O:306:ILE:CD1	2.39	0.51
11:c:126:PHE:O	11:c:130:ILE:HD12	2.09	0.51
17:B:194:VAL:HG13	17:B:194:VAL:O	2.09	0.51
1:E:240:LEU:HD12	1:E:439:TRP:CE2	2.46	0.51
7:R:176:MET:SD	7:R:176:MET:N	2.83	0.51
17:B:391:MET:O	17:B:392:THR:OG1	2.26	0.51
8:S:40:GLU:OE1	8:S:40:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:330:ILE:HG22	6:O:332:VAL:HG23	1.93	0.51
7:R:96:LYS:N	7:R:170:ASP:OD2	2.44	0.51
17:D:102:ILE:HD12	17:D:258:LEU:CD2	2.41	0.50
1:A:303:GLU:O	1:A:304:MET:HE2	2.11	0.50
7:R:229:ASN:HB3	7:R:232:VAL:HG23	1.93	0.50
16:Q:647:TRP:CD2	16:Q:651:VAL:HG11	2.46	0.50
17:D:103:PRO:HB2	17:D:128:ALA:HB2	1.94	0.50
1:A:465:ASN:OD1	1:A:466:VAL:N	2.45	0.50
11:b:110:ILE:HD12	13:e:247:LEU:HD11	1.92	0.50
1:E:442:ASP:OD1	1:E:443:LYS:N	2.45	0.50
12:d:30:GLN:O	12:d:34:ARG:N	2.45	0.50
16:Q:305:GLU:O	16:Q:308:SER:OG	2.26	0.50
16:Q:624:ASP:OD1	16:Q:625:GLU:N	2.45	0.50
12:d:67:LEU:HD22	14:f:42:ILE:HA	1.94	0.49
1:C:292:GLU:OE2	17:D:146:TYR:OH	2.27	0.49
10:U:104:CYS:O	11:V:22:ILE:HD11	2.12	0.49
6:O:330:ILE:CG2	6:O:332:VAL:HG23	2.42	0.49
11:a:121:GLN:N	11:a:121:GLN:OE1	2.45	0.49
11:c:77:SER:O	11:c:82:GLN:NE2	2.45	0.49
17:F:374:ASN:OD1	17:F:375:VAL:N	2.45	0.49
1:C:75:GLU:OE1	1:C:75:GLU:N	2.45	0.49
6:O:107:VAL:HG12	6:O:392:LEU:HD22	1.93	0.49
2:I:219:ARG:NH1	17:F:129:GLU:OE1	2.45	0.49
6:O:387:MET:SD	6:O:387:MET:N	2.85	0.49
17:B:361:ASP:OD1	17:B:362:ARG:N	2.46	0.49
1:E:349:ASN:CG	1:E:409:SER:HG	2.14	0.49
10:U:104:CYS:HA	11:V:22:ILE:HD11	1.93	0.49
7:R:315:LEU:HD21	7:R:332:VAL:HA	1.94	0.49
11:c:54:ILE:O	11:c:54:ILE:HG22	2.13	0.49
17:D:51:GLU:OE2	17:D:97:GLY:N	2.38	0.49
17:D:392:THR:HG21	17:D:396:HIS:ND1	2.27	0.49
11:V:95:LEU:HD11	11:W:18:ALA:HB1	1.95	0.49
1:E:428:THR:O	1:E:432:LEU:HG	2.13	0.48
12:d:32:VAL:HG13	16:Q:409:LEU:HD22	1.95	0.48
1:C:455:ASN:CG	1:C:458:VAL:HG12	2.38	0.48
6:O:58:LEU:HD22	16:Q:245:ILE:HD13	1.93	0.48
17:B:355:GLU:N	17:B:355:GLU:OE1	2.46	0.48
17:B:392:THR:HG22	17:B:393:ARG:N	2.28	0.48
17:D:334:ILE:O	17:D:335:LEU:HD12	2.13	0.48
1:C:281:VAL:HG13	1:C:281:VAL:O	2.13	0.48
7:R:556:GLY:O	7:R:560:GLN:NE2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:138:ASN:O	9:T:141:THR:OG1	2.27	0.48
11:W:55:VAL:N	11:W:56:PRO:CD	2.76	0.48
17:F:39:VAL:HG12	17:F:40:ILE:N	2.27	0.48
2:K:147:ASP:OD1	2:K:147:ASP:N	2.45	0.48
6:O:96:ALA:O	6:O:100:LEU:HD12	2.12	0.48
7:R:505:LEU:HD23	7:R:506:ILE:O	2.13	0.48
11:c:6:PRO:HG2	11:c:9:ALA:HB2	1.95	0.48
14:f:38:PHE:O	14:f:39:VAL:HG13	2.14	0.48
7:R:43:GLU:OE1	7:R:43:GLU:N	2.46	0.48
1:A:540:ILE:HG23	1:A:541:TRP:N	2.28	0.48
1:E:269:LEU:HD23	1:E:269:LEU:C	2.39	0.48
15:P:50:ILE:HG23	15:P:51:LEU:HD12	1.95	0.48
17:B:178:LEU:HD12	17:B:360:VAL:HG12	1.95	0.48
1:E:235:THR:O	1:E:235:THR:HG22	2.14	0.48
9:T:115:LEU:O	9:T:119:ILE:HD12	2.12	0.48
1:A:362:GLU:OE1	1:A:365:ARG:NH2	2.46	0.48
1:C:252:THR:HG22	1:C:253:CYS:N	2.29	0.48
1:C:335:THR:O	1:C:339:LEU:HD13	2.13	0.48
4:M:85:GLU:O	8:S:116:HIS:NE2	2.46	0.48
17:F:102:ILE:HD12	17:F:258:LEU:HD22	1.96	0.48
1:C:95:GLU:C	1:C:96:LEU:HD12	2.39	0.47
1:A:38:GLU:OE1	1:A:39:ASN:N	2.48	0.47
1:A:442:ASP:OD1	1:A:443:LYS:N	2.47	0.47
15:P:417:LYS:NZ	15:P:458:ASP:OD2	2.41	0.47
1:E:264:VAL:HG11	18:E:701:ADP:C5	2.49	0.47
1:C:157:ILE:HD11	1:C:406:ARG:NE	2.29	0.47
2:K:142:LEU:N	2:K:142:LEU:HD12	2.29	0.47
6:O:12:ILE:C	6:O:390:ILE:HD11	2.39	0.47
6:O:47:ASP:OD1	6:O:49:LYS:NZ	2.44	0.47
15:P:356:PHE:O	15:P:360:VAL:HG23	2.15	0.47
17:F:79:VAL:HG12	17:F:80:PHE:O	2.14	0.47
7:R:548:ASP:OD1	7:R:549:ARG:N	2.48	0.47
17:D:217:VAL:HG22	17:D:221:THR:HB	1.97	0.47
1:E:255:PRO:HG2	1:E:438:PHE:HE1	1.80	0.47
1:E:59:GLU:OE1	1:E:73:TYR:OH	2.33	0.47
17:B:468:TYR:HB2	17:B:473:LEU:HD21	1.97	0.47
6:O:318:ARG:HA	16:Q:208:ARG:HB3	1.97	0.46
15:P:280:ILE:O	15:P:281:THR:HG23	2.14	0.46
17:B:79:VAL:HG23	17:B:79:VAL:O	2.15	0.46
14:f:7:THR:O	14:f:7:THR:HG22	2.15	0.46
1:E:231:TYR:O	1:E:247:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:85:ILE:HG23	6:O:149:TYR:CD1	2.51	0.46
17:F:369:ILE:HG22	17:F:370:TYR:N	2.30	0.46
1:C:432:LEU:HD11	1:C:438:PHE:CG	2.51	0.46
7:R:51:LEU:HD22	7:R:107:LEU:HD23	1.96	0.46
11:Z:135:PHE:O	11:Z:138:VAL:HG22	2.15	0.46
17:B:350:THR:O	17:B:354:THR:HG22	2.15	0.46
1:C:172:ILE:C	1:C:173:LEU:HD12	2.41	0.46
6:O:380:THR:HG21	16:Q:205:ARG:CB	2.46	0.46
11:Z:132:ILE:HG22	11:a:57:VAL:HG11	1.96	0.46
16:Q:753:MET:SD	16:Q:754:THR:HG23	2.56	0.46
17:D:310:THR:O	17:D:313:SER:OG	2.20	0.46
1:E:477:GLU:OE1	1:E:477:GLU:N	2.45	0.46
11:c:55:VAL:N	11:c:56:PRO:CD	2.78	0.46
1:A:239:VAL:HG13	1:A:240:LEU:N	2.29	0.46
2:G:129:LEU:O	2:G:133:LEU:N	2.42	0.46
7:R:424:TYR:HE2	7:R:475:PHE:CZ	2.33	0.46
12:d:26:PRO:HA	12:d:29:ASN:HB2	1.98	0.46
8:S:205:LYS:O	8:S:209:GLN:N	2.45	0.45
11:b:113:ASP:OD1	11:b:117:ARG:NH1	2.47	0.45
16:Q:622:ILE:HG22	16:Q:634:GLN:HB3	1.97	0.45
3:J:3:GLN:HG3	3:J:4:LYS:H	1.82	0.45
4:M:123:THR:OG1	4:M:136:LYS:NZ	2.49	0.45
11:a:48:ASP:OD1	11:a:48:ASP:N	2.50	0.45
1:C:338:THR:O	1:C:341:GLU:N	2.49	0.45
7:R:290:VAL:HG22	7:R:291:MET:N	2.31	0.45
8:S:141:VAL:HG12	8:S:142:ALA:N	2.31	0.45
10:U:37:GLY:O	10:U:41:SER:OG	2.34	0.45
17:D:67:VAL:HG23	17:D:76:ILE:O	2.16	0.45
1:C:362:GLU:OE1	1:C:365:ARG:NH1	2.50	0.45
6:O:300:PHE:O	6:O:304:PHE:N	2.45	0.45
6:O:389:ILE:O	6:O:390:ILE:HG23	2.16	0.45
17:D:151:ILE:O	17:D:151:ILE:HG23	2.17	0.45
1:C:540:ILE:HG23	1:C:541:TRP:N	2.31	0.45
7:R:422:ASP:OD1	7:R:423:ILE:N	2.49	0.45
2:G:192:ASN:ND2	2:G:194:SER:OG	2.50	0.45
4:M:8:VAL:HG23	4:M:188:ILE:HD11	1.97	0.45
7:R:341:LEU:HD21	7:R:466:PHE:HE2	1.82	0.45
8:S:245:ILE:O	8:S:245:ILE:HG23	2.17	0.45
11:a:39:ILE:CG1	11:a:116:VAL:HG21	2.47	0.45
1:C:293:VAL:HG23	1:C:294:LEU:N	2.31	0.45
6:O:1:MET:HB2	6:O:389:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:347:GLU:O	15:P:351:GLN:NE2	2.45	0.45
17:F:81:GLU:HA	17:F:248:PRO:HG2	1.99	0.45
2:K:192:ASN:OD1	2:K:193:ALA:N	2.50	0.45
11:W:113:ASP:OD1	11:W:113:ASP:N	2.44	0.45
6:O:174:SER:C	6:O:175:LEU:HD22	2.41	0.45
11:V:67:GLY:HA2	11:V:97:VAL:HG11	1.99	0.45
12:d:57:HIS:N	12:d:58:PRO:CD	2.80	0.45
12:d:63:ARG:NH1	14:f:36:GLU:OE1	2.50	0.45
1:A:521:ILE:HD11	1:A:550:PHE:CB	2.46	0.44
1:E:468:ASN:OD1	1:E:469:LYS:N	2.49	0.44
1:A:223:VAL:HG22	1:A:224:THR:N	2.33	0.44
1:E:95:GLU:C	1:E:96:LEU:HD12	2.42	0.44
2:G:84:MET:SD	3:H:72:ALA:HB1	2.57	0.44
2:K:115:ASP:OD1	2:K:116:GLU:N	2.49	0.44
7:R:437:ILE:HD12	7:R:437:ILE:H	1.82	0.44
17:D:103:PRO:CB	17:D:128:ALA:HB2	2.47	0.44
17:D:343:THR:HG22	17:D:343:THR:O	2.18	0.44
17:D:436:LEU:C	17:D:436:LEU:HD23	2.43	0.44
11:a:9:ALA:N	11:a:10:PRO:HD2	2.31	0.44
14:f:51:VAL:HG11	16:Q:759:PHE:CZ	2.52	0.44
17:D:175:ALA:HB3	17:D:178:LEU:HD13	1.98	0.44
1:A:472:ASP:OD1	1:A:473:SER:N	2.50	0.44
6:O:284:LEU:O	6:O:288:LEU:HD13	2.17	0.44
7:R:362:TYR:CZ	7:R:366:LEU:HD21	2.52	0.44
7:R:451:LYS:N	7:R:454:SER:O	2.48	0.44
16:Q:16:LEU:HD22	16:Q:373:THR:CG2	2.47	0.44
17:D:249:THR:HG23	17:D:250:ILE:N	2.33	0.44
17:D:428:GLU:OE1	17:D:472:MET:HE2	2.18	0.44
1:C:356:SER:O	1:C:357:SER:C	2.60	0.44
3:H:95:VAL:HG23	3:H:96:LYS:N	2.32	0.44
11:X:55:VAL:N	11:X:56:PRO:HD2	2.33	0.44
17:B:36:GLY:O	17:B:83:THR:HG21	2.18	0.44
1:C:27:ILE:HD12	1:C:83:ASP:HB2	2.00	0.44
2:G:142:LEU:HD11	2:G:184:VAL:HG11	1.99	0.44
6:O:322:PRO:N	6:O:323:PRO:HD2	2.33	0.44
6:O:364:ILE:O	6:O:375:ALA:N	2.48	0.44
16:Q:647:TRP:O	16:Q:651:VAL:HG13	2.18	0.44
1:A:35:VAL:HG12	1:A:36:ILE:N	2.32	0.44
1:E:261:GLY:N	18:E:701:ADP:O2A	2.46	0.44
7:R:445:ASP:OD1	7:R:445:ASP:N	2.47	0.44
8:S:88:SER:O	8:S:92:ARG:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:131:GLU:OE1	9:T:132:ASN:N	2.50	0.44
17:B:100:LEU:HD23	17:B:134:ILE:HD13	1.99	0.44
17:F:133:ASP:OD1	17:F:134:ILE:N	2.51	0.44
7:R:252:THR:HG21	7:R:489:LEU:HA	1.99	0.44
9:T:60:ALA:HA	9:T:145:LEU:HD11	2.00	0.44
11:c:135:PHE:O	11:c:138:VAL:HG12	2.17	0.44
1:C:315:THR:HG22	1:C:316:THR:N	2.33	0.44
5:N:11:ILE:O	5:N:69:ILE:HA	2.18	0.44
16:Q:194:ASP:OD2	16:Q:195:LYS:NZ	2.43	0.44
9:T:145:LEU:HA	9:T:205:MET:HE2	2.00	0.43
5:N:85:THR:OG1	7:R:533:GLU:OE2	2.31	0.43
7:R:111:ILE:HG21	7:R:269:PHE:CZ	2.53	0.43
1:A:515:LEU:HD23	1:A:515:LEU:C	2.44	0.43
2:K:164:ALA:HB1	2:K:166:ARG:HG2	2.00	0.43
6:O:62:ILE:HD13	16:Q:245:ILE:HG22	1.99	0.43
7:R:193:ILE:HD11	7:R:214:TRP:HA	2.01	0.43
11:W:38:GLY:O	11:W:117:ARG:NH2	2.49	0.43
11:Z:9:ALA:HB3	11:Z:10:PRO:HD3	2.00	0.43
11:c:17:CYS:O	11:c:21:ILE:HG22	2.18	0.43
15:P:394:ILE:H	15:P:394:ILE:HD12	1.83	0.43
16:Q:191:ILE:HD13	16:Q:199:LEU:HD22	2.00	0.43
1:C:455:ASN:OD1	1:C:457:SER:N	2.51	0.43
11:W:58:ILE:HG22	11:W:58:ILE:O	2.18	0.43
15:P:73:ASN:HD22	15:P:116:PHE:HZ	1.66	0.43
17:D:80:PHE:CD1	17:D:250:ILE:HG21	2.54	0.43
1:E:103:THR:HG22	1:E:104:ILE:N	2.34	0.43
6:O:62:ILE:HD13	16:Q:245:ILE:CG2	2.49	0.43
17:B:18:GLN:O	17:B:21:ASN:ND2	2.51	0.43
17:D:484:PHE:HA	17:D:487:ARG:HG2	2.01	0.43
2:G:130:LEU:HD22	2:G:164:ALA:HB2	1.99	0.43
2:K:103:THR:HG22	3:L:95:VAL:HG13	2.01	0.43
3:L:76:VAL:O	3:L:79:GLU:N	2.50	0.43
7:R:566:SER:HB2	17:D:383:MET:HE2	1.99	0.43
11:a:55:VAL:N	11:a:56:PRO:HD2	2.33	0.43
11:b:49:LEU:HD21	11:b:116:VAL:HG22	2.00	0.43
15:P:168:ASN:OD1	15:P:169:ASN:N	2.51	0.43
16:Q:828:GLU:N	16:Q:828:GLU:OE1	2.52	0.43
17:D:420:VAL:HG22	17:D:424:ALA:HB3	2.01	0.43
17:F:67:VAL:O	17:F:68:LEU:HD12	2.19	0.43
2:K:191:SER:HA	2:K:198:GLU:HA	2.00	0.43
17:B:171:PRO:HA	17:B:333:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:30:THR:HG23	6:O:31:ASP:N	2.33	0.43
7:R:125:THR:HG22	7:R:166:ILE:HD12	2.00	0.43
17:B:395:ASP:OD1	17:B:395:ASP:N	2.51	0.43
1:A:192:THR:N	1:A:195:GLU:OE1	2.50	0.43
10:U:132:ARG:O	10:U:135:VAL:HG22	2.19	0.43
17:B:249:THR:HG23	17:B:250:ILE:N	2.34	0.43
16:Q:80:ASP:OD1	16:Q:81:ILE:N	2.52	0.43
1:E:333:ILE:HD11	1:E:360:TRP:CD2	2.54	0.42
1:E:357:SER:O	1:E:360:TRP:HB3	2.18	0.42
1:E:581:VAL:HG23	1:E:582:SER:N	2.34	0.42
2:I:35:ILE:HG21	3:J:24:ALA:HB1	2.01	0.42
7:R:490:SER:O	7:R:495:GLU:N	2.50	0.42
11:W:110:ILE:HG21	11:X:33:ALA:HB1	2.00	0.42
17:F:249:THR:HG23	17:F:250:ILE:N	2.34	0.42
4:M:72:SER:O	4:M:76:GLY:N	2.50	0.42
16:Q:370:VAL:HG22	16:Q:371:LEU:N	2.35	0.42
17:B:260:LEU:HD11	17:B:315:ILE:HG23	2.01	0.42
17:D:153:THR:HG22	17:D:155:VAL:H	1.84	0.42
7:R:202:ASN:OD1	7:R:202:ASN:C	2.62	0.42
1:E:576:ASP:OD1	1:E:577:VAL:N	2.52	0.42
17:B:44:VAL:HG12	17:B:45:LYS:N	2.35	0.42
5:N:72:HIS:CE1	5:N:73:ILE:CG1	3.02	0.42
7:R:204:LYS:N	7:R:276:VAL:O	2.44	0.42
12:d:26:PRO:CA	12:d:29:ASN:HB2	2.49	0.42
17:F:114:ASP:OD1	17:F:117:GLY:N	2.53	0.42
1:A:247:VAL:HG12	1:A:463:TYR:CD2	2.55	0.42
1:A:315:THR:HG22	1:A:316:THR:N	2.34	0.42
6:O:366:LYS:NZ	6:O:368:ASP:OD2	2.47	0.42
16:Q:406:ASN:OD1	16:Q:408:GLY:N	2.46	0.42
17:B:111:ARG:NE	17:B:121:ASP:OD2	2.43	0.42
1:C:176:PRO:O	1:C:177:ARG:HG3	2.19	0.42
1:E:264:VAL:HG11	18:E:701:ADP:C6	2.55	0.42
6:O:118:THR:O	6:O:118:THR:HG22	2.18	0.42
15:P:418:ILE:HD12	15:P:421:GLN:HE21	1.85	0.42
16:Q:39:VAL:HG22	16:Q:40:GLN:N	2.35	0.42
17:D:211:VAL:HG23	17:D:211:VAL:O	2.20	0.42
1:A:128:ILE:HG13	1:A:130:THR:HG23	2.02	0.42
1:C:283:CYS:SG	1:C:356:SER:OG	2.55	0.42
2:I:50:ILE:HG13	2:I:51:VAL:N	2.35	0.42
2:K:120:ILE:O	2:K:123:SER:OG	2.13	0.42
15:P:458:ASP:HB3	15:P:461:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:VAL:O	1:C:327:ALA:C	2.61	0.42
1:C:333:ILE:O	1:C:336:GLY:N	2.53	0.42
1:E:499:VAL:HG13	1:E:504:LYS:N	2.35	0.42
1:E:501:LEU:HD23	1:E:501:LEU:H	1.85	0.42
4:M:29:TYR:HB2	4:M:173:ILE:HG21	2.01	0.42
7:R:290:VAL:HG22	7:R:291:MET:H	1.85	0.42
7:R:316:TYR:OH	7:R:322:GLY:O	2.37	0.42
11:Z:45:LEU:H	11:Z:45:LEU:HD23	1.83	0.42
11:c:5:CYS:N	11:c:6:PRO:CD	2.82	0.42
15:P:466:LEU:HD21	16:Q:291:THR:HG22	2.02	0.42
17:F:332:ILE:O	17:F:332:ILE:HG22	2.20	0.42
5:N:72:HIS:CE1	5:N:73:ILE:HG13	2.54	0.41
1:A:147:GLN:O	1:A:182:ILE:HD11	2.19	0.41
2:I:28:ALA:HB2	3:J:20:ILE:HG21	2.02	0.41
8:S:64:THR:HG23	8:S:64:THR:O	2.19	0.41
15:P:217:ILE:HG22	15:P:243:GLN:HG3	2.02	0.41
17:D:86:ILE:HG23	17:D:91:THR:HG21	2.01	0.41
2:I:128:ALA:HB3	2:I:190:VAL:HG21	2.02	0.41
17:B:171:PRO:HG3	17:B:354:THR:HG21	2.02	0.41
17:B:301:ARG:NH2	17:B:343:THR:O	2.54	0.41
17:F:114:ASP:HB3	17:F:120:ILE:HG21	2.01	0.41
1:A:140:GLN:HA	1:A:140:GLN:OE1	2.20	0.41
1:A:326:VAL:HG13	1:A:327:ALA:N	2.36	0.41
1:E:337:ILE:HD11	1:E:412:ILE:HD11	2.02	0.41
2:I:141:ALA:CB	2:I:188:VAL:HG12	2.50	0.41
11:V:55:VAL:N	11:V:56:PRO:CD	2.82	0.41
16:Q:242:GLY:N	16:Q:245:ILE:HD11	2.34	0.41
17:F:144:ARG:NH2	17:F:319:ALA:O	2.53	0.41
1:C:254:ILE:HG23	1:C:254:ILE:O	2.20	0.41
1:E:343:PHE:O	1:E:346:GLN:N	2.54	0.41
15:P:309:ILE:HG13	15:P:310:LYS:N	2.36	0.41
15:P:372:PRO:N	15:P:373:PRO:HD2	2.36	0.41
15:P:466:LEU:HD22	16:Q:124:MET:SD	2.61	0.41
1:A:80:THR:HG22	17:B:48:ARG:HG2	2.03	0.41
2:K:215:LEU:N	2:K:216:PRO:HD2	2.34	0.41
9:T:96:ILE:HD12	9:T:174:ASP:HB3	2.03	0.41
11:W:144:LEU:O	11:W:148:LEU:HD23	2.21	0.41
11:c:20:ALA:O	11:c:24:THR:OG1	2.28	0.41
15:P:107:ASP:OD1	15:P:108:LYS:N	2.52	0.41
17:D:210:ILE:HG22	17:D:211:VAL:N	2.36	0.41
17:D:243:ASN:ND2	17:D:252:ARG:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:TYR:O	1:C:247:VAL:HG23	2.21	0.41
3:L:51:ASP:OD1	3:L:51:ASP:C	2.64	0.41
7:R:92:PHE:CG	7:R:93:PRO:HD3	2.56	0.41
16:Q:450:LYS:C	16:Q:451:ARG:HD3	2.46	0.41
1:C:324:MET:HB3	1:C:325:PRO:HD2	2.01	0.41
4:M:71:VAL:HG22	4:M:131:GLN:HB3	2.03	0.41
7:R:180:PRO:HA	7:R:240:SER:HA	2.02	0.41
11:W:139:LEU:HD21	11:X:28:ALA:HB3	2.03	0.41
11:Y:113:ASP:OD1	11:Y:114:ALA:N	2.54	0.41
11:a:62:ILE:O	11:a:62:ILE:HG22	2.20	0.41
12:d:30:GLN:O	12:d:31:ALA:C	2.62	0.41
16:Q:62:LEU:HD11	16:Q:320:PHE:CZ	2.56	0.41
16:Q:442:ASN:O	16:Q:446:ILE:HG12	2.21	0.41
17:D:388:GLY:O	17:D:389:GLU:HB3	2.21	0.41
1:A:425:ASP:OD1	1:A:428:THR:OG1	2.33	0.41
1:E:129:ASP:O	1:E:130:THR:HG23	2.21	0.41
1:E:531:TYR:CZ	17:F:384:LYS:HD2	2.56	0.41
1:E:603:LEU:C	1:E:603:LEU:HD23	2.45	0.41
2:G:147:ASP:OD1	2:G:147:ASP:N	2.53	0.41
2:K:175:SER:OG	2:K:177:ASP:O	2.31	0.41
4:M:5:ARG:NH1	4:M:6:GLU:O	2.54	0.41
4:M:72:SER:HA	4:M:75:THR:HG22	2.03	0.41
7:R:432:ILE:HG22	7:R:433:TYR:N	2.35	0.41
8:S:259:ALA:HB1	8:S:264:GLY:HA3	2.02	0.41
11:W:50:LEU:HG	11:W:51:PHE:H	1.85	0.41
11:Y:55:VAL:N	11:Y:56:PRO:CD	2.84	0.41
11:a:42:THR:HG1	11:a:120:SER:HG	1.67	0.41
11:c:21:ILE:HG23	11:c:22:ILE:N	2.36	0.41
16:Q:537:MET:HE2	16:Q:734:LEU:HD11	2.02	0.41
17:B:68:LEU:HD22	17:B:295:ARG:CZ	2.51	0.41
17:B:168:GLN:CG	17:B:169:LYS:N	2.84	0.41
1:A:96:LEU:HD13	1:A:342:TYR:HB2	2.03	0.41
1:A:222:PRO:HB2	1:A:401:LEU:HD13	2.02	0.41
1:C:570:LEU:HD12	1:C:614:SER:OG	2.21	0.41
6:O:12:ILE:O	6:O:390:ILE:HD11	2.21	0.41
16:Q:238:VAL:HG12	16:Q:239:PHE:N	2.35	0.41
16:Q:476:GLY:O	16:Q:480:ASN:N	2.54	0.41
1:C:282:GLY:N	1:C:318:VAL:O	2.48	0.40
1:C:373:GLU:OE2	1:C:383:TYR:CE2	2.74	0.40
2:I:51:VAL:HG23	2:I:52:ARG:N	2.36	0.40
11:W:135:PHE:O	11:W:139:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:42:THR:OG1	11:a:120:SER:OG	2.38	0.40
15:P:40:ASP:O	15:P:43:THR:HG22	2.20	0.40
17:D:49:TYR:CD2	17:D:50:ASN:HB2	2.56	0.40
17:D:111:ARG:NH1	17:D:124:PRO:O	2.40	0.40
17:D:426:SER:OG	17:D:427:ILE:N	2.54	0.40
1:C:28:TYR:O	1:C:28:TYR:CG	2.74	0.40
1:C:161:VAL:O	1:C:170:HIS:N	2.49	0.40
1:C:264:VAL:HG13	1:C:265:ILE:N	2.37	0.40
1:E:309:GLU:HB3	1:E:310:PRO:HD2	2.03	0.40
3:J:97:ILE:HD12	17:F:20:PHE:CZ	2.56	0.40
6:O:380:THR:HG21	16:Q:205:ARG:HB3	2.04	0.40
16:Q:124:MET:HG3	16:Q:295:LEU:HD23	2.01	0.40
3:L:109:VAL:HG22	3:L:110:HIS:N	2.36	0.40
7:R:548:ASP:O	7:R:551:LEU:HB3	2.21	0.40
1:A:33:PRO:CG	1:A:370:ARG:HD3	2.52	0.40
1:A:441:LEU:HD23	1:A:454:ILE:HD13	2.03	0.40
1:C:302:THR:HG23	1:C:302:THR:O	2.21	0.40
4:M:10:PRO:HA	4:M:188:ILE:HD12	2.02	0.40
6:O:302:ASN:OD1	6:O:303:TRP:N	2.55	0.40
7:R:244:GLN:HG2	7:R:245:GLN:N	2.37	0.40
10:U:55:LEU:HD12	10:U:127:TYR:HE2	1.87	0.40
11:X:104:ALA:O	11:X:108:ILE:HD12	2.21	0.40
11:Z:107:ALA:O	11:Z:111:VAL:HG22	2.21	0.40
16:Q:440:VAL:HG13	16:Q:441:LEU:N	2.36	0.40
17:B:93:VAL:HG12	17:B:94:GLU:N	2.36	0.40
17:D:135:ASN:OD1	17:D:135:ASN:N	2.54	0.40
1:E:499:VAL:HG13	1:E:503:GLY:C	2.46	0.40
2:I:39:ALA:HB2	3:J:28:ARG:HG2	2.04	0.40
2:K:114:ARG:NH2	2:K:145:ASP:OD1	2.47	0.40
5:N:88:PHE:HB2	5:N:89:PRO:CD	2.52	0.40
11:c:126:PHE:CE1	11:c:127:VAL:HG13	2.56	0.40
14:f:29:HIS:CE1	14:f:33:THR:HG21	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	592/617 (96%)	566 (96%)	26 (4%)	0	100	100
1	C	592/617 (96%)	564 (95%)	28 (5%)	0	100	100
1	E	592/617 (96%)	565 (95%)	27 (5%)	0	100	100
2	G	223/233 (96%)	221 (99%)	2 (1%)	0	100	100
2	I	223/233 (96%)	217 (97%)	6 (3%)	0	100	100
2	K	223/233 (96%)	218 (98%)	5 (2%)	0	100	100
3	H	109/114 (96%)	107 (98%)	2 (2%)	0	100	100
3	J	109/114 (96%)	107 (98%)	2 (2%)	0	100	100
3	L	109/114 (96%)	108 (99%)	1 (1%)	0	100	100
4	M	219/256 (86%)	215 (98%)	4 (2%)	0	100	100
5	N	113/118 (96%)	103 (91%)	10 (9%)	0	100	100
6	O	390/392 (100%)	367 (94%)	23 (6%)	0	100	100
7	R	554/567 (98%)	543 (98%)	11 (2%)	0	100	100
8	S	342/345 (99%)	326 (95%)	16 (5%)	0	100	100
9	T	198/213 (93%)	193 (98%)	5 (2%)	0	100	100
10	U	155/164 (94%)	152 (98%)	3 (2%)	0	100	100
11	V	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
11	W	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
11	X	157/160 (98%)	157 (100%)	0	0	100	100
11	Y	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
11	Z	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
11	a	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
11	b	158/160 (99%)	158 (100%)	0	0	100	100
11	c	157/160 (98%)	157 (100%)	0	0	100	100
12	d	67/73 (92%)	56 (84%)	11 (16%)	0	100	100
13	e	50/265 (19%)	45 (90%)	5 (10%)	0	100	100
14	f	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
15	P	455/478 (95%)	443 (97%)	12 (3%)	0	100	100
16	Q	741/840 (88%)	704 (95%)	37 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	B	467/517 (90%)	445 (95%)	22 (5%)	0	100	100
17	D	467/517 (90%)	446 (96%)	21 (4%)	0	100	100
17	F	469/517 (91%)	448 (96%)	21 (4%)	0	100	100
All	All	8791/9519 (92%)	8476 (96%)	315 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/516 (96%)	498 (100%)	0	100	100
1	C	498/516 (96%)	498 (100%)	0	100	100
1	E	498/516 (96%)	498 (100%)	0	100	100
2	G	202/208 (97%)	202 (100%)	0	100	100
2	I	202/208 (97%)	202 (100%)	0	100	100
2	K	202/208 (97%)	202 (100%)	0	100	100
3	H	92/94 (98%)	92 (100%)	0	100	100
3	J	92/94 (98%)	92 (100%)	0	100	100
3	L	92/94 (98%)	92 (100%)	0	100	100
4	M	192/221 (87%)	192 (100%)	0	100	100
5	N	102/104 (98%)	102 (100%)	0	100	100
6	O	348/348 (100%)	348 (100%)	0	100	100
7	R	499/510 (98%)	499 (100%)	0	100	100
8	S	308/309 (100%)	308 (100%)	0	100	100
9	T	156/168 (93%)	156 (100%)	0	100	100
10	U	119/125 (95%)	119 (100%)	0	100	100
11	V	118/119 (99%)	118 (100%)	0	100	100
11	W	118/119 (99%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	X	118/119 (99%)	118 (100%)	0	100	100
11	Y	119/119 (100%)	119 (100%)	0	100	100
11	Z	118/119 (99%)	118 (100%)	0	100	100
11	a	118/119 (99%)	118 (100%)	0	100	100
11	b	119/119 (100%)	119 (100%)	0	100	100
11	c	118/119 (99%)	118 (100%)	0	100	100
12	d	62/65 (95%)	62 (100%)	0	100	100
13	e	47/244 (19%)	47 (100%)	0	100	100
14	f	63/72 (88%)	63 (100%)	0	100	100
15	P	424/439 (97%)	424 (100%)	0	100	100
16	Q	657/728 (90%)	657 (100%)	0	100	100
17	B	403/444 (91%)	403 (100%)	0	100	100
17	D	403/444 (91%)	403 (100%)	0	100	100
17	F	404/444 (91%)	404 (100%)	0	100	100
All	All	7509/8071 (93%)	7509 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	436	GLN
1	A	450	HIS
1	A	527	GLN
1	A	554	HIS
1	C	55	ASN
1	C	267	GLN
1	C	474	ASN
2	G	14	ASN
2	G	165	GLN
3	H	5	ASN
2	K	14	ASN
4	M	175	HIS
4	M	189	ASN
5	N	72	HIS
7	R	278	HIS

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Mol	Chain	Res	Type
7	R	310	HIS
7	R	503	HIS
7	R	523	GLN
8	S	255	HIS
8	S	260	GLN
8	S	271	ASN
10	U	129	HIS
11	Z	151	ASN
14	f	35	HIS
15	P	73	ASN
15	P	152	GLN
15	P	172	ASN
15	P	241	GLN
16	Q	185	ASN
16	Q	201	GLN
16	Q	523	HIS
16	Q	559	HIS
17	B	186	GLN
17	B	243	ASN
17	D	12	ASN
17	D	29	ASN
17	F	12	ASN
17	F	162	ASN
17	F	207	ASN
17	F	365	HIS
17	F	396	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	ADP	E	701	-	28,29,29	1.38	5 (17%)	43,45,45	1.87	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ADP	E	701	-	-	6/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	E	701	ADP	C5-C4	4.36	1.46	1.39
18	E	701	ADP	C5-C6	2.54	1.48	1.41
18	E	701	ADP	C5-N7	-2.49	1.34	1.39
18	E	701	ADP	C8-N7	2.24	1.36	1.31
18	E	701	ADP	C4-N9	-2.08	1.33	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	E	701	ADP	C5-C4-N3	-5.64	118.95	126.72
18	E	701	ADP	N3-C4-N9	4.50	134.83	127.17
18	E	701	ADP	C2-N3-C4	3.78	121.05	111.83
18	E	701	ADP	N3-C2-N1	-3.69	122.99	128.58
18	E	701	ADP	C4-C5-N7	-3.51	106.57	110.58
18	E	701	ADP	C4-N9-C8	2.98	108.86	105.74
18	E	701	ADP	C5-N7-C8	2.64	107.60	103.45
18	E	701	ADP	N9-C8-N7	-2.25	110.74	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	E	701	ADP	C3'-C2'-C1'	2.16	105.56	101.46
18	E	701	ADP	C2-N1-C6	2.14	122.25	118.73
18	E	701	ADP	C6-C5-N7	2.12	136.18	132.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

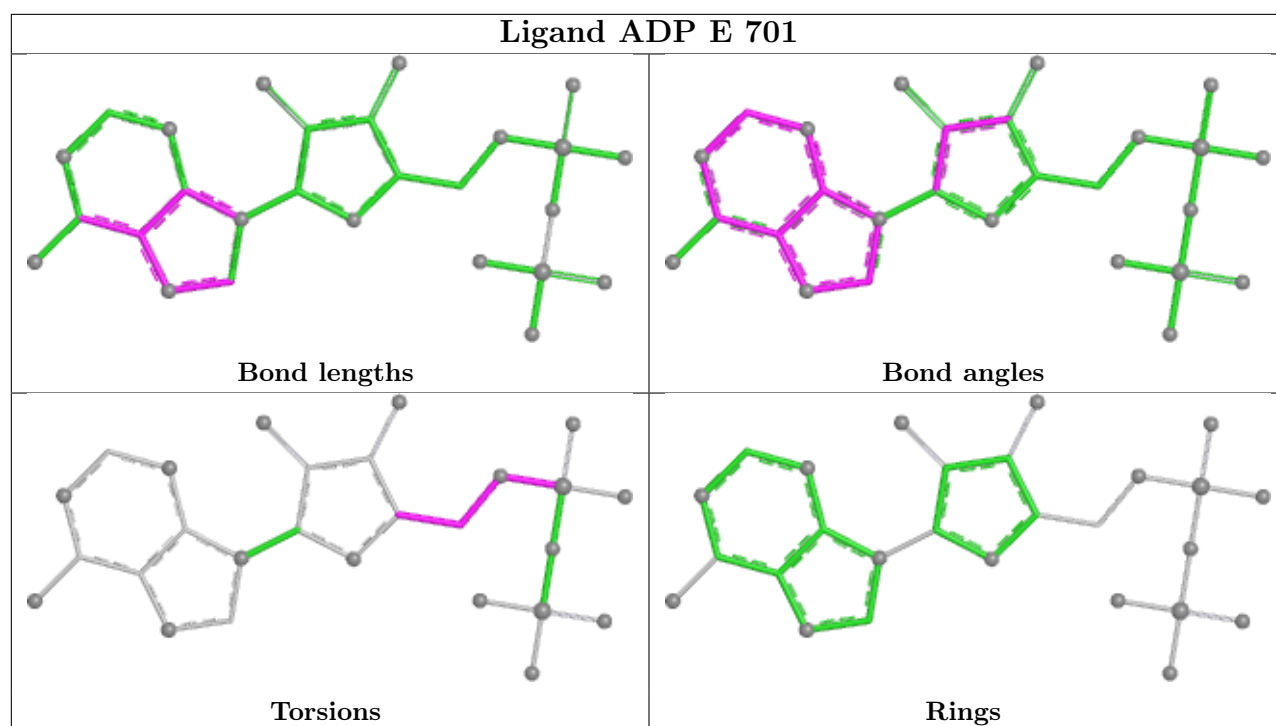
Mol	Chain	Res	Type	Atoms
18	E	701	ADP	C5'-O5'-PA-O1A
18	E	701	ADP	C5'-O5'-PA-O2A
18	E	701	ADP	C5'-O5'-PA-O3A
18	E	701	ADP	O4'-C4'-C5'-O5'
18	E	701	ADP	C3'-C4'-C5'-O5'
18	E	701	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	E	701	ADP	7	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



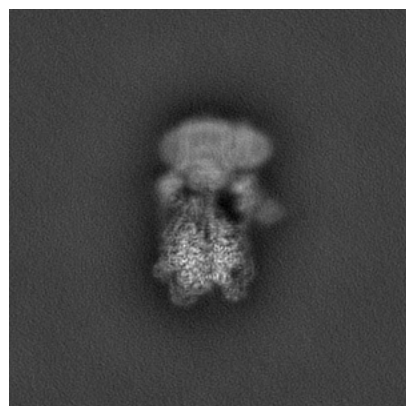
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70377. These allow visual inspection of the internal detail of the map and identification of artifacts.

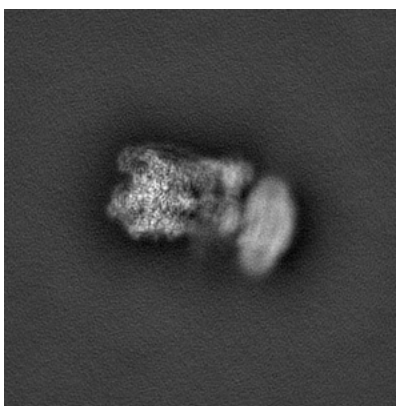
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

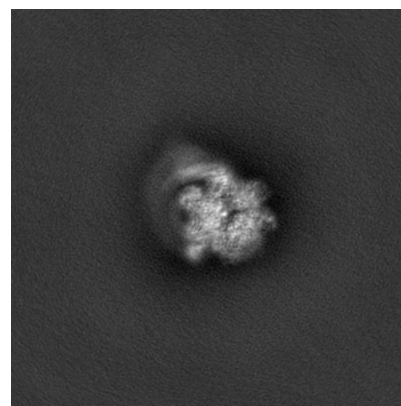
#### 6.1.1 Primary map



X

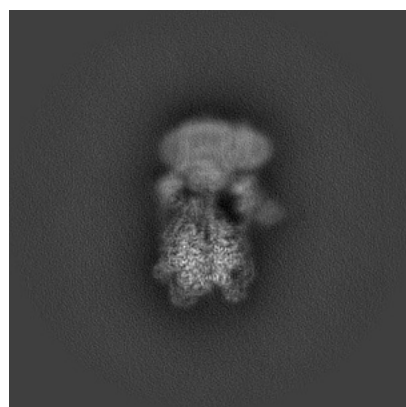


Y

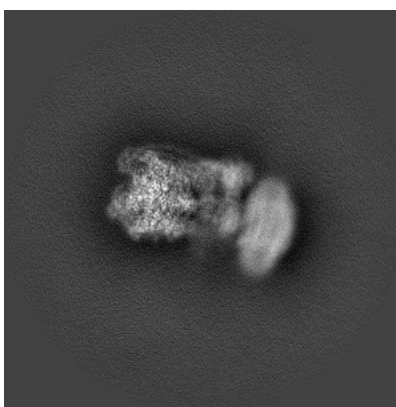


Z

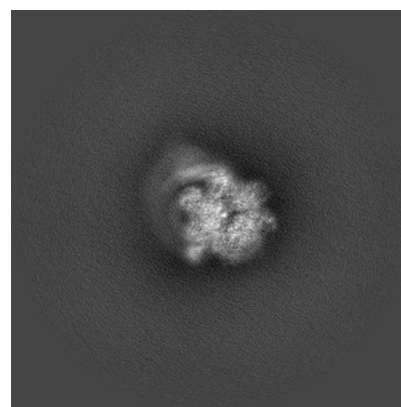
#### 6.1.2 Raw map



X



Y



Z

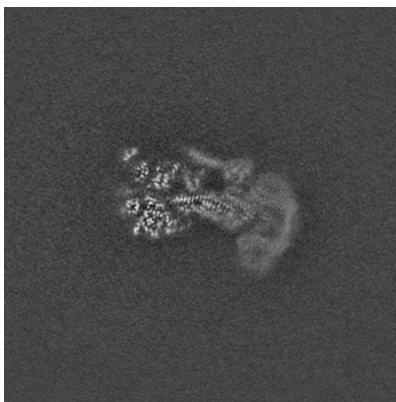
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

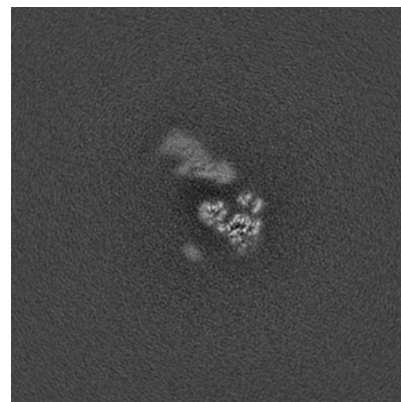
### 6.2.1 Primary map



X Index: 160

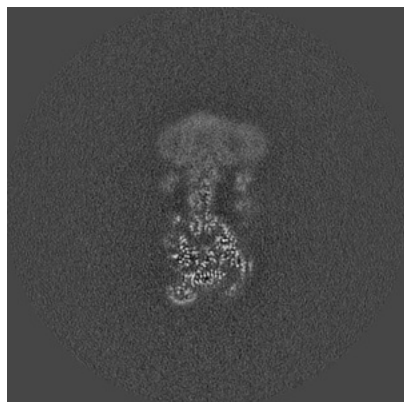


Y Index: 160

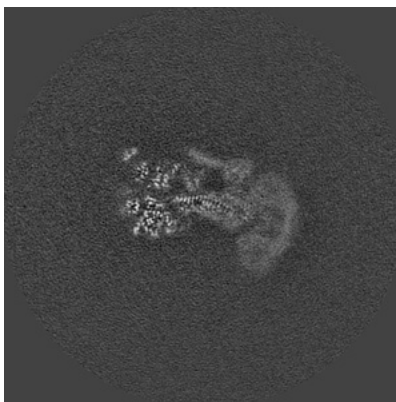


Z Index: 160

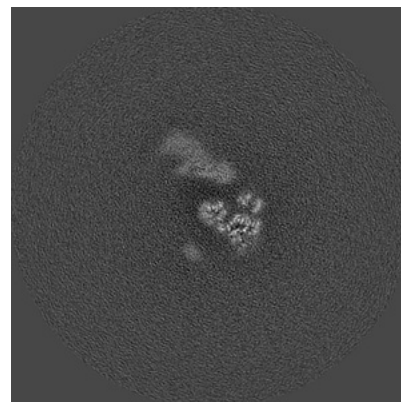
### 6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

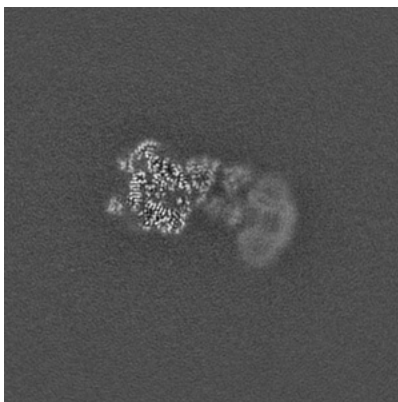
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

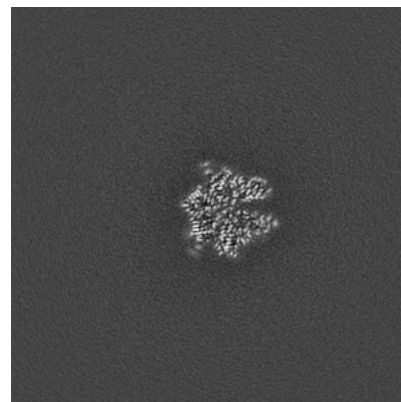
### 6.3.1 Primary map



X Index: 167

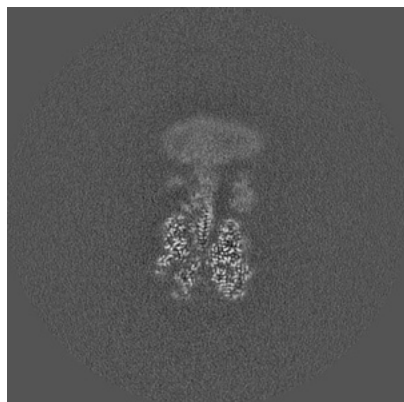


Y Index: 145

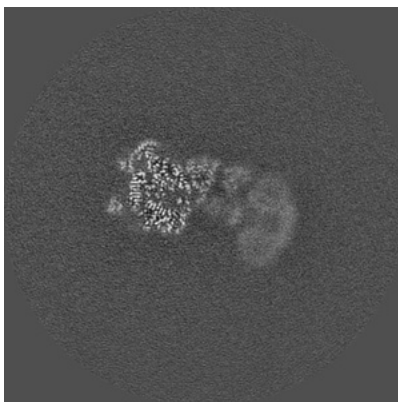


Z Index: 118

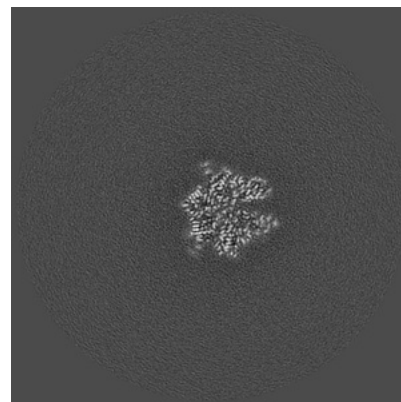
### 6.3.2 Raw map



X Index: 167



Y Index: 145

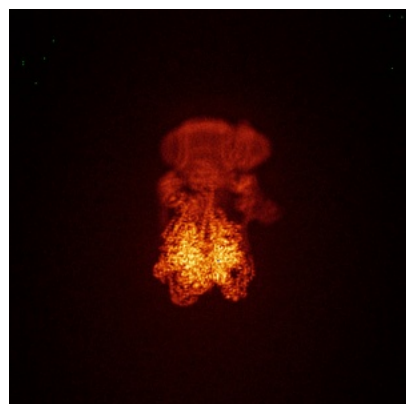


Z Index: 118

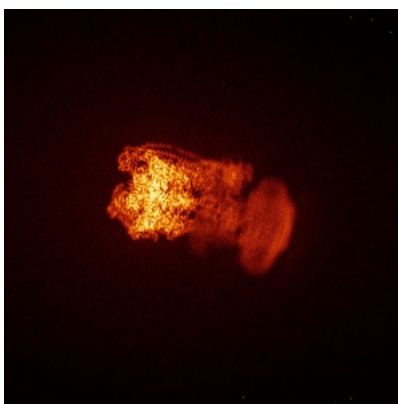
The images above show the largest variance slices of the map in three orthogonal directions.

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

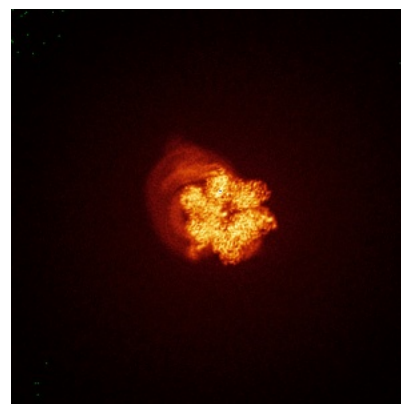
### 6.4.1 Primary map



X

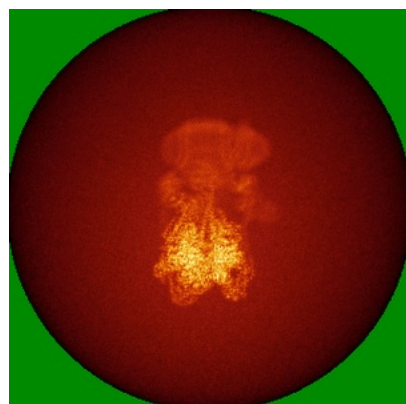


Y

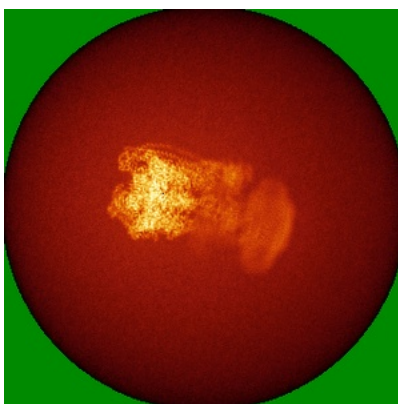


Z

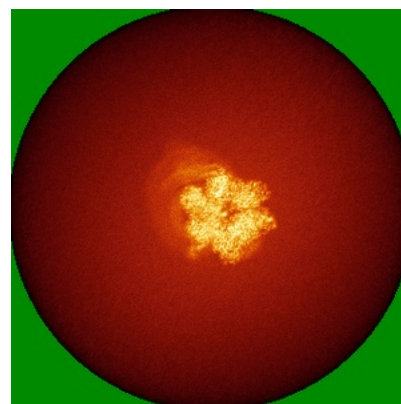
### 6.4.2 Raw map



X



Y



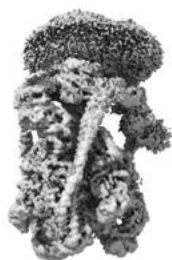
Z

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](#)

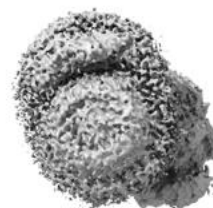
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

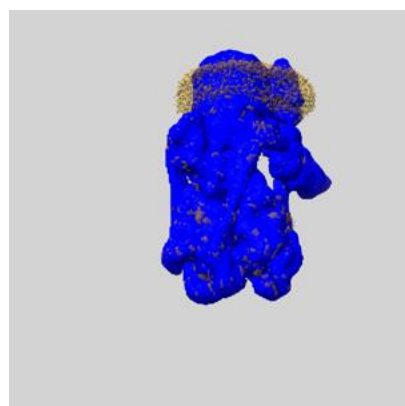
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

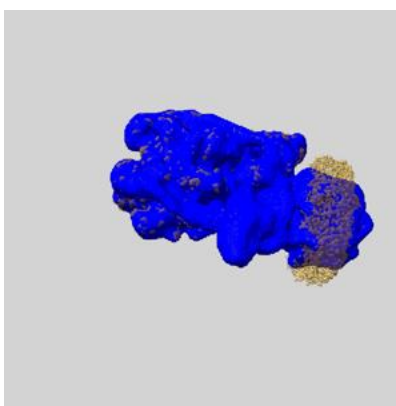
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

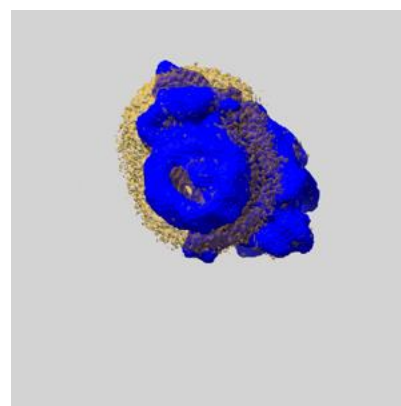
### 6.6.1 emd\_70377\_msk\_1.map [i](#)



X



Y

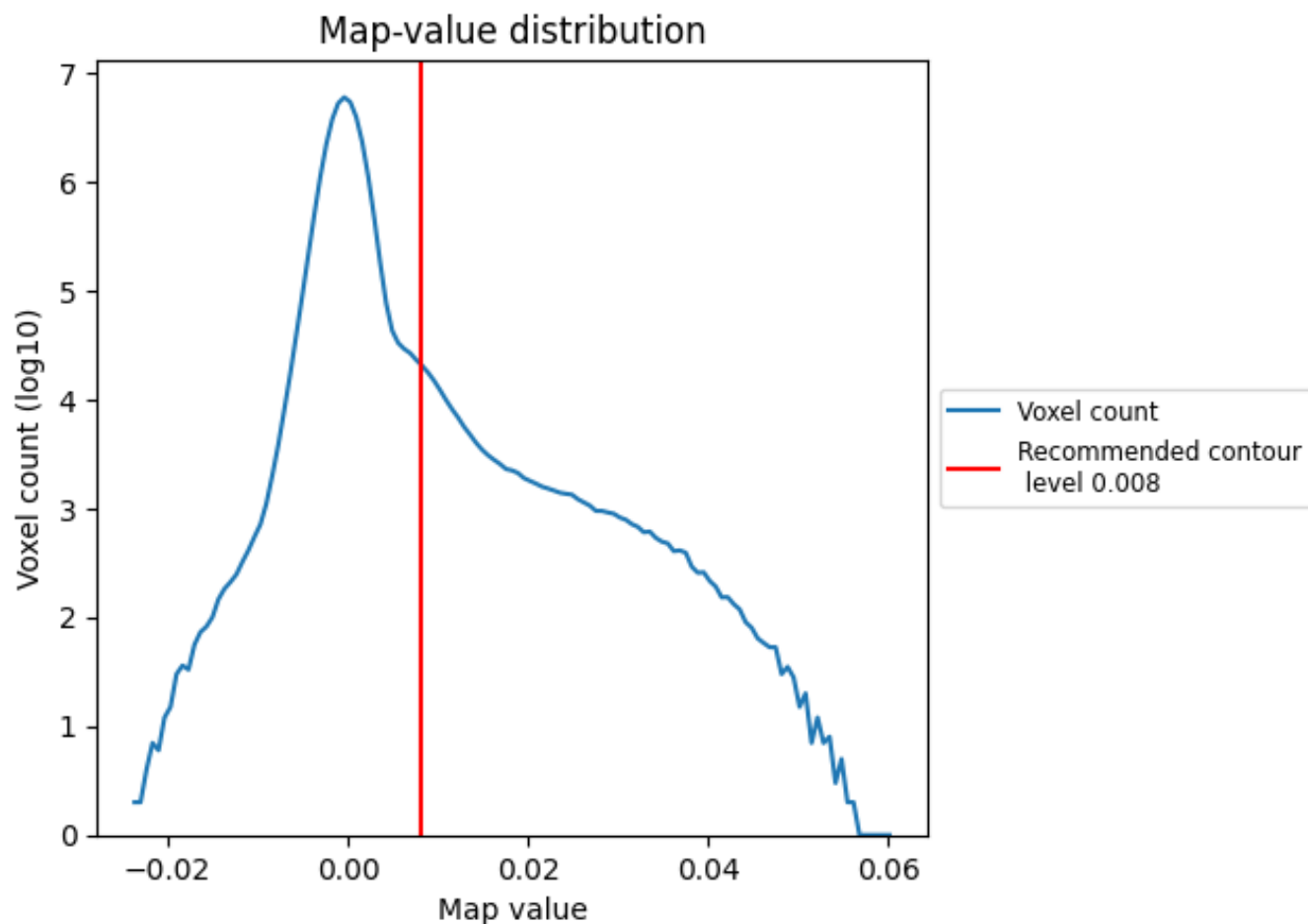


Z

## 7 Map analysis [i](#)

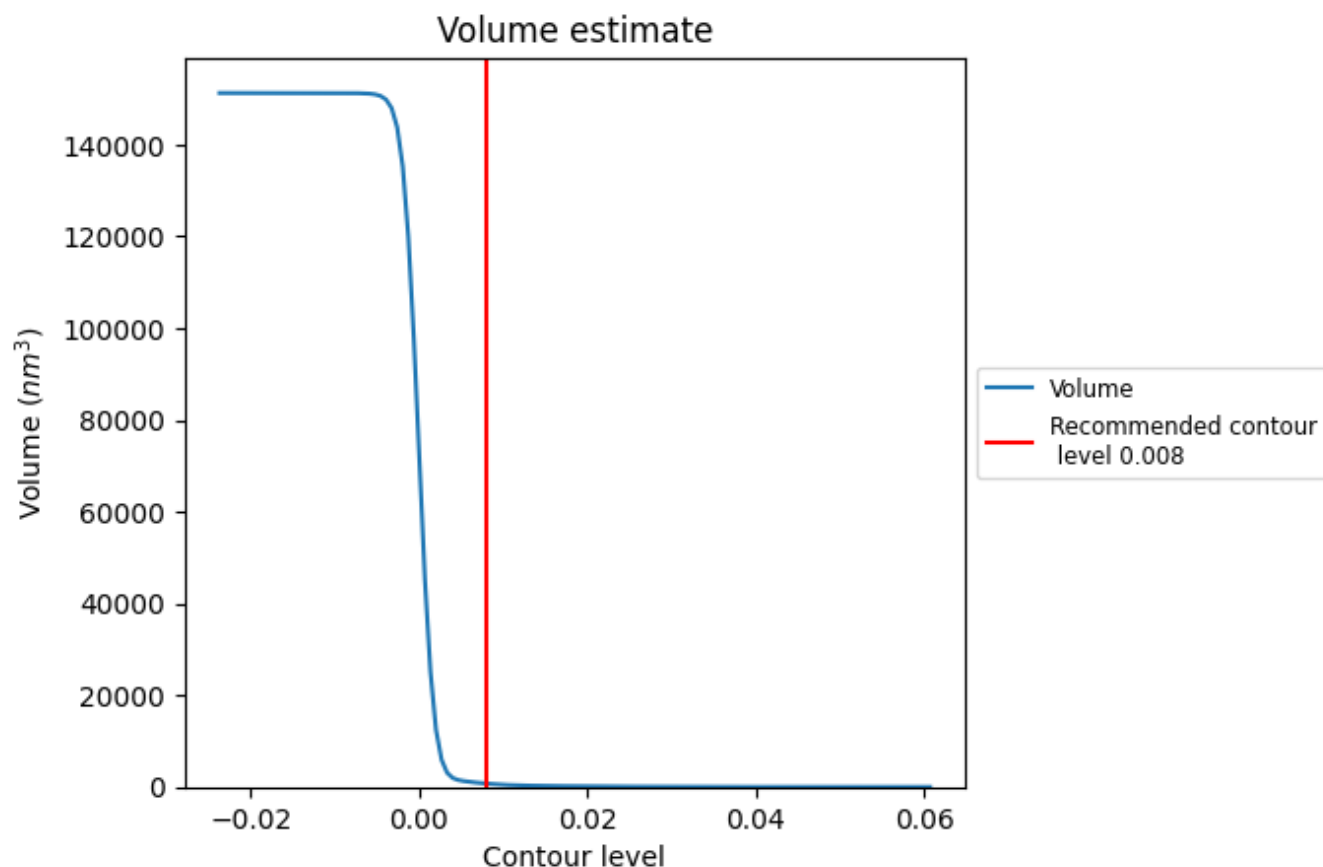
This section contains the results of statistical analysis of the map.

### 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](#)

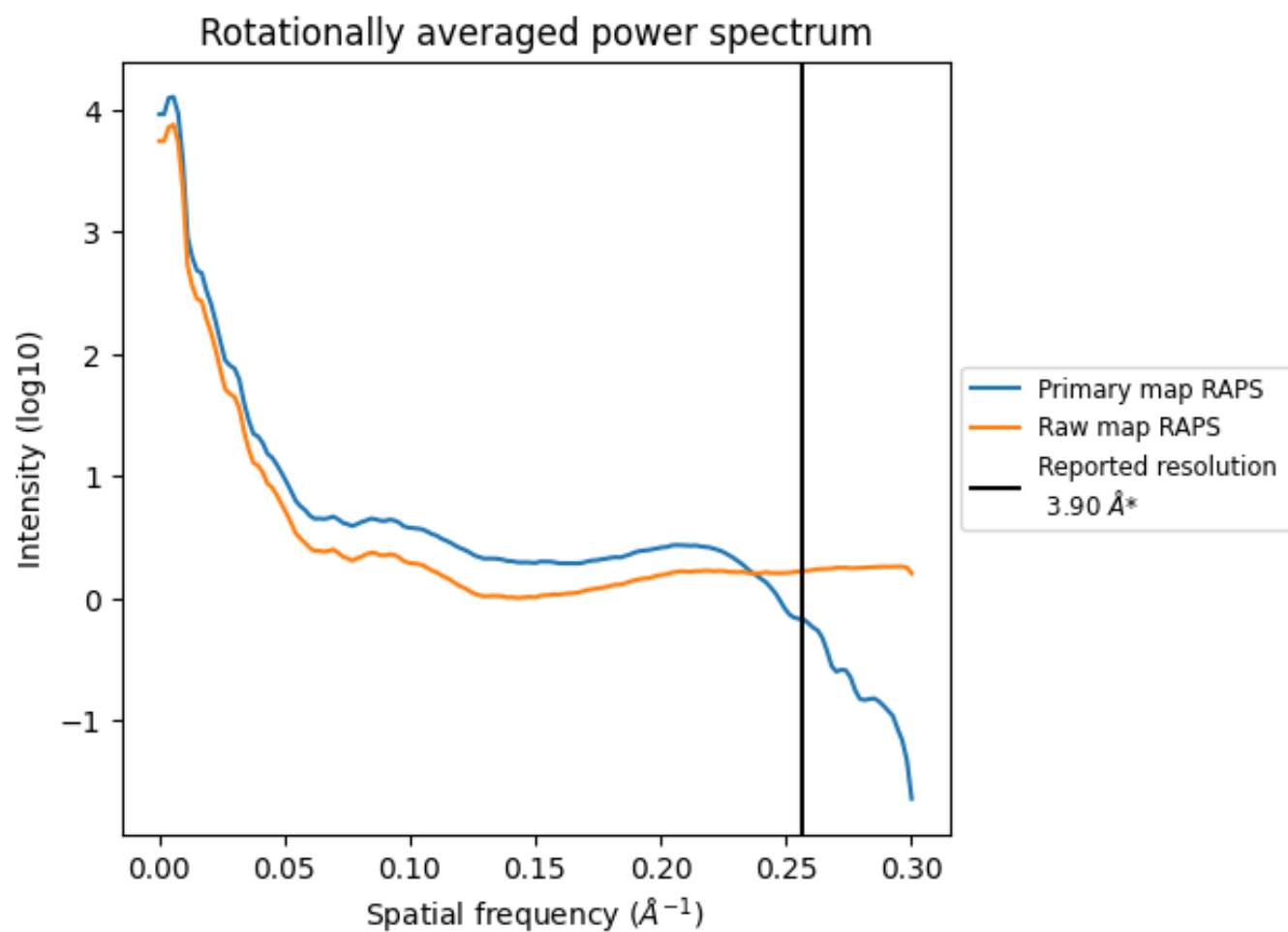


The volume at the recommended contour level is 743 nm<sup>3</sup>; this corresponds to an approximate mass of 671 kDa.

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 ⓘ

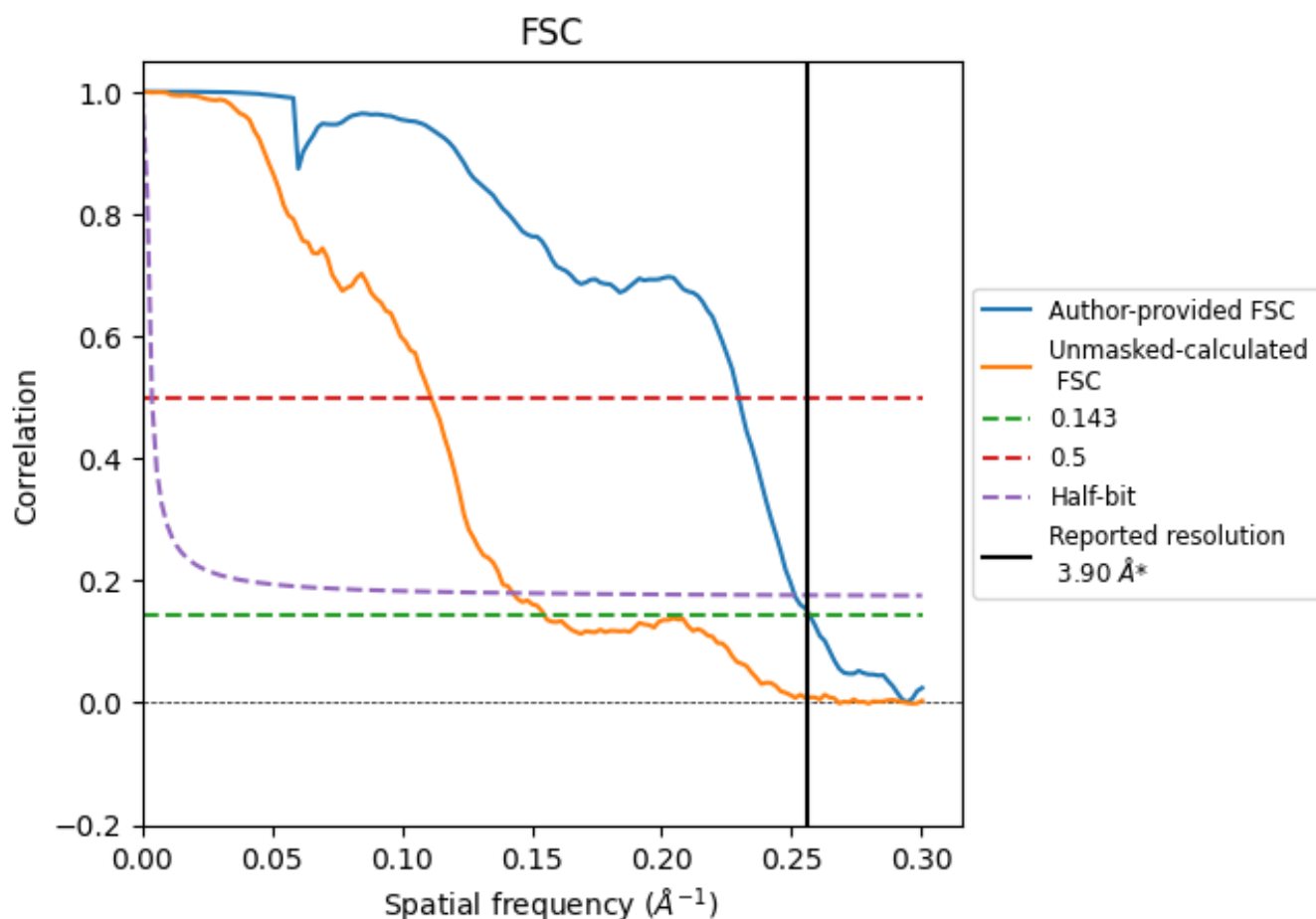


\*Reported resolution corresponds to spatial frequency of 0.256  $\text{\AA}^{-1}$

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

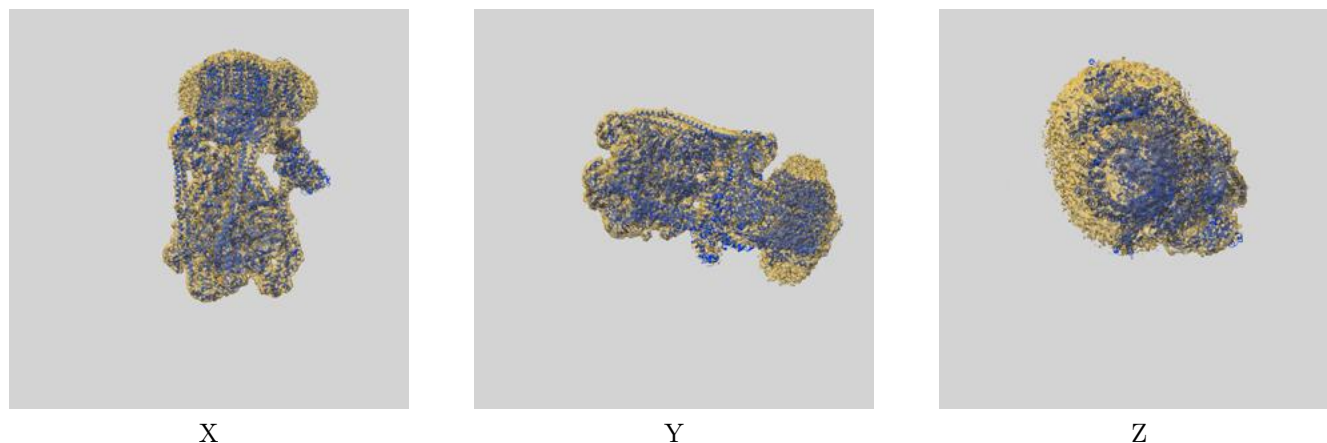
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	4.36	3.98
Unmasked-calculated*	6.46	8.99	7.00

\*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 6.46 differs from the reported value 3.9 by more than 10 %

## 9 Map-model fit [i](#)

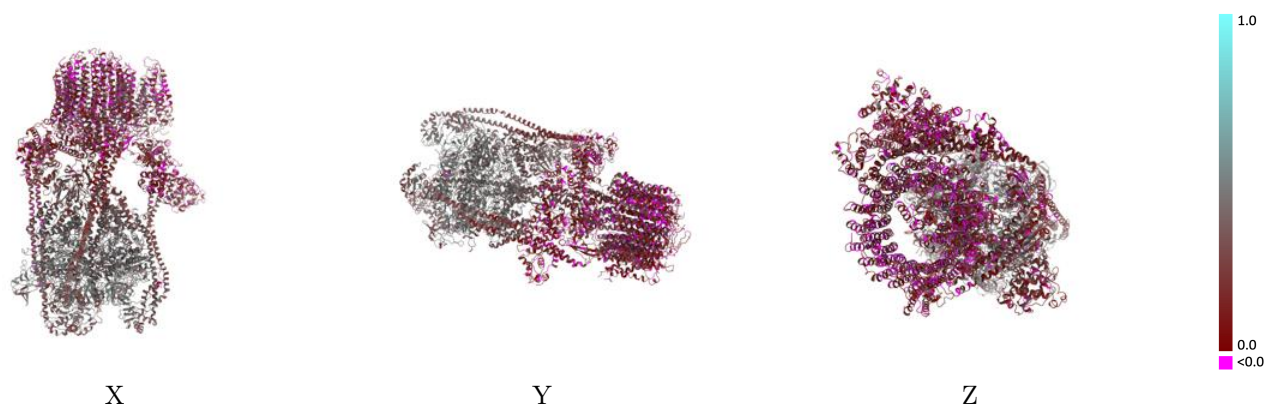
This section contains information regarding the fit between EMDB map EMD-70377 and PDB model 9ODU. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

### 9.1 Map-model overlay [i](#)



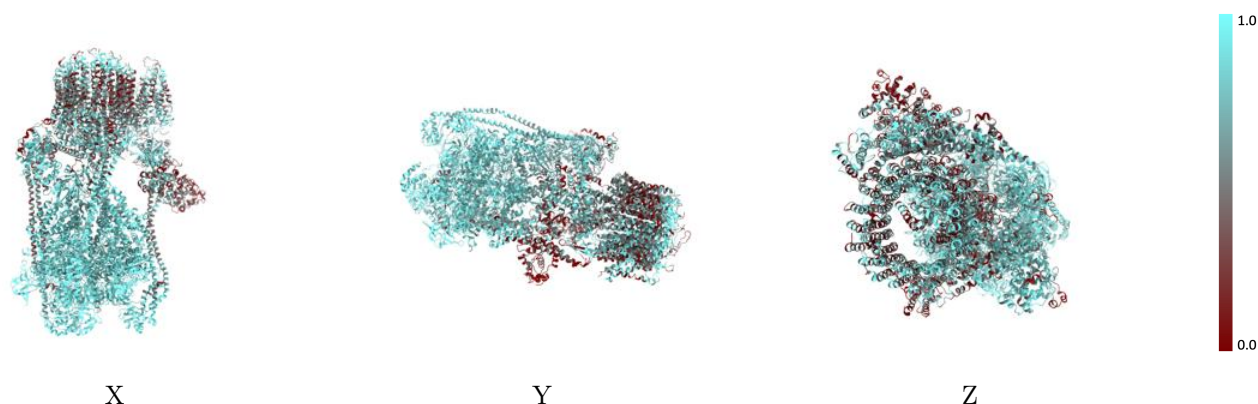
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



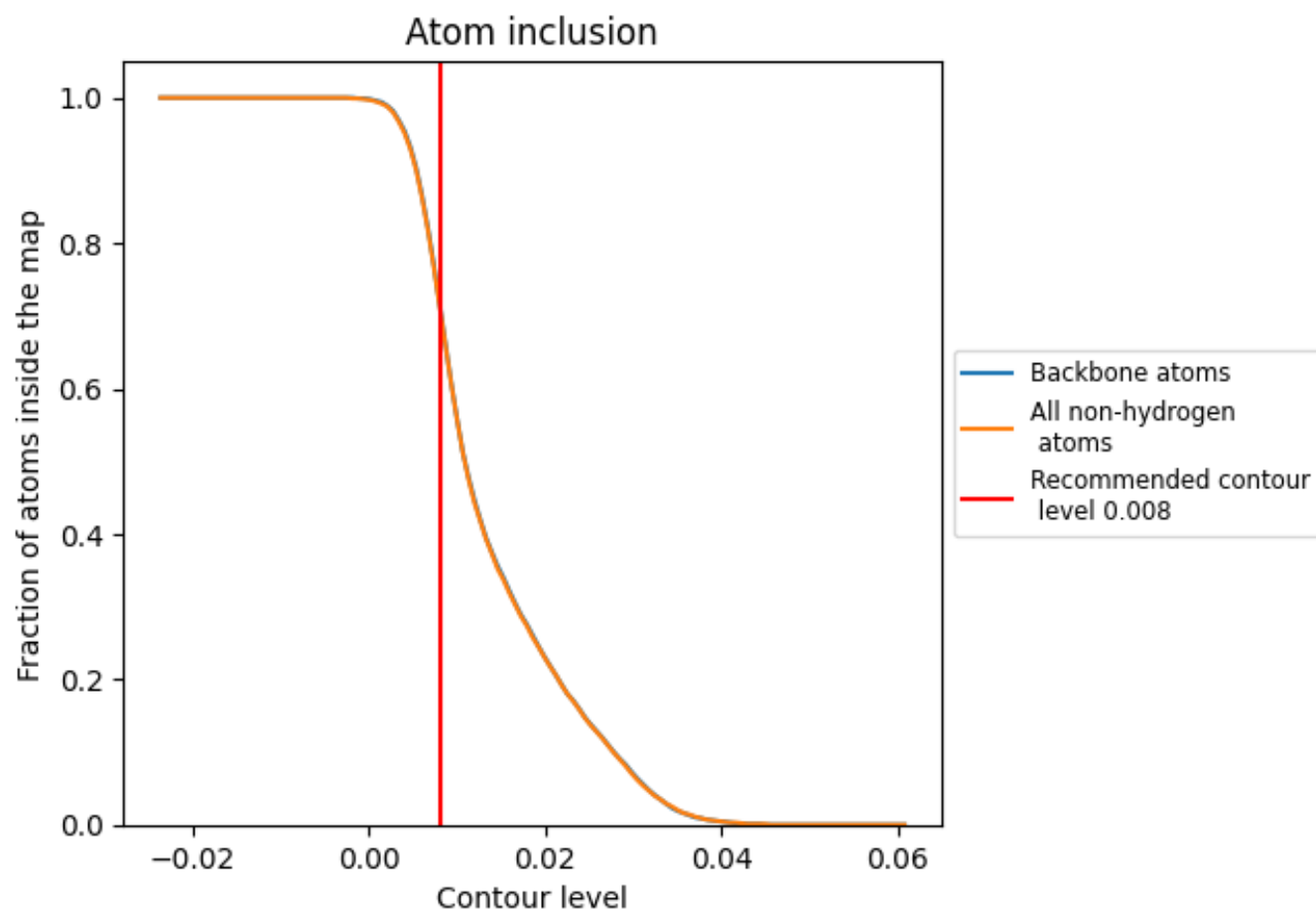
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).



































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7140	 0.2810
A	 0.9090	 0.4210
B	 0.8990	 0.4440
C	 0.9120	 0.4280
D	 0.8990	 0.4400
E	 0.9230	 0.4410
F	 0.9060	 0.4520
G	 0.7260	 0.2950
H	 0.4890	 0.2010
I	 0.8360	 0.3240
J	 0.7960	 0.2740
K	 0.7660	 0.3230
L	 0.5560	 0.2360
M	 0.7990	 0.3300
N	 0.6450	 0.2170
O	 0.5900	 0.1610
P	 0.3510	 0.1350
Q	 0.6640	 0.1560
R	 0.7680	 0.2830
S	 0.4900	 0.1650
T	 0.5350	 0.1250
U	 0.4690	 0.1440
V	 0.5070	 0.1410
W	 0.5990	 0.1520
X	 0.4780	 0.1370
Y	 0.4200	 0.0920
Z	 0.5010	 0.0980
a	 0.5920	 0.1390
b	 0.6460	 0.1280
c	 0.6020	 0.1460
d	 0.6190	 0.1630
e	 0.4170	 0.1180
f	 0.6050	 0.1030

