Full wwPDB EM Validation Report ⓘ

Mar 9, 2024 – 09:02 AM EST

PDB ID	:	6O7X
EMDB ID	:	EMD-0648
Title	:	Saccharomyces cerevisiae V-ATPase Stv1-V1VO State 3
Authors	:	Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.
Deposited on	:	2019-03-08
Resolution	:	8.70 Å(reported)

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

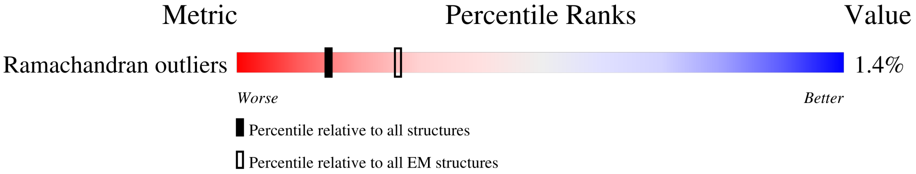
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

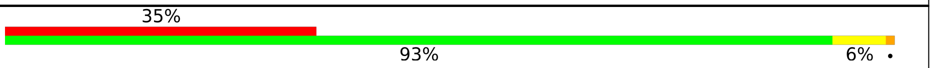
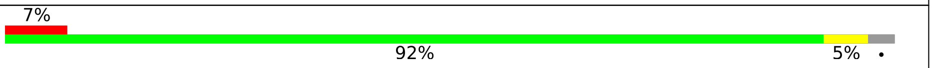
The reported resolution of this entry is 8.70 Å.

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)
Ramachandran outliers	154571	4023

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	O	392	 35% 93% 6% •
2	M	256	 • 76% 6% 18%
3	N	118	 7% 92% 5% •
4	A	639	 • 87% 5% 7%
4	C	639	 • 87% 6% 7%
4	E	639	 • 84% 8% 7%
5	B	517	 83% 5% 12%
5	D	517	 • 81% 7% 12%
5	F	517	 • 81% 7% 12%
6	H	114	 89% • 8%
6	J	114	 86% 6% 8%

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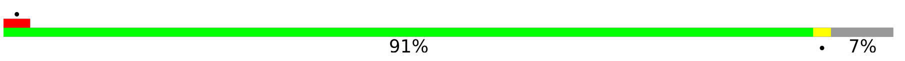
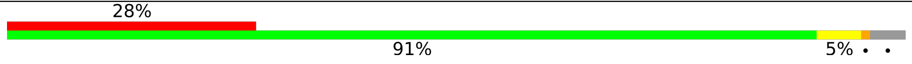
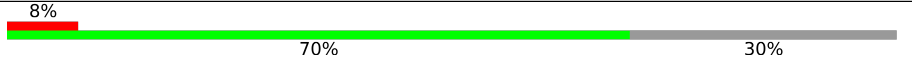
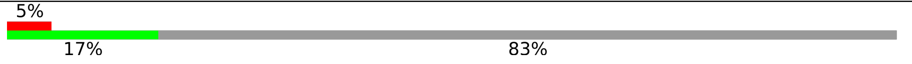
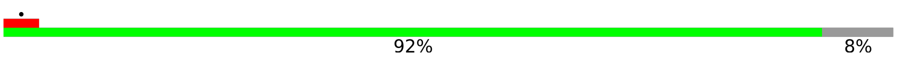
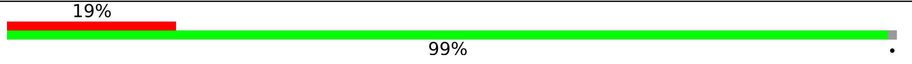
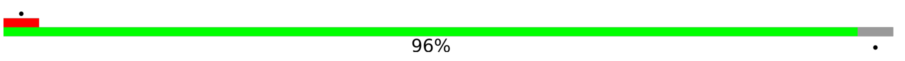
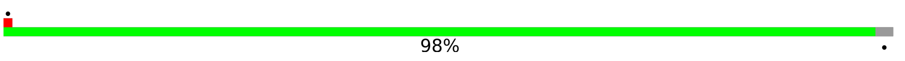
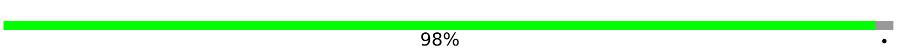
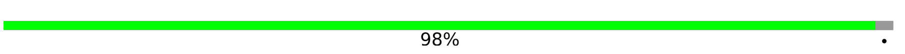
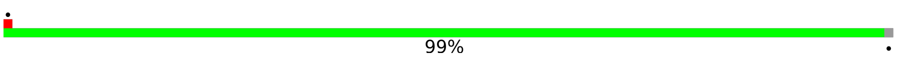
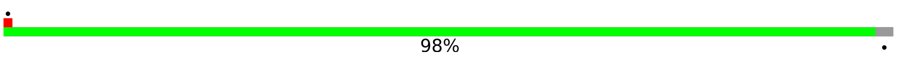
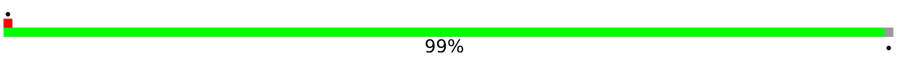
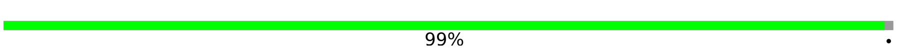
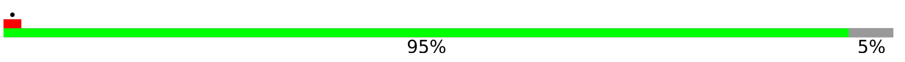
Mol	Chain	Length	Quality of chain
6	L	114	 5% 86% 5% • 8%
7	G	233	 85% 8% 7%
7	I	233	 • 89% • 7%
7	K	233	 • 91% • 7%
8	P	478	 28% 91% 5% • •
9	a	890	 8% 70% 30%
10	b	265	 5% 17% 83%
11	c	213	 • 92% 8%
12	d	345	 19% 99% •
13	g	160	 • 96% •
13	h	160	 • 98% •
13	i	160	 98% •
13	j	160	 98% •
13	k	160	 • 99% •
13	l	160	 • 98% •
13	m	160	 • 99% •
13	n	160	 99% •
14	o	164	 • 95% 5%
15	e	73	 88% 12%
16	f	85	 72% 28%

2 Entry composition ⓘ

There are 16 unique types of molecules in this entry. The entry contains 39578 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	O	392	1947	1163	392	392	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	M	210	1039	619	210	210	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	N	115	571	341	115	115	0	0

- Molecule 4 is a protein called Vacuolar ATP synthase catalytic subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	593	2915	1729	593	593	0	0
4	A	593	2915	1729	593	593	0	0
4	C	593	2915	1729	593	593	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	617	ASP	-	SEE REMARK 999	UNP B3LH69
E	618	TYR	-	SEE REMARK 999	UNP B3LH69
E	619	LYS	-	SEE REMARK 999	UNP B3LH69
E	620	ASP	-	SEE REMARK 999	UNP B3LH69
E	621	HIS	-	SEE REMARK 999	UNP B3LH69

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Chain	Residue	Modelled	Actual	Comment	Reference
E	622	ASP	-	SEE REMARK 999	UNP B3LH69
E	623	GLY	-	SEE REMARK 999	UNP B3LH69
E	624	ASP	-	SEE REMARK 999	UNP B3LH69
E	625	TYR	-	SEE REMARK 999	UNP B3LH69
E	626	LYS	-	SEE REMARK 999	UNP B3LH69
E	627	ASP	-	SEE REMARK 999	UNP B3LH69
E	628	HIS	-	SEE REMARK 999	UNP B3LH69
E	629	ASP	-	SEE REMARK 999	UNP B3LH69
E	630	ILE	-	SEE REMARK 999	UNP B3LH69
E	631	ASP	-	SEE REMARK 999	UNP B3LH69
E	632	TYR	-	SEE REMARK 999	UNP B3LH69
E	633	LYS	-	SEE REMARK 999	UNP B3LH69
E	634	ASP	-	SEE REMARK 999	UNP B3LH69
E	635	ASP	-	SEE REMARK 999	UNP B3LH69
E	636	ASP	-	SEE REMARK 999	UNP B3LH69
E	637	ASP	-	SEE REMARK 999	UNP B3LH69
E	638	LYS	-	SEE REMARK 999	UNP B3LH69
A	617	ASP	-	SEE REMARK 999	UNP B3LH69
A	618	TYR	-	SEE REMARK 999	UNP B3LH69
A	619	LYS	-	SEE REMARK 999	UNP B3LH69
A	620	ASP	-	SEE REMARK 999	UNP B3LH69
A	621	HIS	-	SEE REMARK 999	UNP B3LH69
A	622	ASP	-	SEE REMARK 999	UNP B3LH69
A	623	GLY	-	SEE REMARK 999	UNP B3LH69
A	624	ASP	-	SEE REMARK 999	UNP B3LH69
A	625	TYR	-	SEE REMARK 999	UNP B3LH69
A	626	LYS	-	SEE REMARK 999	UNP B3LH69
A	627	ASP	-	SEE REMARK 999	UNP B3LH69
A	628	HIS	-	SEE REMARK 999	UNP B3LH69
A	629	ASP	-	SEE REMARK 999	UNP B3LH69
A	630	ILE	-	SEE REMARK 999	UNP B3LH69
A	631	ASP	-	SEE REMARK 999	UNP B3LH69
A	632	TYR	-	SEE REMARK 999	UNP B3LH69
A	633	LYS	-	SEE REMARK 999	UNP B3LH69
A	634	ASP	-	SEE REMARK 999	UNP B3LH69
A	635	ASP	-	SEE REMARK 999	UNP B3LH69
A	636	ASP	-	SEE REMARK 999	UNP B3LH69
A	637	ASP	-	SEE REMARK 999	UNP B3LH69
A	638	LYS	-	SEE REMARK 999	UNP B3LH69
C	617	ASP	-	SEE REMARK 999	UNP B3LH69
C	618	TYR	-	SEE REMARK 999	UNP B3LH69
C	619	LYS	-	SEE REMARK 999	UNP B3LH69

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Chain	Residue	Modelled	Actual	Comment	Reference
C	620	ASP	-	SEE REMARK 999	UNP B3LH69
C	621	HIS	-	SEE REMARK 999	UNP B3LH69
C	622	ASP	-	SEE REMARK 999	UNP B3LH69
C	623	GLY	-	SEE REMARK 999	UNP B3LH69
C	624	ASP	-	SEE REMARK 999	UNP B3LH69
C	625	TYR	-	SEE REMARK 999	UNP B3LH69
C	626	LYS	-	SEE REMARK 999	UNP B3LH69
C	627	ASP	-	SEE REMARK 999	UNP B3LH69
C	628	HIS	-	SEE REMARK 999	UNP B3LH69
C	629	ASP	-	SEE REMARK 999	UNP B3LH69
C	630	ILE	-	SEE REMARK 999	UNP B3LH69
C	631	ASP	-	SEE REMARK 999	UNP B3LH69
C	632	TYR	-	SEE REMARK 999	UNP B3LH69
C	633	LYS	-	SEE REMARK 999	UNP B3LH69
C	634	ASP	-	SEE REMARK 999	UNP B3LH69
C	635	ASP	-	SEE REMARK 999	UNP B3LH69
C	636	ASP	-	SEE REMARK 999	UNP B3LH69
C	637	ASP	-	SEE REMARK 999	UNP B3LH69
C	638	LYS	-	SEE REMARK 999	UNP B3LH69

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	F	457	2250	1336	457	457	0	0
5	B	457	2250	1336	457	457	0	0
5	D	457	2250	1336	457	457	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	J	105	519	309	105	105	0	0
6	L	105	519	309	105	105	0	0
6	H	105	519	309	105	105	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	217	Total	C	N	O	0	0
			1078	644	217	217		
7	K	217	Total	C	N	O	0	0
			1078	644	217	217		
7	G	217	Total	C	N	O	0	0
			1078	644	217	217		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	461	Total	C	N	O	0	0
			2292	1370	461	461		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	a	625	Total	C	N	O	0	0
			3092	1842	625	625		

- Molecule 10 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	b	44	Total	C	N	O	0	0
			218	130	44	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	c	197	Total	C	N	O	0	0
			962	568	197	197		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	d	343	Total	C	N	O	0	0
			1699	1013	343	343		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	153	Total	C	N	O	0	0
			743	437	153	153		

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Mol	Chain	Residues	Atoms				AltConf	Trace
13	h	157	Total 763	C 449	N 157	O 157	0	0
13	i	157	Total 763	C 449	N 157	O 157	0	0
13	j	156	Total 758	C 446	N 156	O 156	0	0
13	k	158	Total 768	C 452	N 158	O 158	0	0
13	l	157	Total 763	C 449	N 157	O 157	0	0
13	m	158	Total 768	C 452	N 158	O 158	0	0
13	n	158	Total 768	C 452	N 158	O 158	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	o	156	Total 758	C 446	N 156	O 156	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	e	64	Total 319	C 191	N 64	O 64	0	0

- Molecule 16 is a protein called Putative protein YPR170W-B.

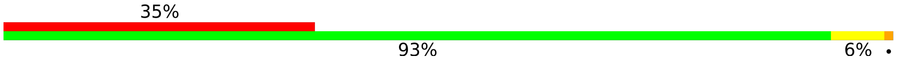
Mol	Chain	Residues	Atoms				AltConf	Trace
16	f	61	Total 301	C 179	N 61	O 61	0	0

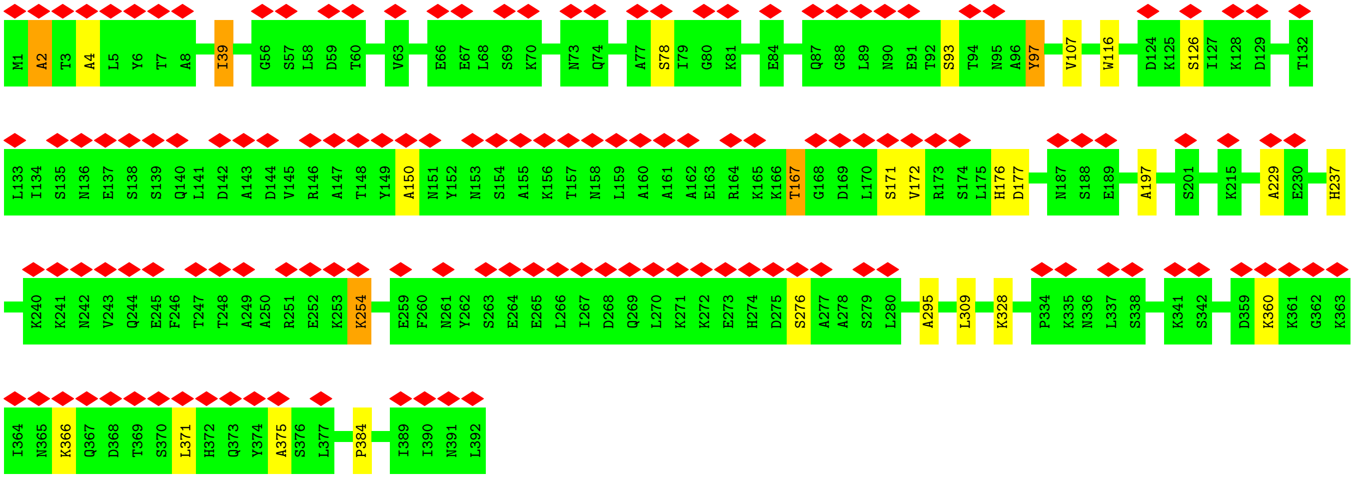
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: V-type proton ATPase subunit C

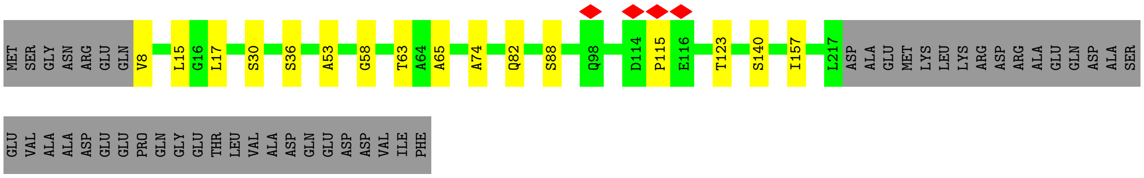
Chain O:





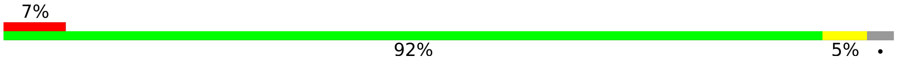
- Molecule 2: V-type proton ATPase subunit D

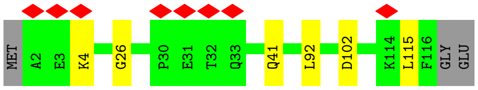
Chain M:



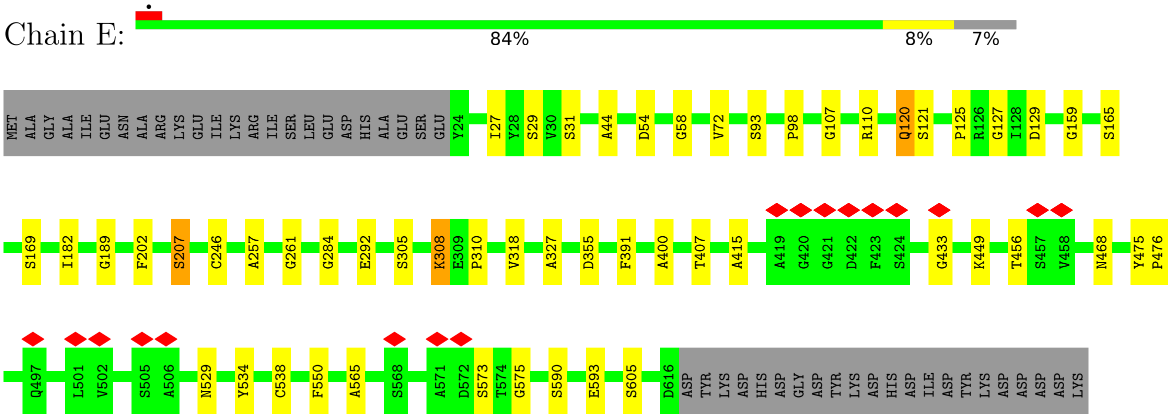
- Molecule 3: V-type proton ATPase subunit F

Chain N:

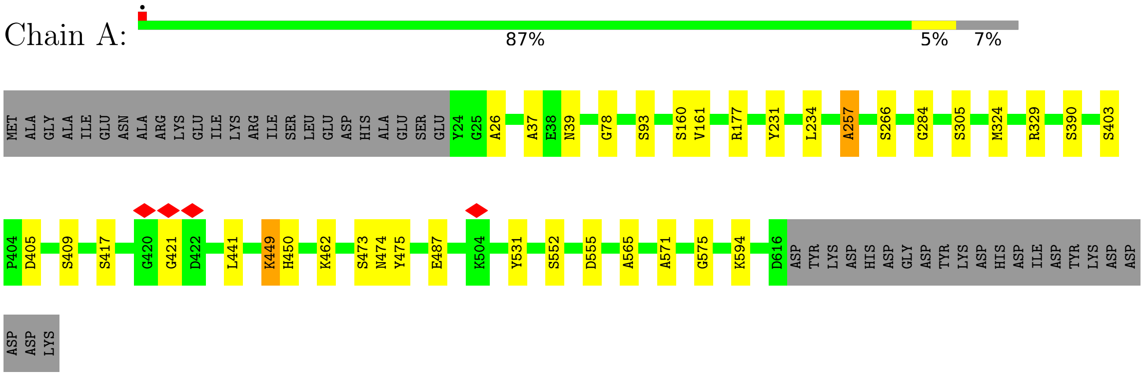




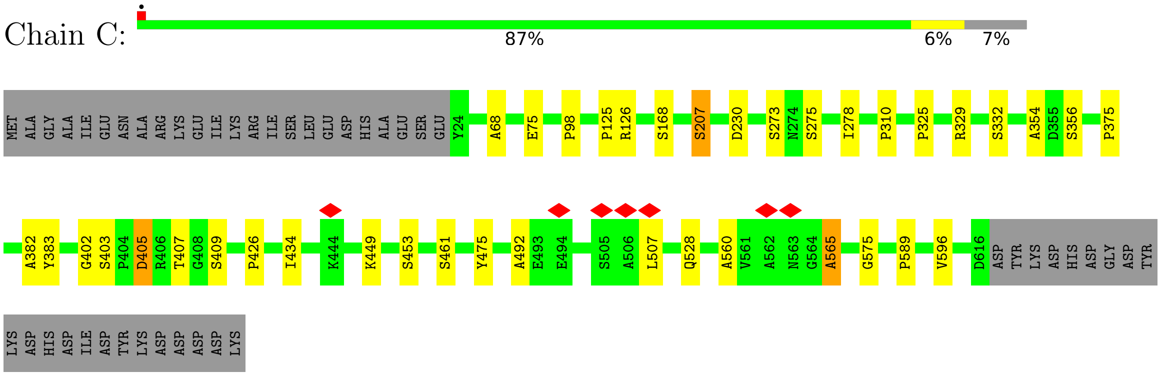
- Molecule 4: Vacuolar ATP synthase catalytic subunit A



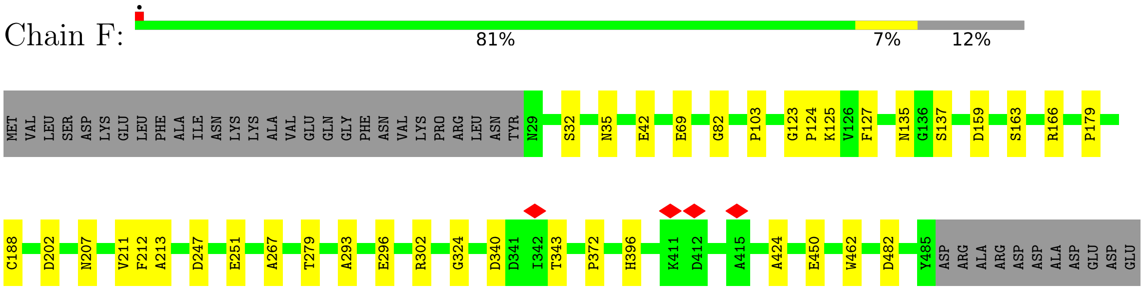
- Molecule 4: Vacuolar ATP synthase catalytic subunit A



- Molecule 4: Vacuolar ATP synthase catalytic subunit A

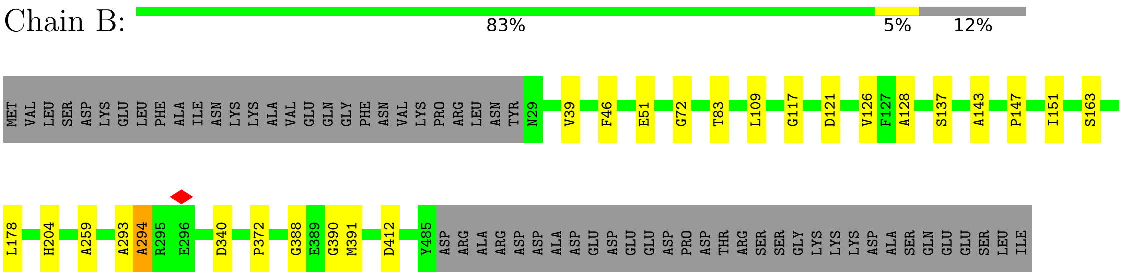


- Molecule 5: V-type proton ATPase subunit B



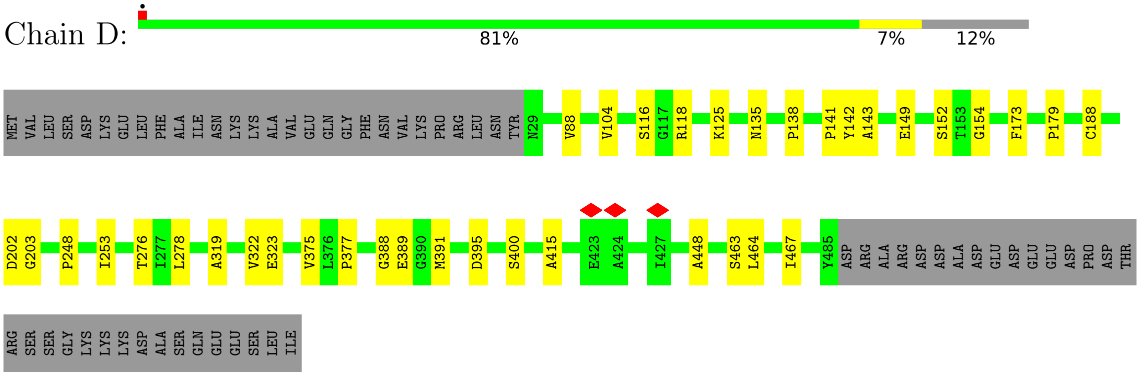
- Molecule 5: V-type proton ATPase subunit B

Chain B:



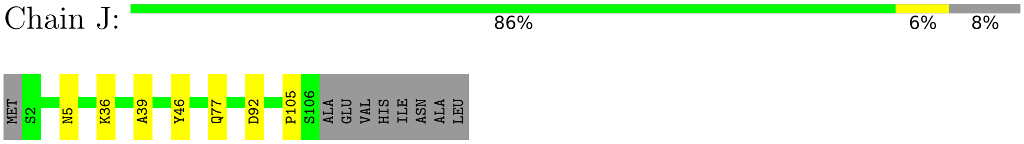
- Molecule 5: V-type proton ATPase subunit B

Chain D:



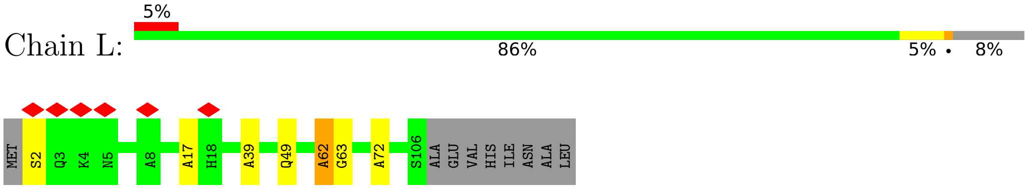
- Molecule 6: V-type proton ATPase subunit G

Chain J:



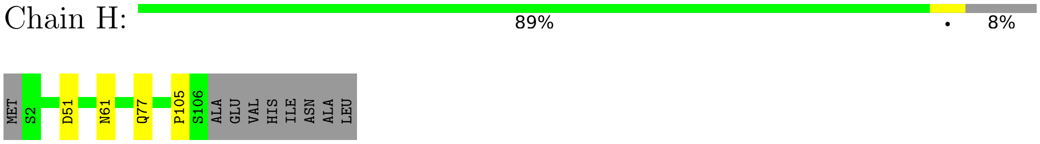
- Molecule 6: V-type proton ATPase subunit G

Chain L:

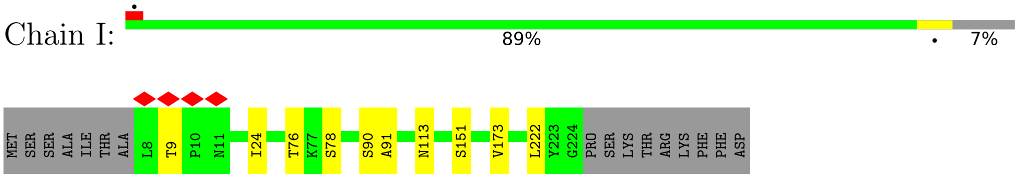


- Molecule 6: V-type proton ATPase subunit G

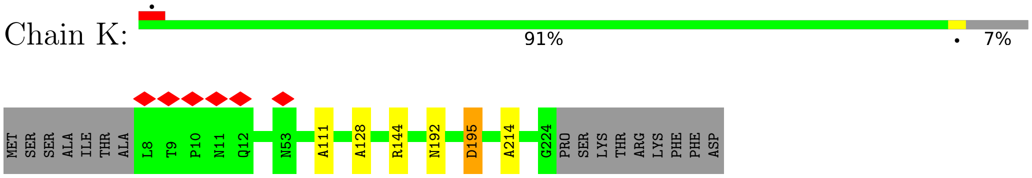
Chain H:



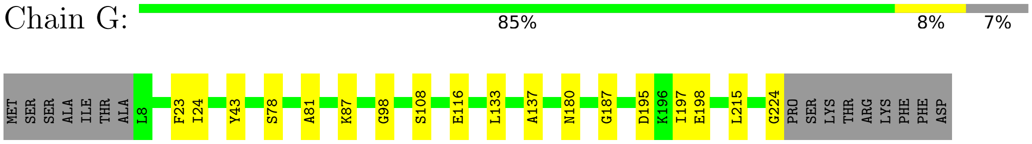
- Molecule 7: V-type proton ATPase subunit E



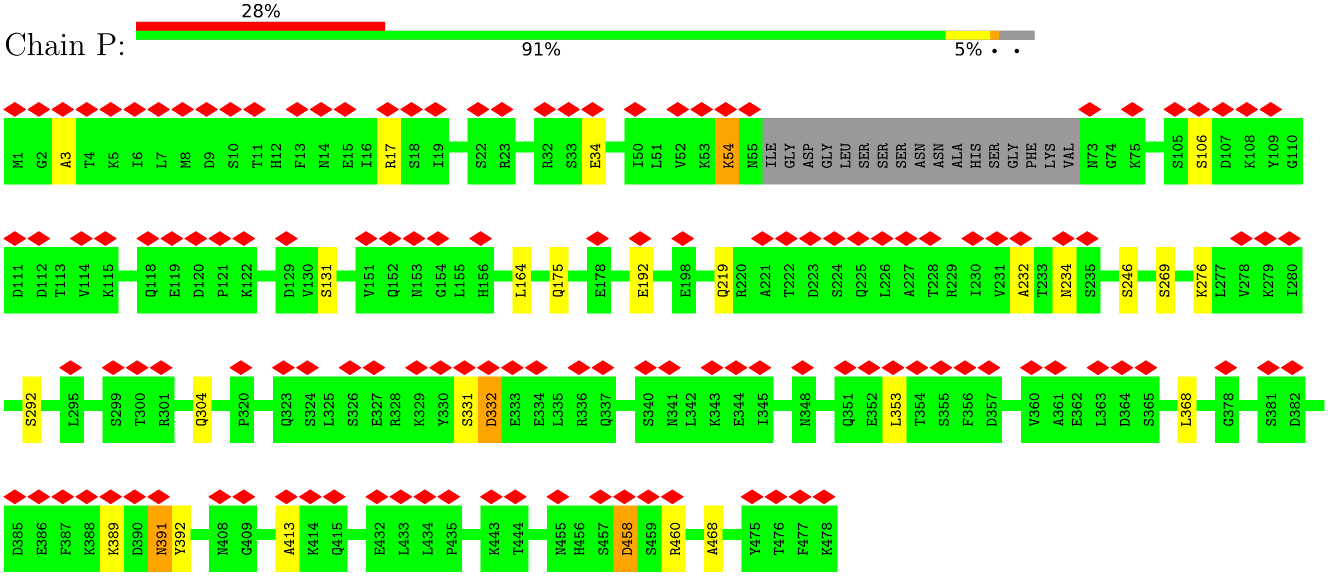
- Molecule 7: V-type proton ATPase subunit E



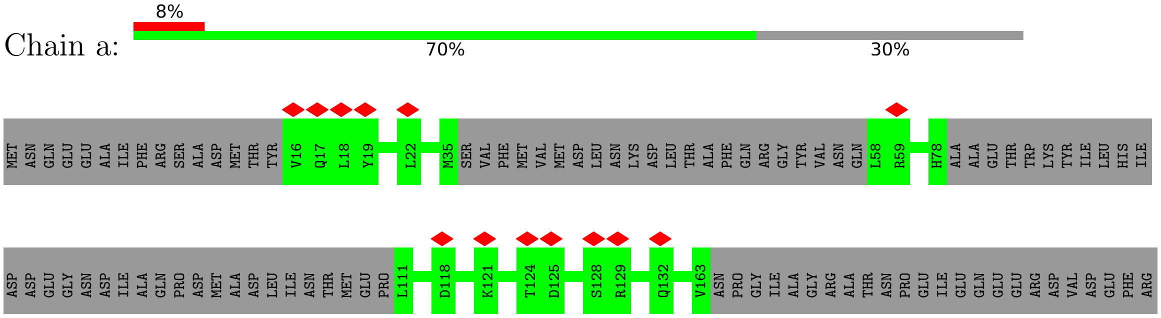
- Molecule 7: V-type proton ATPase subunit E

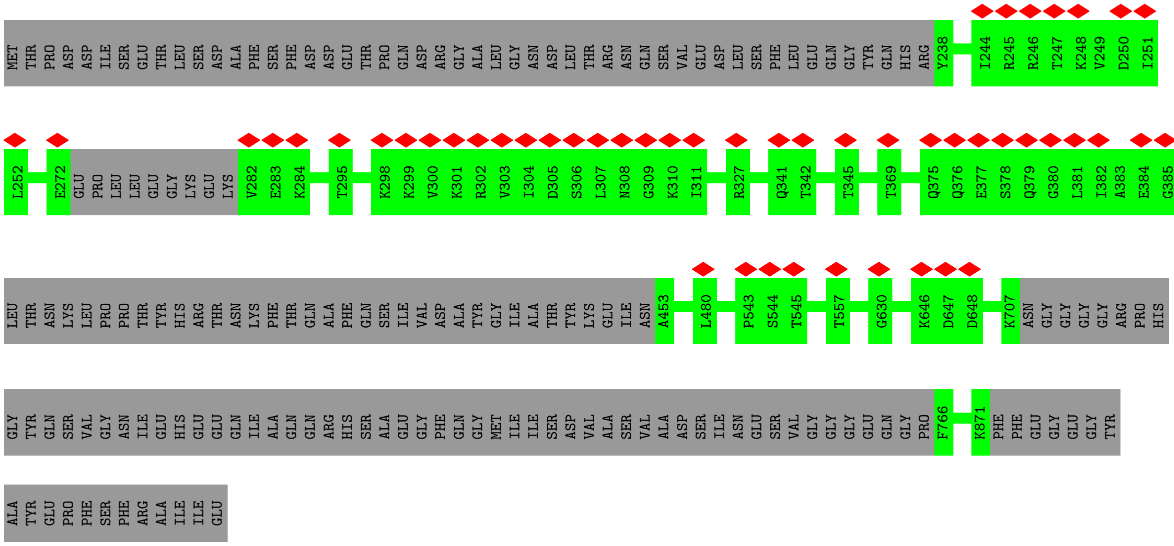


- Molecule 8: V-type proton ATPase subunit H



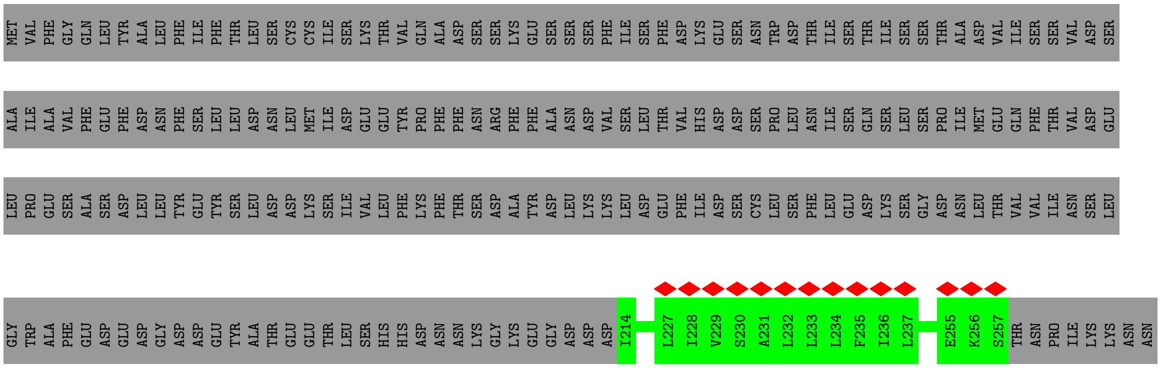
- Molecule 9: V-type proton ATPase subunit a, Golgi isoform





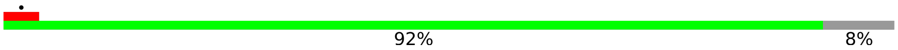
- Molecule 10: V0 assembly protein 1

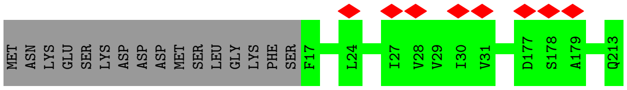
Chain b:



- Molecule 11: V-type proton ATPase subunit c”

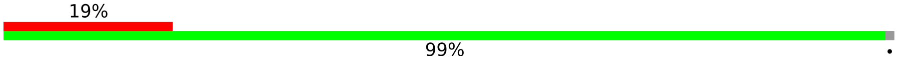
Chain c:

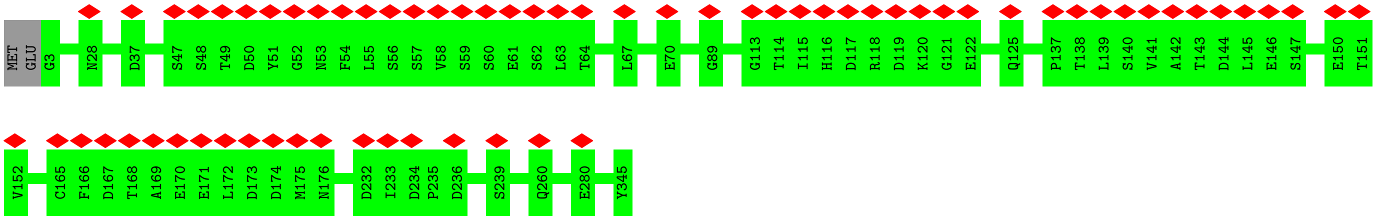




- Molecule 12: V-type proton ATPase subunit d

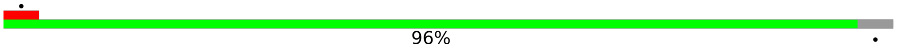
Chain d:

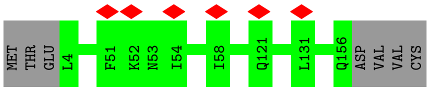




- Molecule 13: V-type proton ATPase subunit c

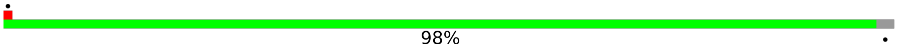
Chain g:

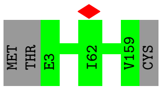




- Molecule 13: V-type proton ATPase subunit c

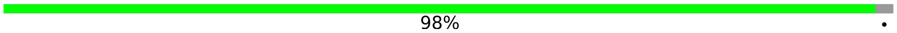
Chain h:

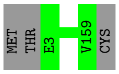




- Molecule 13: V-type proton ATPase subunit c

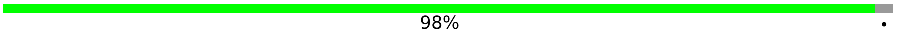
Chain i:

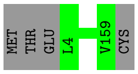




- Molecule 13: V-type proton ATPase subunit c

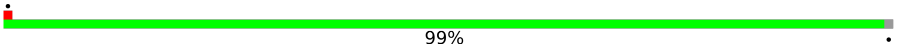
Chain j:

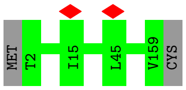




- Molecule 13: V-type proton ATPase subunit c

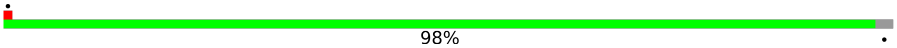
Chain k:

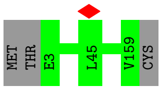




- Molecule 13: V-type proton ATPase subunit c

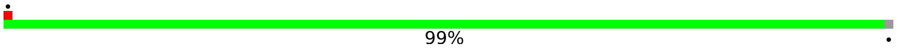
Chain l:

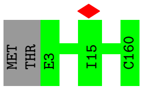




- Molecule 13: V-type proton ATPase subunit c

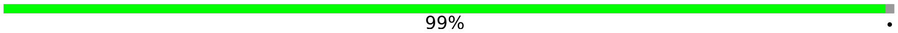
Chain m:

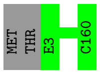




- Molecule 13: V-type proton ATPase subunit c

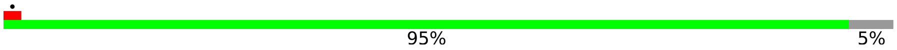
Chain n:

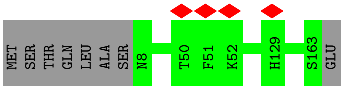




- Molecule 14: V-type proton ATPase subunit c’

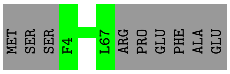
Chain o:





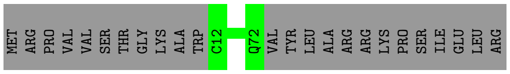
- Molecule 15: V-type proton ATPase subunit e

Chain e:



- Molecule 16: Putative protein YPR170W-B

Chain f:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.402	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	O	1.56	4/1946 (0.2%)	1.72	18/2715 (0.7%)
2	M	1.58	7/1038 (0.7%)	1.66	9/1445 (0.6%)
3	N	1.58	1/570 (0.2%)	1.64	3/794 (0.4%)
4	A	1.57	8/2914 (0.3%)	1.73	17/4048 (0.4%)
4	C	1.58	6/2914 (0.2%)	1.74	22/4048 (0.5%)
4	E	1.60	20/2914 (0.7%)	1.72	26/4048 (0.6%)
5	B	1.52	5/2249 (0.2%)	1.73	15/3126 (0.5%)
5	D	1.56	4/2249 (0.2%)	1.75	19/3126 (0.6%)
5	F	1.58	8/2249 (0.4%)	1.73	19/3126 (0.6%)
6	H	1.54	0/518	1.64	2/720 (0.3%)
6	J	1.51	2/518 (0.4%)	1.64	3/720 (0.4%)
6	L	1.50	0/518	1.64	6/720 (0.8%)
7	G	1.50	3/1077 (0.3%)	1.73	13/1502 (0.9%)
7	I	1.57	2/1077 (0.2%)	1.68	8/1502 (0.5%)
7	K	1.52	0/1077	1.65	4/1502 (0.3%)
8	P	1.57	7/2290 (0.3%)	1.71	17/3195 (0.5%)
9	a	0.25	0/3085	0.49	0/4288
10	b	0.24	0/217	0.45	0/301
11	c	0.27	0/961	0.50	0/1330
12	d	0.25	0/1698	0.48	0/2366
13	g	0.27	0/742	0.49	0/1024
13	h	0.27	0/762	0.48	0/1052
13	i	0.27	0/762	0.52	0/1052
13	j	0.26	0/757	0.48	0/1045
13	k	0.25	0/767	0.49	0/1059
13	l	0.26	0/762	0.49	0/1052
13	m	0.25	0/767	0.49	0/1059
13	n	0.26	0/767	0.49	0/1059
14	o	0.26	0/757	0.50	0/1045
15	e	0.23	0/318	0.45	0/443
16	f	0.24	0/300	0.44	0/416
All	All	1.28	77/39540 (0.2%)	1.42	201/54928 (0.4%)

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
5	B	0	1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	246	SER	CA-CB	9.62	1.67	1.52
5	F	123	GLY	N-CA	-8.02	1.34	1.46
4	E	573	SER	CA-CB	7.91	1.64	1.52
5	D	463	SER	CA-CB	7.62	1.64	1.52
4	E	433	GLY	N-CA	-7.34	1.35	1.46
4	A	473	SER	CA-CB	7.31	1.64	1.52
4	E	169	SER	CA-CB	7.17	1.63	1.52
4	E	207	SER	CA-CB	7.05	1.63	1.52
2	M	88	SER	CA-CB	6.70	1.62	1.52
5	F	163	SER	CA-CB	6.66	1.62	1.52
8	P	304	GLN	CA-CB	6.65	1.68	1.53
4	C	402	GLY	N-CA	-6.60	1.36	1.46
7	G	98	GLY	CA-C	-6.48	1.41	1.51
4	A	552	SER	CA-CB	6.46	1.62	1.52
5	D	116	SER	CA-CB	6.45	1.62	1.52
3	N	26	GLY	CA-C	-6.44	1.41	1.51
4	A	421	GLY	CA-C	-6.42	1.41	1.51
8	P	460	ARG	CA-CB	6.37	1.68	1.53
5	B	390	GLY	CA-C	-6.36	1.41	1.51
5	D	135	ASN	C-N	6.31	1.44	1.33
7	I	78	SER	CA-CB	6.23	1.62	1.52
7	G	187	GLY	CA-C	-6.16	1.42	1.51
5	B	117	GLY	CA-C	-6.15	1.42	1.51
4	E	127	GLY	CA-C	-6.05	1.42	1.51
5	F	32	SER	CA-CB	6.04	1.62	1.52
4	A	409	SER	CA-CB	5.87	1.61	1.52
2	M	30	SER	CA-CB	5.86	1.61	1.52
4	E	605	SER	CA-CB	5.83	1.61	1.52
4	E	58	GLY	CA-C	-5.69	1.42	1.51
8	P	219	GLN	CA-CB	5.69	1.66	1.53
4	E	107	GLY	CA-C	-5.66	1.42	1.51
2	M	140	SER	CA-C	-5.63	1.38	1.52
4	E	27	ILE	CA-CB	-5.60	1.42	1.54
5	B	388	GLY	CA-C	-5.57	1.43	1.51
7	G	43	TYR	CA-CB	5.55	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	261	GLY	CA-C	-5.54	1.43	1.51
4	E	165	SER	CA-CB	5.53	1.61	1.52
6	J	5	ASN	N-CA	-5.53	1.35	1.46
5	F	324	GLY	CA-C	-5.51	1.43	1.51
4	C	507	LEU	C-N	5.50	1.46	1.34
7	I	90	SER	CA-CB	5.49	1.61	1.52
8	P	331	SER	CA-CB	5.49	1.61	1.52
8	P	54	LYS	CA-CB	5.48	1.66	1.53
4	E	189	GLY	N-CA	-5.48	1.37	1.46
4	E	407	THR	C-N	5.46	1.42	1.33
5	F	267	ALA	N-CA	-5.46	1.35	1.46
4	C	275	SER	CA-CB	5.44	1.61	1.52
1	O	93	SER	CA-CB	5.41	1.61	1.52
4	E	534	TYR	N-CA	-5.39	1.35	1.46
4	A	555	ASP	CA-CB	5.39	1.65	1.53
4	E	182	ILE	N-CA	-5.36	1.35	1.46
1	O	39	ILE	C-N	5.34	1.42	1.33
4	A	231	TYR	C-O	-5.34	1.13	1.23
2	M	17	LEU	N-CA	-5.32	1.35	1.46
5	F	188	CYS	N-CA	-5.28	1.35	1.46
4	A	403	SER	CA-CB	5.23	1.60	1.52
2	M	15	LEU	C-N	5.23	1.42	1.33
2	M	58	GLY	CA-C	-5.22	1.43	1.51
4	E	159	GLY	CA-C	-5.20	1.43	1.51
4	E	590	SER	CA-CB	5.18	1.60	1.52
5	B	109	LEU	C-N	5.17	1.42	1.33
6	J	46	TYR	CA-CB	5.17	1.65	1.53
8	P	276	LYS	N-CA	-5.17	1.36	1.46
5	B	178	LEU	N-CA	-5.13	1.36	1.46
2	M	123	THR	C-N	5.13	1.42	1.33
4	C	168	SER	CA-CB	5.12	1.60	1.52
4	E	31	SER	C-N	5.11	1.42	1.33
4	C	329	ARG	C-N	5.11	1.45	1.34
4	C	356	SER	CA-CB	5.11	1.60	1.52
1	O	309	LEU	N-CA	-5.10	1.36	1.46
5	D	389	GLU	C-N	5.10	1.42	1.33
4	E	305	SER	CA-CB	5.09	1.60	1.52
5	F	462	TRP	CA-C	-5.05	1.39	1.52
5	F	82	GLY	N-CA	-5.03	1.38	1.46
1	O	177	ASP	C-N	5.02	1.45	1.34
4	E	415	ALA	N-CA	-5.01	1.36	1.46
4	A	487	GLU	CA-CB	5.00	1.65	1.53

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	332	SER	N-CA-CB	9.17	124.25	110.50
4	C	565	ALA	N-CA-CB	8.45	121.93	110.10
8	P	391	ASN	CB-CA-C	8.40	127.20	110.40
1	O	167	THR	N-CA-CB	8.06	125.61	110.30
4	E	257	ALA	N-CA-CB	8.00	121.30	110.10
4	C	409	SER	N-CA-CB	7.64	121.96	110.50
5	D	415	ALA	N-CA-CB	7.44	120.51	110.10
8	P	468	ALA	N-CA-CB	7.40	120.47	110.10
4	E	565	ALA	N-CA-CB	7.38	120.43	110.10
7	K	128	ALA	N-CA-CB	7.28	120.29	110.10
5	B	128	ALA	N-CA-CB	7.28	120.29	110.10
7	K	111	ALA	N-CA-CB	7.21	120.19	110.10
7	G	137	ALA	N-CA-CB	7.20	120.17	110.10
4	A	26	ALA	N-CA-CB	7.01	119.92	110.10
4	E	121	SER	CB-CA-C	-6.87	97.05	110.10
7	G	224	GLY	N-CA-C	-6.79	96.12	113.10
1	O	366	LYS	O-C-N	-6.78	111.85	122.70
5	F	213	ALA	N-CA-CB	6.76	119.57	110.10
4	E	327	ALA	CB-CA-C	-6.73	100.00	110.10
4	E	29	SER	N-CA-CB	6.73	120.59	110.50
4	C	356	SER	N-CA-CB	6.68	120.52	110.50
4	A	266	SER	N-CA-CB	6.68	120.52	110.50
5	D	149	GLU	N-CA-CB	6.66	122.59	110.60
7	I	113	ASN	N-CA-C	-6.62	93.13	111.00
7	G	116	GLU	CB-CA-C	-6.61	97.19	110.40
7	I	9	THR	N-CA-CB	6.57	122.78	110.30
4	E	44	ALA	CB-CA-C	-6.56	100.26	110.10
2	M	74	ALA	CB-CA-C	-6.54	100.29	110.10
4	C	68	ALA	CB-CA-C	-6.54	100.29	110.10
2	M	36	SER	N-CA-CB	6.50	120.25	110.50
1	O	78	SER	CB-CA-C	-6.48	97.79	110.10
8	P	368	LEU	N-CA-CB	6.42	123.23	110.40
7	G	180	ASN	CB-CA-C	-6.37	97.66	110.40
4	A	449	LYS	N-CA-CB	6.34	122.02	110.60
6	L	2	SER	N-CA-CB	6.28	119.92	110.50
4	E	120	GLN	N-CA-CB	6.22	121.79	110.60
5	F	450	GLU	N-CA-C	-6.21	94.24	111.00
1	O	366	LYS	CA-C-O	6.15	133.01	120.10
2	M	63	THR	N-CA-CB	6.13	121.96	110.30
4	C	453	SER	CB-CA-C	-6.12	98.46	110.10
7	G	198	GLU	CB-CA-C	-6.06	98.27	110.40
5	F	247	ASP	N-CA-CB	6.05	121.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	39	ALA	CB-CA-C	-6.03	101.05	110.10
4	E	318	VAL	N-CA-C	-6.02	94.74	111.00
8	P	332	ASP	N-CA-CB	6.01	121.42	110.60
5	D	400	SER	N-CA-CB	6.01	119.51	110.50
4	E	400	ALA	N-CA-CB	-6.00	101.70	110.10
5	D	142	TYR	C-N-CA	5.97	136.62	121.70
5	F	159	ASP	O-C-N	-5.96	113.16	122.70
6	L	62	ALA	CB-CA-C	-5.94	101.19	110.10
5	D	173	PHE	CB-CA-C	-5.93	98.53	110.40
4	A	390	SER	N-CA-CB	5.93	119.40	110.50
8	P	131	SER	N-CA-CB	5.93	119.39	110.50
4	C	560	ALA	CB-CA-C	-5.90	101.25	110.10
4	E	308	LYS	N-CA-CB	5.88	121.19	110.60
7	G	24	ILE	O-C-N	5.88	132.11	122.70
1	O	2	ALA	N-CA-CB	5.88	118.33	110.10
4	C	207	SER	N-CA-CB	5.87	119.30	110.50
5	D	395	ASP	CB-CA-C	-5.87	98.67	110.40
4	A	160	SER	CB-CA-C	-5.86	98.97	110.10
5	F	166	ARG	N-CA-CB	5.82	121.08	110.60
5	B	151	ILE	N-CA-C	-5.80	95.35	111.00
7	I	151	SER	O-C-N	-5.79	113.43	122.70
5	D	188	CYS	CB-CA-C	-5.79	98.82	110.40
1	O	197	ALA	N-CA-CB	5.78	118.19	110.10
5	F	42	GLU	CB-CA-C	-5.78	98.84	110.40
5	F	396	HIS	CB-CA-C	-5.78	98.84	110.40
5	D	253	ILE	N-CA-CB	5.78	124.09	110.80
5	D	118	ARG	N-CA-CB	5.77	120.99	110.60
2	M	65	ALA	N-CA-CB	5.77	118.17	110.10
8	P	106	SER	N-CA-CB	5.76	119.15	110.50
4	A	324	MET	N-CA-CB	5.76	120.96	110.60
5	F	482	ASP	N-CA-CB	5.75	120.94	110.60
7	G	87	LYS	O-C-N	-5.74	113.51	122.70
7	I	76	THR	N-CA-CB	5.74	121.20	110.30
8	P	17	ARG	N-CA-CB	5.73	120.92	110.60
6	J	36	LYS	N-CA-CB	5.72	120.89	110.60
4	C	492	ALA	N-CA-CB	5.72	118.10	110.10
5	F	127	PHE	N-CA-CB	5.71	120.88	110.60
7	I	222	LEU	CB-CA-C	-5.70	99.37	110.20
4	C	434	ILE	C-N-CA	5.68	135.91	121.70
7	G	197	ILE	N-CA-C	-5.68	95.67	111.00
4	E	246	CYS	N-CA-CB	5.67	120.80	110.60
8	P	413	ALA	N-CA-CB	5.65	118.01	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	98	PRO	N-CA-CB	5.63	110.06	103.30
1	O	150	ALA	CB-CA-C	5.63	118.55	110.10
6	H	61	ASN	N-CA-CB	5.62	120.72	110.60
1	O	328	LYS	N-CA-CB	5.62	120.71	110.60
4	A	39	ASN	CB-CA-C	5.61	121.62	110.40
6	J	92	ASP	CB-CA-C	-5.61	99.18	110.40
7	I	91	ALA	CB-CA-C	-5.60	101.69	110.10
5	B	137	SER	O-C-N	-5.59	110.48	121.10
1	O	97	TYR	N-CA-CB	5.59	120.66	110.60
5	B	143	ALA	C-N-CA	5.58	135.65	121.70
5	B	51	GLU	N-CA-CB	5.57	120.63	110.60
8	P	458	ASP	N-CA-CB	5.54	120.58	110.60
4	C	405	ASP	N-CA-CB	5.53	120.56	110.60
7	G	108	SER	CA-C-N	5.53	127.26	116.20
4	E	550	PHE	O-C-N	5.49	131.49	122.70
7	K	195	ASP	N-CA-CB	5.49	120.49	110.60
5	B	46	PHE	CA-C-N	5.49	132.46	117.10
2	M	8	VAL	CB-CA-C	5.48	121.81	111.40
4	C	426	PRO	N-CA-CB	5.47	109.86	103.30
4	E	292	GLU	O-C-N	-5.46	113.97	122.70
4	E	538	CYS	N-CA-CB	5.46	120.42	110.60
5	D	104	VAL	O-C-N	-5.45	113.97	122.70
1	O	237	HIS	O-C-N	-5.45	113.98	122.70
4	C	354	ALA	N-CA-C	-5.44	96.32	111.00
6	L	17	ALA	CB-CA-C	-5.43	101.95	110.10
3	N	92	LEU	N-CA-C	-5.43	96.35	111.00
5	D	388	GLY	N-CA-C	-5.41	99.56	113.10
7	G	81	ALA	N-CA-CB	5.41	117.68	110.10
5	B	204	HIS	N-CA-CB	5.40	120.31	110.60
4	C	461	SER	N-CA-C	-5.40	96.43	111.00
5	D	152	SER	N-CA-C	-5.39	96.45	111.00
1	O	371	LEU	CB-CA-C	-5.38	99.98	110.20
4	C	461	SER	N-CA-CB	5.37	118.56	110.50
5	B	294	ALA	N-CA-CB	5.37	117.62	110.10
5	B	340	ASP	N-CA-CB	5.37	120.26	110.60
8	P	175	GLN	N-CA-CB	5.36	120.25	110.60
5	D	464	LEU	C-N-CA	5.35	135.08	121.70
4	E	110	ARG	N-CA-C	-5.35	96.56	111.00
4	C	382	ALA	CB-CA-C	-5.34	102.08	110.10
3	N	41	GLN	N-CA-C	-5.34	96.58	111.00
6	L	72	ALA	N-CA-CB	5.33	117.57	110.10
5	F	103	PRO	O-C-N	-5.33	114.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	417	SER	N-CA-C	-5.33	96.60	111.00
4	E	72	VAL	CB-CA-C	5.33	121.53	111.40
4	C	278	ILE	N-CA-C	-5.32	96.63	111.00
1	O	295	ALA	CB-CA-C	-5.32	102.12	110.10
4	A	531	TYR	N-CA-CB	5.31	120.16	110.60
4	E	93	SER	N-CA-CB	5.30	118.45	110.50
6	H	51	ASP	N-CA-CB	5.29	120.13	110.60
5	F	343	THR	N-CA-CB	5.29	120.35	110.30
8	P	192	GLU	N-CA-CB	5.29	120.12	110.60
4	C	383	TYR	CB-CA-C	-5.29	99.83	110.40
5	B	143	ALA	N-CA-CB	5.28	117.49	110.10
1	O	254	LYS	N-CA-CB	5.27	120.09	110.60
7	K	214	ALA	N-CA-CB	5.27	117.47	110.10
8	P	292	SER	CB-CA-C	5.27	120.11	110.10
8	P	3	ALA	N-CA-CB	5.26	117.47	110.10
5	B	137	SER	CA-C-N	5.26	131.82	117.10
2	M	157	ILE	O-C-N	-5.24	114.31	122.70
2	M	82	GLN	N-CA-CB	5.24	120.04	110.60
4	A	329	ARG	CB-CA-C	-5.24	99.92	110.40
3	N	102	ASP	N-CA-C	-5.24	96.86	111.00
4	E	54	ASP	N-CA-CB	5.24	120.02	110.60
5	F	251	GLU	N-CA-CB	5.24	120.02	110.60
7	G	23	PHE	N-CA-CB	5.24	120.03	110.60
1	O	126	SER	N-CA-CB	5.23	118.35	110.50
4	C	98	PRO	N-CA-CB	5.23	109.57	103.30
2	M	53	ALA	N-CA-CB	5.22	117.41	110.10
4	E	202	PHE	N-CA-C	-5.22	96.90	111.00
5	D	154	GLY	O-C-N	-5.22	114.35	122.70
5	D	276	THR	N-CA-CB	5.22	120.22	110.30
4	E	468	ASN	N-CA-CB	5.21	119.99	110.60
6	L	49	GLN	N-CA-CB	5.21	119.97	110.60
1	O	4	ALA	N-CA-CB	5.21	117.39	110.10
4	A	257	ALA	CB-CA-C	-5.21	102.29	110.10
4	C	273	SER	N-CA-CB	5.20	118.31	110.50
2	M	17	LEU	C-N-CA	5.20	134.70	121.70
4	E	129	ASP	N-CA-CB	5.20	119.95	110.60
8	P	331	SER	N-CA-CB	5.20	118.29	110.50
5	B	72	GLY	C-N-CA	5.18	134.66	121.70
8	P	164	LEU	N-CA-CB	-5.18	100.05	110.40
4	E	125	PRO	N-CA-C	-5.17	98.65	112.10
5	F	35	ASN	N-CA-CB	5.16	119.90	110.60
5	D	118	ARG	CB-CA-C	-5.16	100.08	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	215	LEU	CA-C-O	-5.16	109.27	120.10
4	A	474	ASN	CB-CA-C	-5.16	100.09	110.40
5	F	211	VAL	N-CA-CB	5.15	122.83	111.50
5	B	39	VAL	C-N-CA	5.15	134.58	121.70
4	A	37	ALA	C-N-CA	5.14	134.55	121.70
5	F	279	THR	O-C-N	-5.12	114.51	122.70
4	C	596	VAL	N-CA-C	-5.12	97.18	111.00
4	E	125	PRO	N-CA-CB	5.12	109.44	103.30
4	C	407	THR	N-CA-C	-5.11	97.19	111.00
5	D	278	LEU	N-CA-C	-5.11	97.20	111.00
5	F	212	PHE	O-C-N	5.11	130.88	122.70
1	O	171	SER	N-CA-CB	5.11	118.16	110.50
5	F	69	GLU	CB-CA-C	-5.10	100.19	110.40
5	D	322	VAL	C-N-CA	5.09	134.43	121.70
4	A	462	LYS	CB-CA-C	-5.09	100.22	110.40
8	P	353	LEU	N-CA-CB	5.09	120.58	110.40
5	B	412	ASP	N-CA-CB	5.08	119.75	110.60
7	G	78	SER	N-CA-CB	5.08	118.12	110.50
5	F	424	ALA	CB-CA-C	-5.08	102.48	110.10
7	I	173	VAL	O-C-N	5.08	130.82	122.70
1	O	276	SER	CB-CA-C	-5.07	100.47	110.10
5	D	448	ALA	CB-CA-C	-5.06	102.50	110.10
4	A	93	SER	O-C-N	5.06	130.80	122.70
6	L	39	ALA	CB-CA-C	-5.06	102.51	110.10
1	O	107	VAL	CA-C-N	5.05	131.25	117.10
8	P	269	SER	N-CA-CB	5.05	118.08	110.50
4	E	391	PHE	CA-C-O	-5.05	109.50	120.10
5	B	259	ALA	CB-CA-C	-5.03	102.55	110.10
7	I	24	ILE	C-N-CA	5.03	134.27	121.70
4	A	571	ALA	N-CA-CB	5.01	117.11	110.10
4	E	355	ASP	N-CA-CB	5.01	119.61	110.60
5	F	302	ARG	C-N-CA	5.00	132.81	122.30
4	A	161	VAL	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	147	PRO	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	O	390/392 (100%)	359 (92%)	19 (5%)	12 (3%)	4	27
2	M	208/256 (81%)	201 (97%)	6 (3%)	1 (0%)	29	69
3	N	113/118 (96%)	103 (91%)	8 (7%)	2 (2%)	8	40
4	A	591/639 (92%)	543 (92%)	34 (6%)	14 (2%)	6	33
4	C	591/639 (92%)	540 (91%)	35 (6%)	16 (3%)	5	31
4	E	591/639 (92%)	536 (91%)	43 (7%)	12 (2%)	7	38
5	B	455/517 (88%)	415 (91%)	32 (7%)	8 (2%)	8	40
5	D	455/517 (88%)	406 (89%)	34 (8%)	15 (3%)	4	26
5	F	455/517 (88%)	405 (89%)	39 (9%)	11 (2%)	6	33
6	H	103/114 (90%)	101 (98%)	0	2 (2%)	8	38
6	J	103/114 (90%)	99 (96%)	2 (2%)	2 (2%)	8	38
6	L	103/114 (90%)	99 (96%)	2 (2%)	2 (2%)	8	38
7	G	215/233 (92%)	205 (95%)	8 (4%)	2 (1%)	17	57
7	I	215/233 (92%)	209 (97%)	6 (3%)	0	100	100
7	K	215/233 (92%)	207 (96%)	5 (2%)	3 (1%)	11	46
8	P	457/478 (96%)	429 (94%)	19 (4%)	9 (2%)	7	38
9	a	611/890 (69%)	588 (96%)	23 (4%)	0	100	100
10	b	42/265 (16%)	42 (100%)	0	0	100	100
11	c	195/213 (92%)	189 (97%)	6 (3%)	0	100	100
12	d	341/345 (99%)	327 (96%)	14 (4%)	0	100	100
13	g	151/160 (94%)	149 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	h	155/160 (97%)	154 (99%)	1 (1%)	0	100	100
13	i	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
13	j	154/160 (96%)	152 (99%)	2 (1%)	0	100	100
13	k	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
13	l	155/160 (97%)	153 (99%)	2 (1%)	0	100	100
13	m	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
13	n	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
14	o	154/164 (94%)	152 (99%)	2 (1%)	0	100	100
15	e	62/73 (85%)	62 (100%)	0	0	100	100
16	f	59/85 (69%)	59 (100%)	0	0	100	100
All	All	7962/9068 (88%)	7499 (94%)	352 (4%)	111 (1%)	15	46

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	167	THR
1	O	172	VAL
4	E	475	TYR
5	F	125	LYS
5	F	207	ASN
5	F	293	ALA
4	A	475	TYR
4	C	475	TYR
4	C	565	ALA
5	D	143	ALA
5	D	319	ALA
7	K	144	ARG
8	P	389	LYS
1	O	39	ILE
1	O	97	TYR
1	O	116	TRP
1	O	176	HIS
4	E	120	GLN
4	E	456	THR
4	E	575	GLY
4	E	593	GLU
5	F	340	ASP
4	A	177	ARG

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Mol	Chain	Res	Type
4	A	234	LEU
4	A	449	LYS
4	A	450	HIS
4	A	565	ALA
4	A	575	GLY
5	B	163	SER
5	B	294	ALA
4	C	75	GLU
4	C	125	PRO
4	C	575	GLY
5	D	88	VAL
5	D	323	GLU
5	D	377	PRO
5	D	467	ILE
6	J	77	GLN
8	P	391	ASN
8	P	392	TYR
6	H	77	GLN
3	N	4	LYS
4	E	308	LYS
4	E	529	ASN
5	F	135	ASN
4	A	305	SER
4	A	405	ASP
4	A	441	LEU
5	B	83	THR
5	B	293	ALA
4	C	325	PRO
5	D	141	PRO
5	D	203	GLY
6	L	63	GLY
7	K	192	ASN
8	P	234	ASN
8	P	332	ASP
1	O	2	ALA
1	O	229	ALA
1	O	360	LYS
1	O	375	ALA
3	N	115	LEU
4	E	207	SER
5	F	202	ASP
5	F	296	GLU

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Mol	Chain	Res	Type
4	A	257	ALA
5	B	121	ASP
5	B	391	MET
4	C	230	ASP
4	C	405	ASP
4	C	449	LYS
5	D	179	PRO
8	P	34	GLU
8	P	232	ALA
8	P	458	ASP
7	G	195	ASP
1	O	254	LYS
4	E	449	LYS
4	E	476	PRO
5	F	372	PRO
4	A	594	LYS
4	C	126	ARG
4	C	207	SER
4	C	528	GLN
5	D	125	LYS
5	D	138	PRO
5	D	391	MET
6	L	62	ALA
7	K	195	ASP
7	G	133	LEU
5	F	124	PRO
4	A	78	GLY
5	D	202	ASP
6	J	105	PRO
8	P	54	LYS
6	H	105	PRO
4	A	284	GLY
5	B	372	PRO
4	C	310	PRO
4	C	403	SER
4	E	284	GLY
1	O	384	PRO
2	M	115	PRO
5	F	137	SER
5	F	179	PRO
4	C	375	PRO
4	E	310	PRO

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Mol	Chain	Res	Type
5	B	126	VAL
5	D	248	PRO
4	C	589	PRO
5	D	375	VAL

5.3.2 Protein sidechains ⓘ

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

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 ⓘ

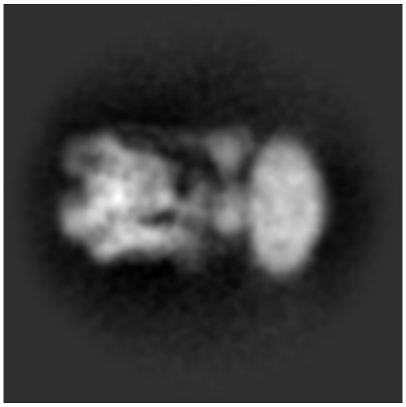
This section contains visualisations of the EMDB entry EMD-0648. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

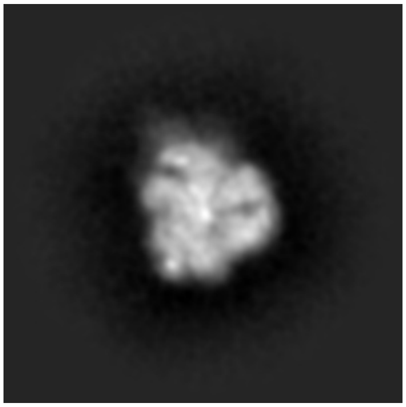
6.1 Orthogonal projections ⓘ

6.1.1 Primary map

X



Y



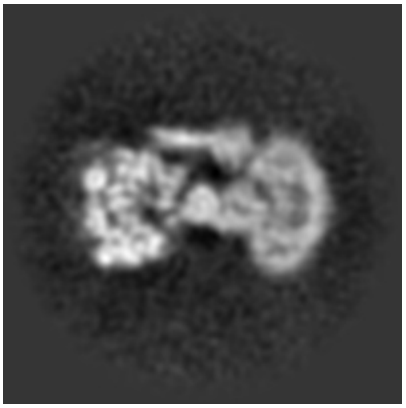
Z

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

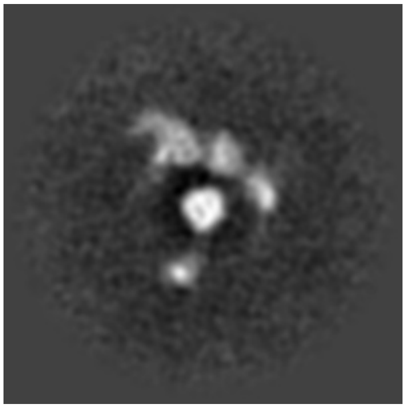
6.2 Central slices ⓘ

6.2.1 Primary map

X Index: 128



Y Index: 128

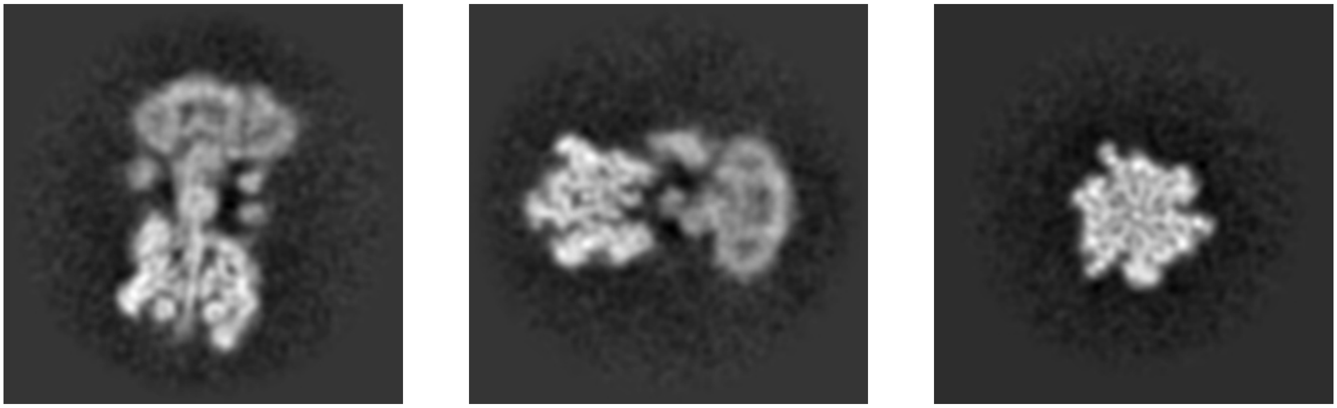


Z Index: 128

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

6.3 Largest variance slices

6.3.1 Primary map

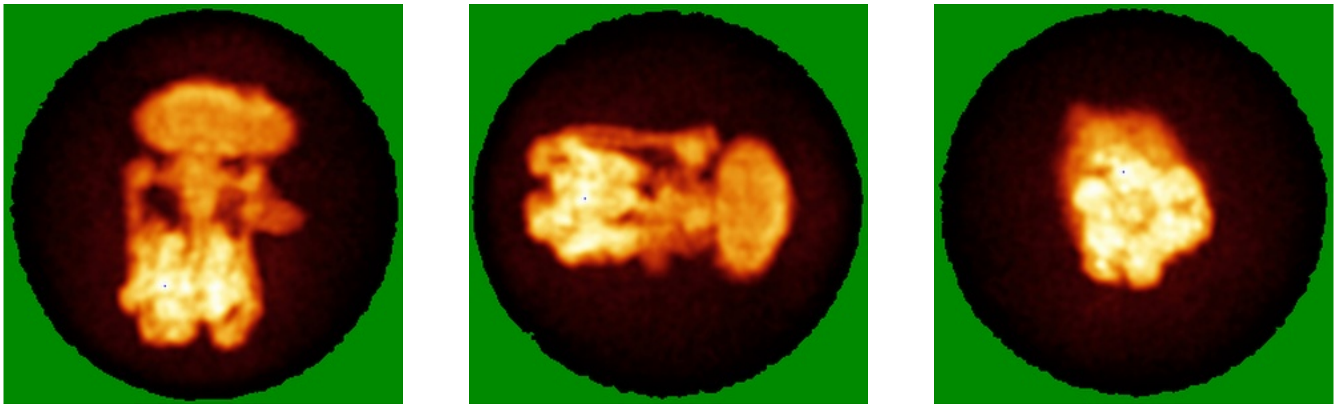


X Index: 128 Y Index: 136 Z Index: 74

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

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 ⓘ

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

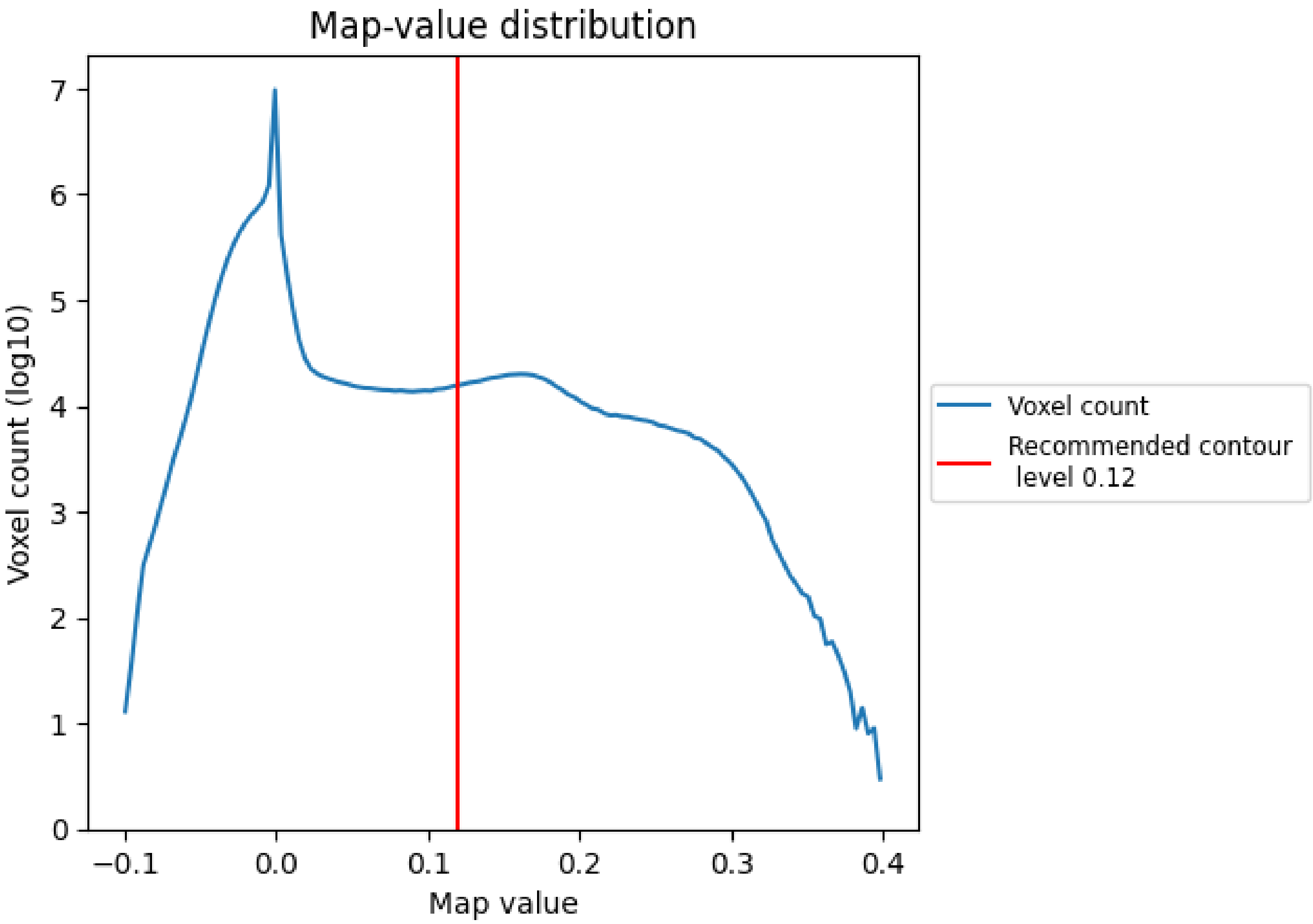
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

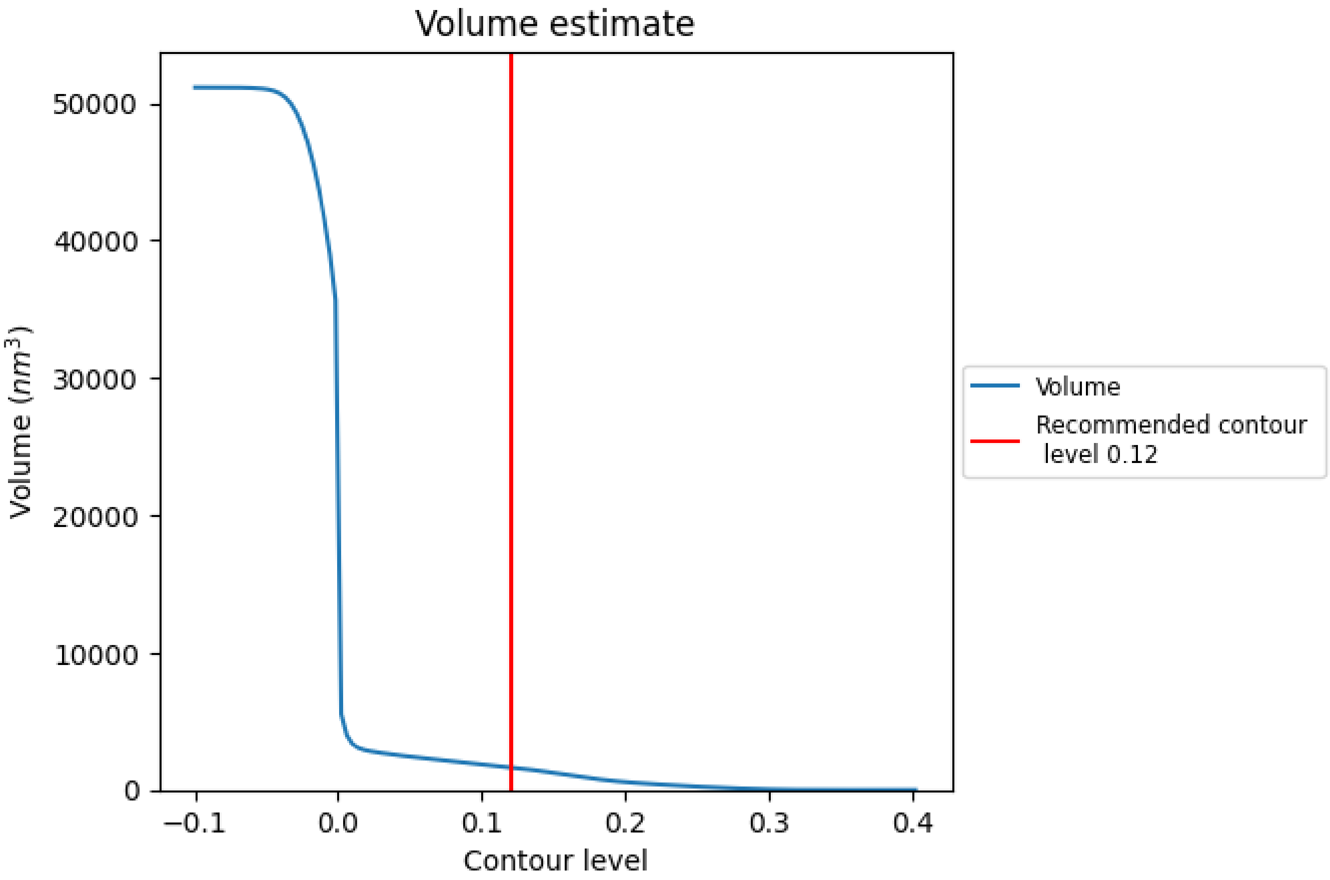
This section contains the results of statistical analysis of the map.

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.

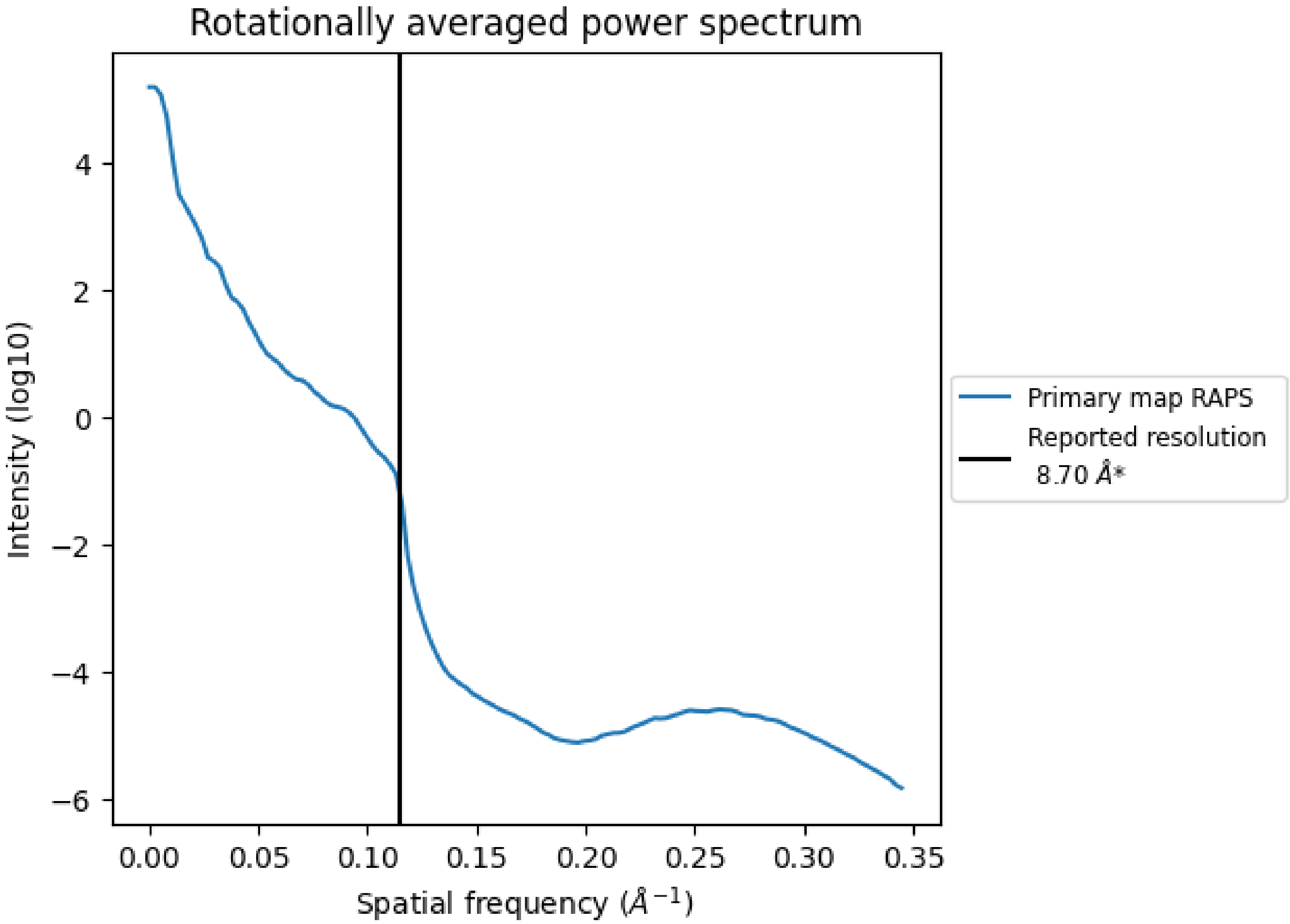
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1646 nm^3; this corresponds to an approximate mass of 1487 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 0.115 Å^{-1}

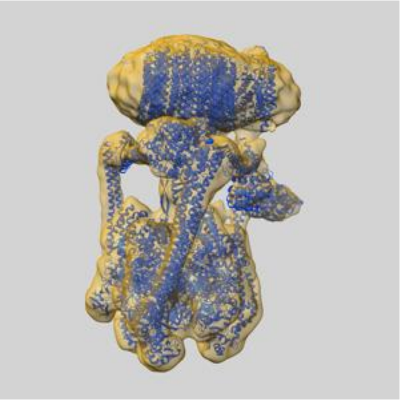
8 Fourier-Shell correlation ⓘ

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

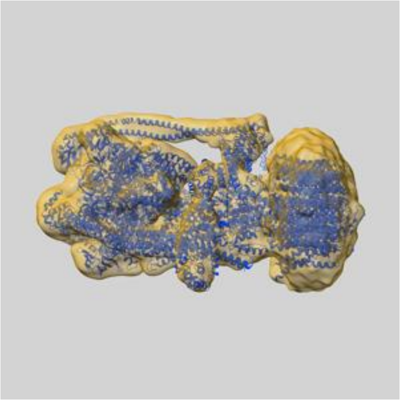
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0648 and PDB model 6O7X. Per-residue inclusion information can be found in section 3 on page 9.

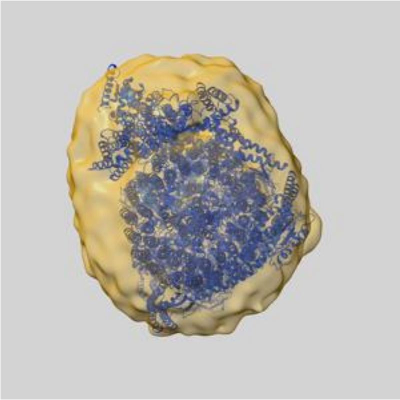
9.1 Map-model overlay



X



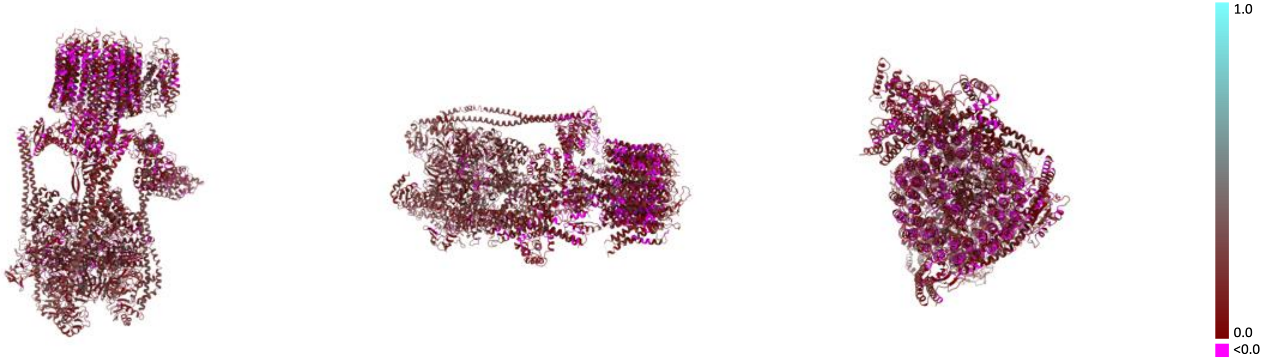
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

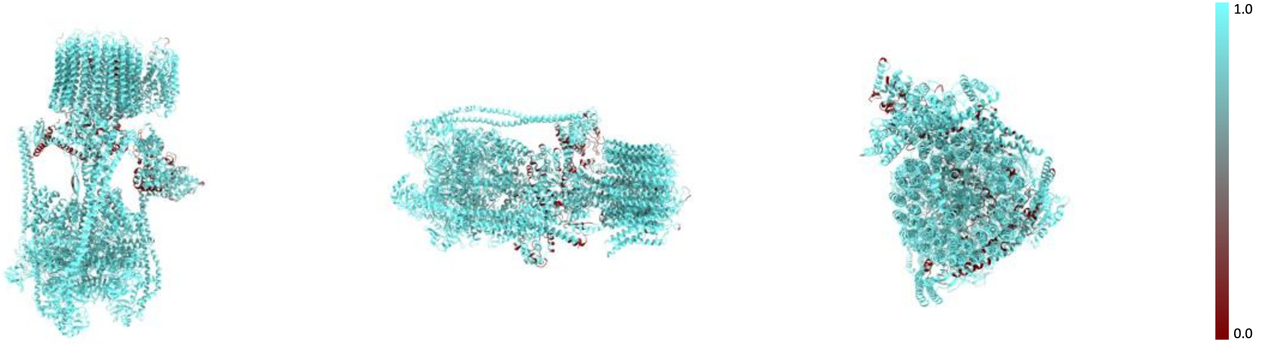
9.2 Q-score mapped to coordinate model ⓘ



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.

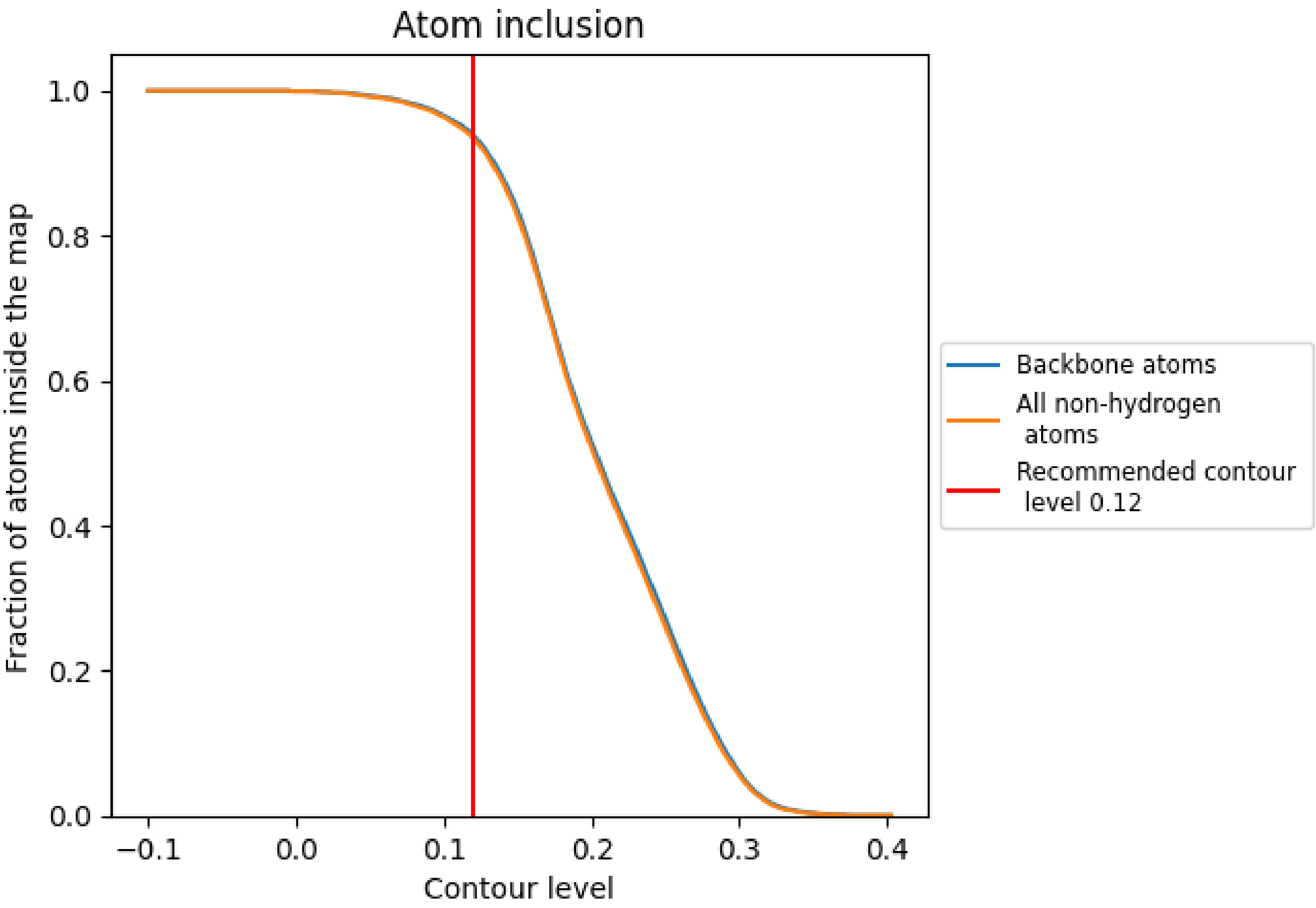
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.1210
A	0.9910	0.1540
B	0.9930	0.1560
C	0.9860	0.1510
D	0.9900	0.1510
E	0.9700	0.1300
F	0.9890	0.1400
G	0.9870	0.1810
H	1.0000	0.2020
I	0.9850	0.1850
J	1.0000	0.1680
K	0.9720	0.1840
L	0.9360	0.1850
M	0.9790	0.1610
N	0.9160	0.1320
O	0.6490	0.0650
P	0.7090	0.1100
a	0.8890	0.1030
b	0.6380	0.0370
c	0.9570	0.0610
d	0.8120	0.0890
e	0.9910	0.1100
f	0.9970	0.1270
g	0.9660	0.0720
h	0.9840	0.0670
i	0.9960	0.0510
j	0.9890	0.0480
k	0.9790	0.0480
l	0.9860	0.0760
m	0.9880	0.0670
n	0.9970	0.0730
o	0.9700	0.0490