Full wwPDB EM Validation Report (i)

Mar 9, 2024 – 10:50 AM EST

PDB ID	:	6O7W
EMDB ID	:	EMD-0647
Title	:	Saccharomyces cerevisiae V-ATPase Stv1-V1VO State 2
Authors	:	Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.
Deposited on	:	2019-03-08
Resolution	:	7.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

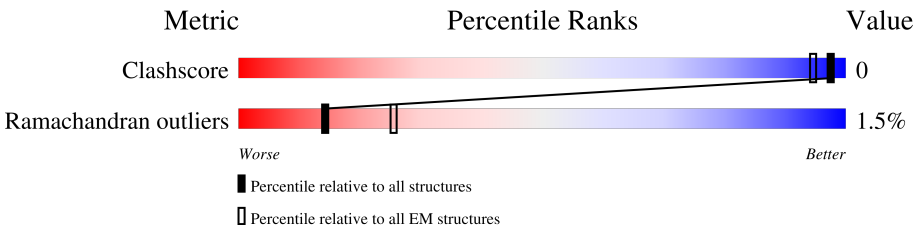
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	M	256	5%, 78%, •, 18%
2	N	118	14%, 88%, 8%, • •
3	A	639	•, 84%, 9%, 7%
3	C	639	•, 87%, 6%, 7%
3	E	639	•, 85%, 7%, •, 7%
4	B	517	•, 81%, 7%, 12%
4	D	517	•, 82%, 6%, 12%
4	F	517	•, 81%, 7%, 12%
5	H	114	•, 89%, •, 8%

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Mol	Chain	Length	Quality of chain
5	J	114	89% · 8%
5	L	114	8% 85% 7% 8%
6	G	233	6% 90% · 7%
6	I	233	· 88% 5% 7%
6	K	233	· 88% 5% 7%
7	P	478	13% 91% 5% ·
8	O	392	39% 92% 8% ·
9	a	890	7% 70% 30%
10	b	265	5% 17% 83%
11	c	213	7% 92% 8%
12	d	345	24% 99% ·
13	g	160	· 96% ·
13	h	160	6% 98% ·
13	i	160	· 98% ·
13	j	160	· 98% ·
13	k	160	· 99% ·
13	l	160	· 98% ·
13	m	160	12% 99% ·
13	n	160	18% 99% ·
14	o	164	9% 95% 5%
15	e	73	88% 12%
16	f	85	72% 28%

2 Entry composition (i)

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 D.

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

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

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

- Molecule 3 is a protein called Vacuolar ATP synthase catalytic subunit A.

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

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	617	ASP	-	SEE REMARK 999	UNP B3LH69
C	618	TYR	-	SEE REMARK 999	UNP B3LH69
C	619	LYS	-	SEE REMARK 999	UNP B3LH69
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	I	217	1078	644	217	217	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	g	153	743	437	153	153	0	0
13	h	157	763	449	157	157	0	0
13	i	157	763	449	157	157	0	0
13	j	156	758	446	156	156	0	0
13	k	158	768	452	158	158	0	0
13	l	157	763	449	157	157	0	0
13	m	158	768	452	158	158	0	0
13	n	158	768	452	158	158	0	0

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

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

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

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

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

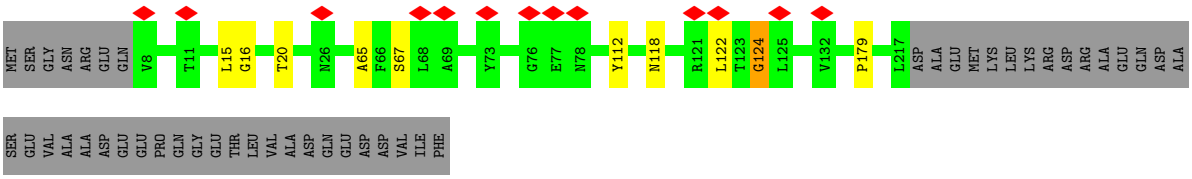
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	f	61	301	179	61	61	0	0

3 Residue-property plots (i)

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

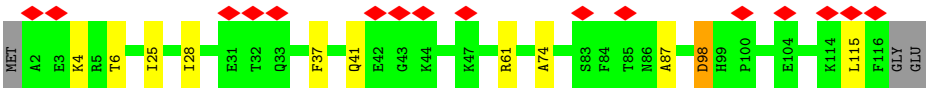
• Molecule 1: V-type proton ATPase subunit D

Chain M:



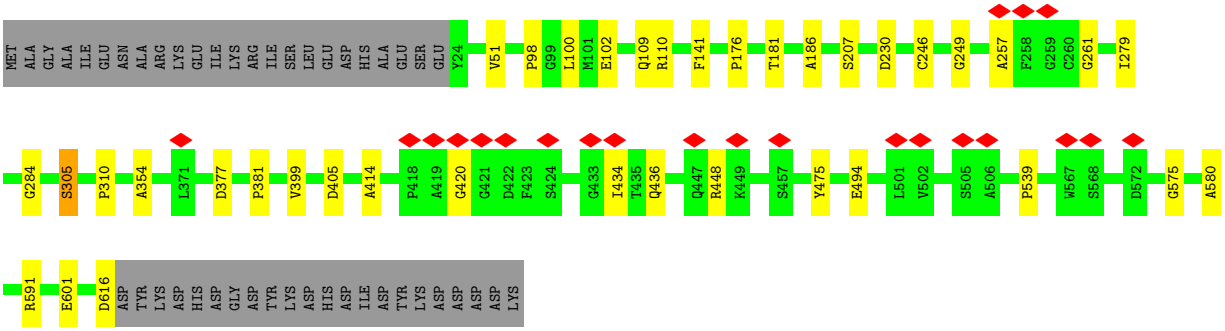
• Molecule 2: V-type proton ATPase subunit F

Chain N:



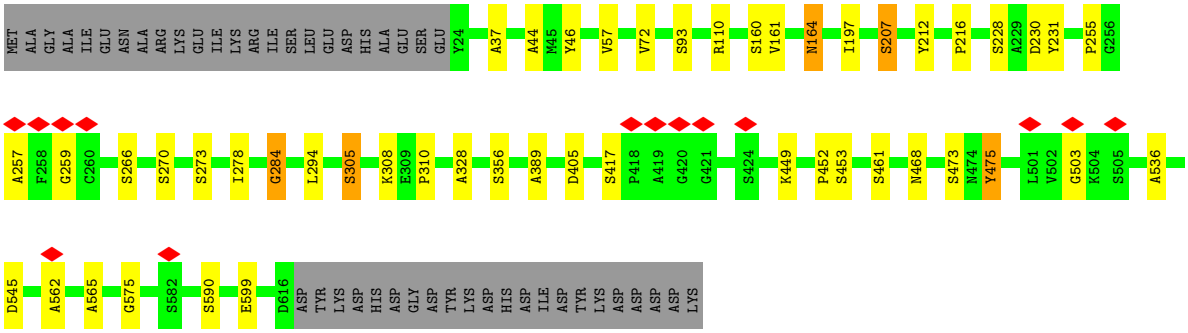
• Molecule 3: Vacuolar ATP synthase catalytic subunit A

Chain C:



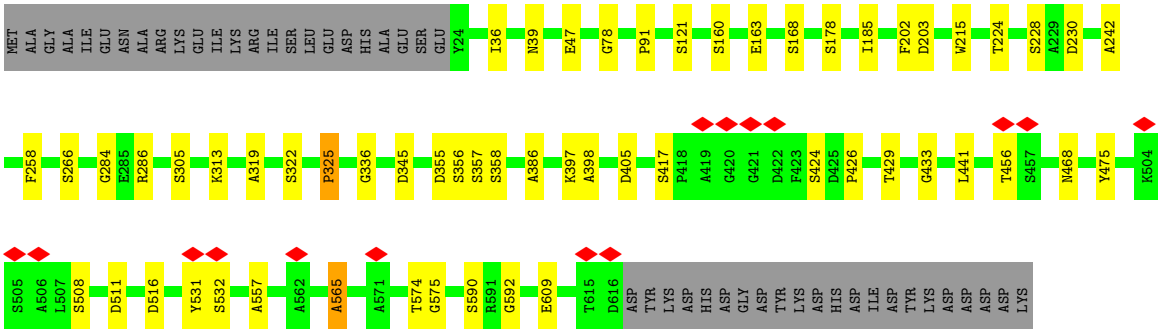
• Molecule 3: Vacuolar ATP synthase catalytic subunit A

Chain E:



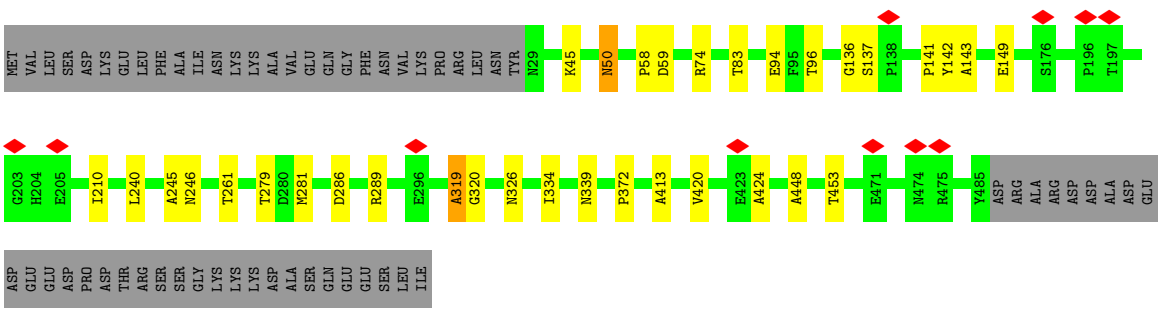
• Molecule 3: Vacuolar ATP synthase catalytic subunit A

Chain A:



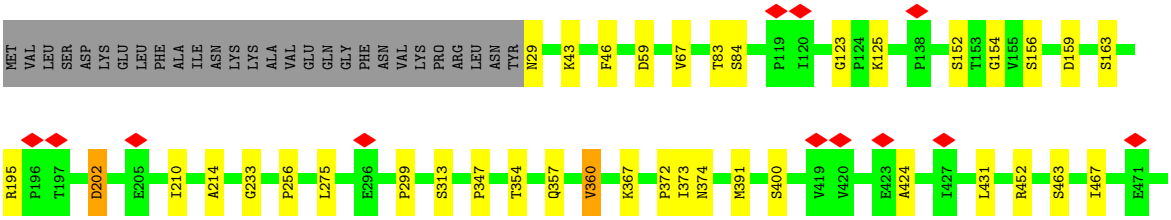
• Molecule 4: V-type proton ATPase subunit B

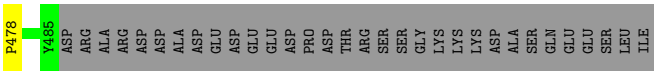
Chain D:



• Molecule 4: V-type proton ATPase subunit B

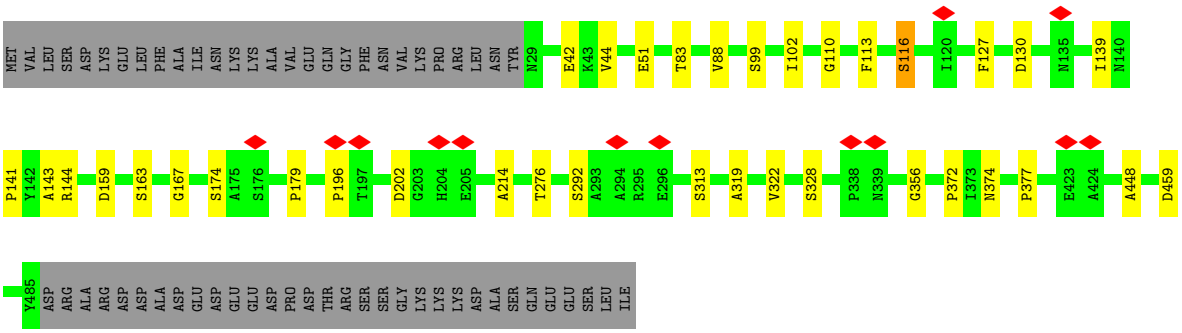
Chain F:





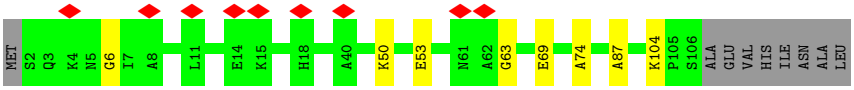
• Molecule 4: V-type proton ATPase subunit B

Chain B:



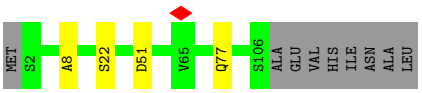
• Molecule 5: V-type proton ATPase subunit G

Chain L:



• Molecule 5: V-type proton ATPase subunit G

Chain H:

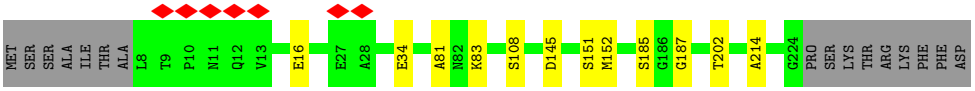


• Molecule 5: V-type proton ATPase subunit G

Chain J:

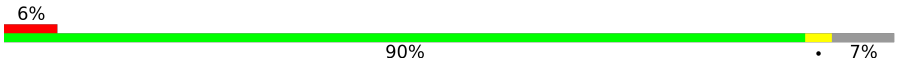
• Molecule 6: V-type proton ATPase subunit E

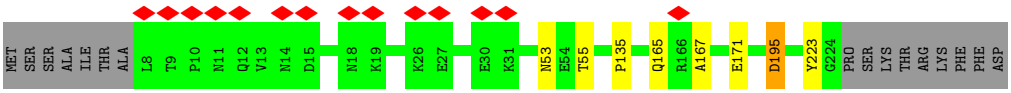
Chain K:



• Molecule 6: V-type proton ATPase subunit E

Chain G:



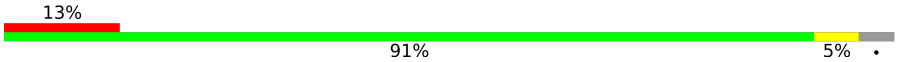


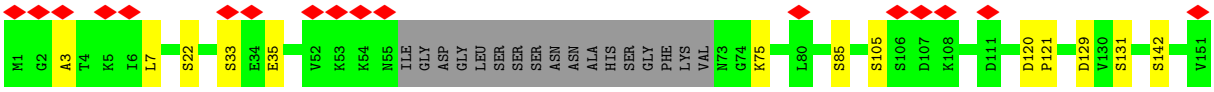
• Molecule 6: V-type proton ATPase subunit E

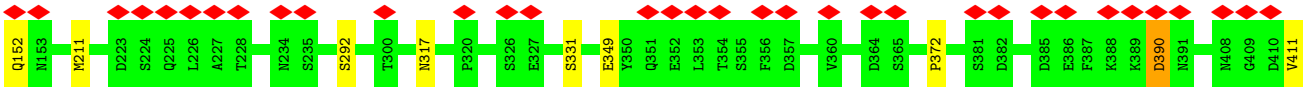
Chain I:

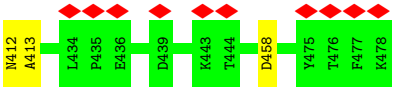
• Molecule 7: V-type proton ATPase subunit H

Chain P:



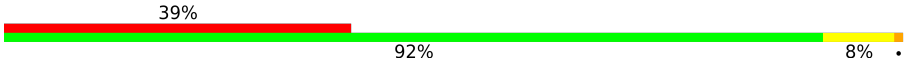


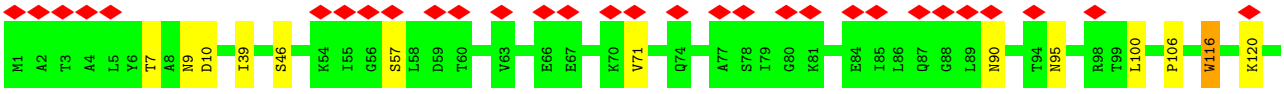


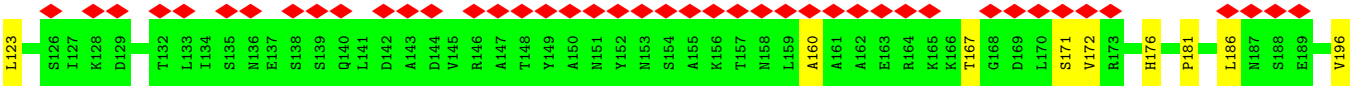


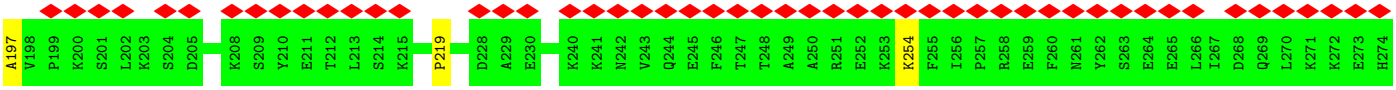
• Molecule 8: V-type proton ATPase subunit C

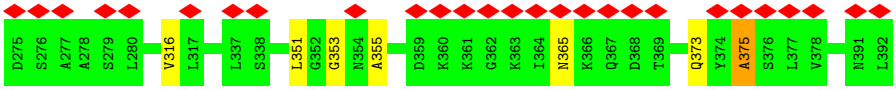
Chain O:





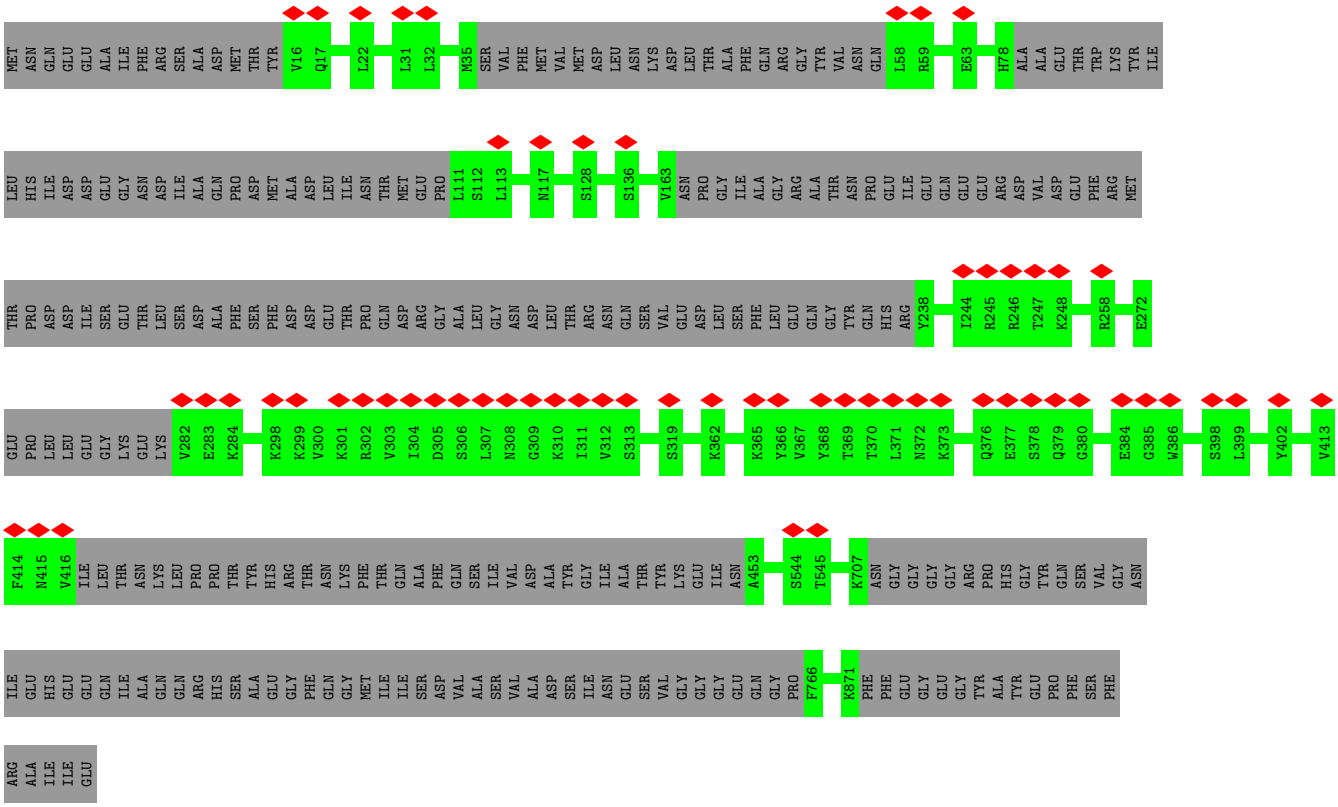






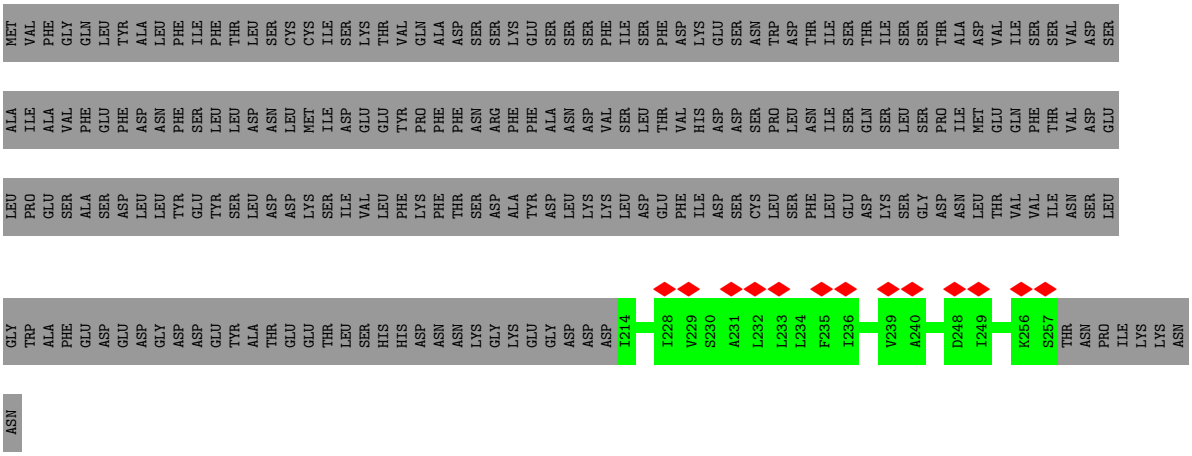
• Molecule 9: V-type proton ATPase subunit a, Golgi isoform

Chain a:



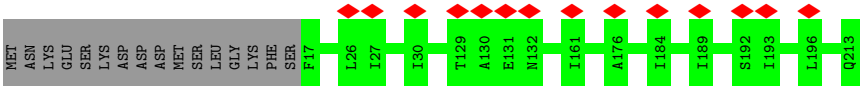
• Molecule 10: V0 assembly protein 1

Chain b: 5% 17% 83%



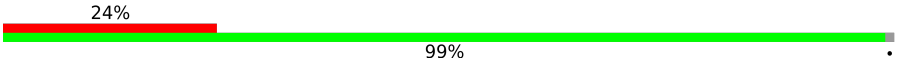
• Molecule 11: V-type proton ATPase subunit c"

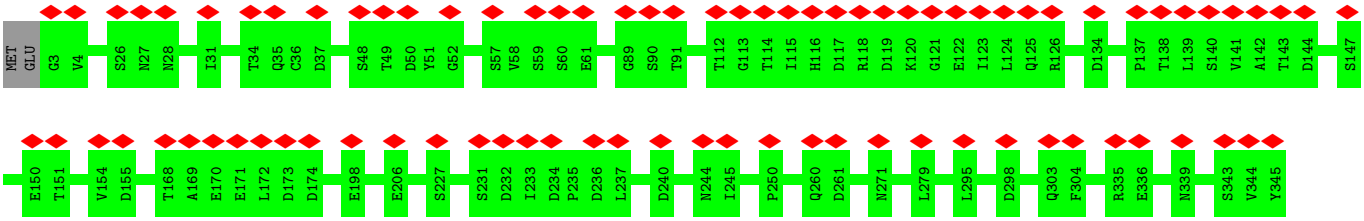
Chain c: 7% 92% 8%



• Molecule 12: V-type proton ATPase subunit d

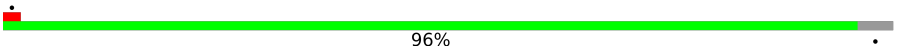
Chain d:

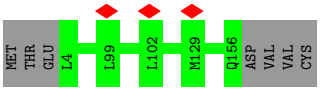




- Molecule 13: V-type proton ATPase subunit c

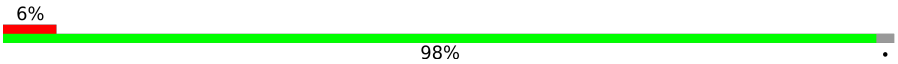
Chain g:

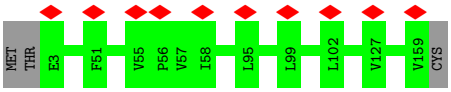




- Molecule 13: V-type proton ATPase subunit c

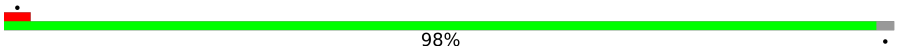
Chain h:

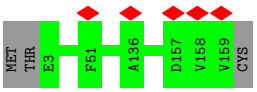




- Molecule 13: V-type proton ATPase subunit c

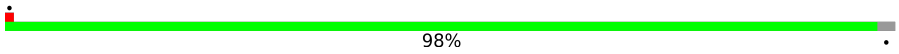
Chain i:

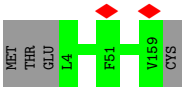




- Molecule 13: V-type proton ATPase subunit c

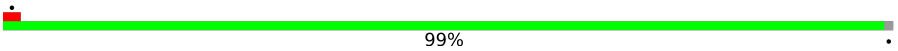
Chain j:

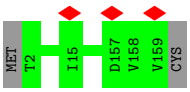




- Molecule 13: V-type proton ATPase subunit c

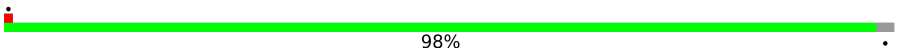
Chain k:

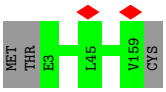




- Molecule 13: V-type proton ATPase subunit c

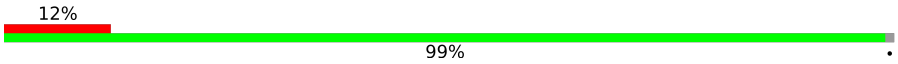
Chain l:

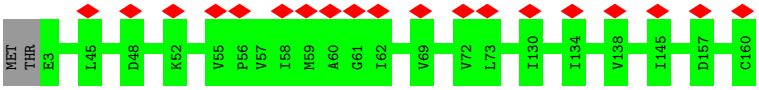




• Molecule 13: V-type proton ATPase subunit c

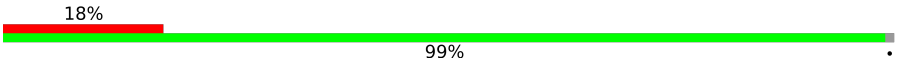
Chain m:

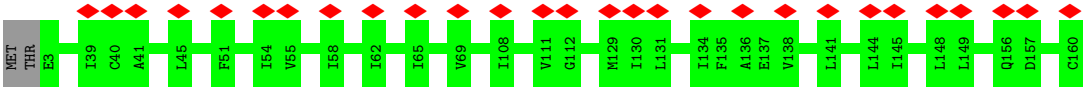




• Molecule 13: V-type proton ATPase subunit c

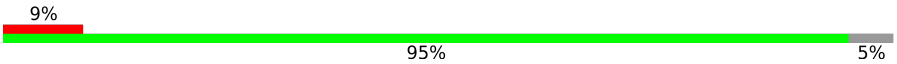
Chain n:

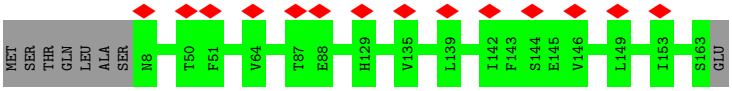




• Molecule 14: V-type proton ATPase subunit c'

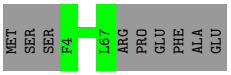
Chain o:





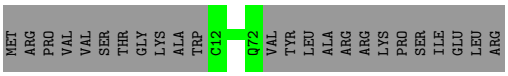
• Molecule 15: V-type proton ATPase subunit e

Chain e:



• Molecule 16: Putative protein YPR170W-B

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19265	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 ($e^-/Å^2$)	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	0.482	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.16	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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	M	1.57	3/1038 (0.3%)	1.69	7/1445 (0.5%)
2	N	1.64	2/570 (0.4%)	1.71	6/794 (0.8%)
3	A	1.62	16/2914 (0.5%)	1.75	25/4048 (0.6%)
3	C	1.55	3/2914 (0.1%)	1.72	22/4048 (0.5%)
3	E	1.57	10/2914 (0.3%)	1.72	26/4048 (0.6%)
4	B	1.53	6/2249 (0.3%)	1.69	15/3126 (0.5%)
4	D	1.57	4/2249 (0.2%)	1.78	18/3126 (0.6%)
4	F	1.62	9/2249 (0.4%)	1.74	16/3126 (0.5%)
5	H	1.47	0/518	1.66	3/720 (0.4%)
5	J	1.51	1/518 (0.2%)	1.57	3/720 (0.4%)
5	L	1.58	2/518 (0.4%)	1.67	5/720 (0.7%)
6	G	1.54	0/1077	1.70	7/1502 (0.5%)
6	I	1.57	2/1077 (0.2%)	1.67	10/1502 (0.7%)
6	K	1.59	3/1077 (0.3%)	1.61	6/1502 (0.4%)
7	P	1.57	6/2290 (0.3%)	1.67	17/3195 (0.5%)
8	O	1.58	6/1946 (0.3%)	1.73	14/2715 (0.5%)
9	a	0.25	0/3085	0.49	0/4288
10	b	0.25	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	1.29	73/39540 (0.2%)	1.42	200/54928 (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
4	B	0	1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	417	SER	CA-CB	7.86	1.64	1.52
3	A	322	SER	CA-CB	7.46	1.64	1.52
6	K	108	SER	CA-CB	7.46	1.64	1.52
7	P	105	SER	CA-CB	7.12	1.63	1.52
3	A	336	GLY	N-CA	-7.02	1.35	1.46
3	A	574	THR	C-N	6.95	1.45	1.33
8	O	181	PRO	N-CA	-6.70	1.35	1.47
3	E	160	SER	CA-CB	6.67	1.62	1.52
8	O	46	SER	CA-CB	6.62	1.62	1.52
4	F	233	GLY	CA-C	-6.50	1.41	1.51
7	P	85	SER	CA-CB	6.10	1.62	1.52
3	A	178	SER	CA-CB	6.10	1.62	1.52
5	J	66	GLY	CA-C	-6.05	1.42	1.51
7	P	372	PRO	CA-C	-6.03	1.40	1.52
3	A	215	TRP	CA-CB	6.03	1.67	1.53
3	C	436	GLN	N-CA	-6.01	1.34	1.46
7	P	292	SER	CA-CB	5.95	1.61	1.52
8	O	254	LYS	N-CA	-5.94	1.34	1.46
1	M	179	PRO	N-CA	-5.92	1.37	1.47
3	A	417	SER	CA-CB	5.91	1.61	1.52
4	B	313	SER	CA-CB	5.89	1.61	1.52
3	A	325	PRO	N-CA	-5.87	1.37	1.47
1	M	16	GLY	N-CA	5.85	1.54	1.46
3	E	255	PRO	C-N	5.79	1.43	1.33
3	E	72	VAL	CA-CB	-5.76	1.42	1.54
4	F	313	SER	CA-CB	5.75	1.61	1.52
3	E	228	SER	CA-CB	5.74	1.61	1.52
6	I	187	GLY	CA-C	-5.73	1.42	1.51
6	K	151	SER	CA-CB	5.72	1.61	1.52
4	F	400	SER	CA-CB	5.71	1.61	1.52
3	E	356	SER	CA-CB	5.69	1.61	1.52
4	F	84	SER	C-N	5.65	1.43	1.33
3	A	433	GLY	N-CA	-5.63	1.37	1.46
3	A	357	SER	CA-CB	5.58	1.61	1.52
4	B	356	GLY	N-CA	-5.55	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	320	GLY	CA-C	-5.53	1.43	1.51
7	P	331	SER	CA-CB	5.53	1.61	1.52
2	N	6	THR	N-CA	-5.51	1.35	1.46
4	F	43	LYS	N-CA	-5.51	1.35	1.46
3	C	249	GLY	N-CA	-5.50	1.37	1.46
3	A	358	SER	N-CA	-5.46	1.35	1.46
5	L	74	ALA	C-N	5.44	1.42	1.33
4	D	289	ARG	CA-CB	5.43	1.65	1.53
4	F	152	SER	CA-CB	5.41	1.61	1.52
4	B	328	SER	CA-CB	5.40	1.61	1.52
1	M	124	GLY	CA-C	-5.38	1.43	1.51
4	F	431	LEU	CA-C	-5.35	1.39	1.52
4	F	59	ASP	C-N	5.34	1.42	1.33
8	O	355	ALA	CA-CB	5.34	1.63	1.52
5	L	6	GLY	N-CA	-5.32	1.38	1.46
7	P	349	GLU	N-CA	-5.31	1.35	1.46
8	O	123	LEU	CA-CB	5.30	1.66	1.53
3	E	231	TYR	CA-CB	5.27	1.65	1.53
3	C	305	SER	CA-CB	5.23	1.60	1.52
3	E	473	SER	CA-CB	5.22	1.60	1.52
3	A	424	SER	CA-CB	5.21	1.60	1.52
3	A	397	LYS	C-N	5.20	1.46	1.34
6	I	167	ALA	CA-CB	5.19	1.63	1.52
4	B	102	ILE	C-N	-5.18	1.24	1.34
3	E	57	VAL	C-N	5.18	1.42	1.33
3	A	121	SER	CA-CB	-5.18	1.45	1.52
3	A	319	ALA	CA-CB	5.17	1.63	1.52
6	K	185	SER	CA-CB	5.15	1.60	1.52
4	F	367	LYS	C-N	5.14	1.42	1.33
3	A	266	SER	CA-CB	5.11	1.60	1.52
4	D	96	THR	C-N	5.08	1.42	1.33
4	D	286	ASP	CA-CB	5.08	1.65	1.53
8	O	71	VAL	CA-CB	-5.08	1.44	1.54
2	N	87	ALA	N-CA	-5.07	1.36	1.46
4	B	174	SER	CA-CB	5.05	1.60	1.52
3	A	185	ILE	CA-C	-5.04	1.39	1.52
3	E	599	GLU	CA-CB	5.02	1.65	1.53
4	B	116	SER	CA-CB	5.01	1.60	1.52

All (200) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	508	SER	N-CA-CB	8.67	123.51	110.50
4	D	74	ARG	N-CA-CB	8.57	126.02	110.60
3	C	414	ALA	N-CA-CB	8.10	121.43	110.10
6	G	195	ASP	N-CA-CB	7.92	124.85	110.60
8	O	375	ALA	N-CA-CB	7.88	121.13	110.10
6	G	167	ALA	N-CA-CB	7.79	121.01	110.10
8	O	160	ALA	CB-CA-C	-7.53	98.81	110.10
3	A	386	ALA	N-CA-CB	7.49	120.59	110.10
3	A	345	ASP	N-CA-CB	7.40	123.92	110.60
5	H	22	SER	N-CA-CB	7.34	121.50	110.50
4	D	319	ALA	N-CA-CB	7.28	120.30	110.10
3	E	110	ARG	N-CA-CB	7.27	123.68	110.60
4	B	448	ALA	CB-CA-C	-7.20	99.30	110.10
3	E	207	SER	N-CA-CB	7.17	121.25	110.50
3	E	284	GLY	N-CA-C	-7.17	95.19	113.10
1	M	65	ALA	N-CA-CB	7.11	120.05	110.10
4	F	400	SER	N-CA-CB	-7.09	99.86	110.50
3	E	164	ASN	N-CA-CB	6.95	123.11	110.60
3	C	98	PRO	N-CA-CB	6.85	111.52	103.30
4	B	319	ALA	CB-CA-C	-6.82	99.87	110.10
3	E	266	SER	CB-CA-C	-6.75	97.28	110.10
3	E	46	TYR	CB-CA-C	-6.73	96.94	110.40
3	A	168	SER	N-CA-CB	6.62	120.43	110.50
4	F	256	PRO	N-CA-CB	6.60	111.22	103.30
3	C	186	ALA	N-CA-CB	6.59	119.33	110.10
6	I	211	SER	N-CA-CB	6.52	120.28	110.50
8	O	353	GLY	O-C-N	6.46	133.04	122.70
4	F	354	THR	N-CA-CB	6.45	122.55	110.30
3	C	354	ALA	N-CA-CB	6.44	119.12	110.10
3	A	468	ASN	CB-CA-C	6.44	123.28	110.40
1	M	67	SER	N-CA-CB	6.43	120.14	110.50
3	E	270	SER	CB-CA-C	-6.41	97.92	110.10
3	A	565	ALA	CB-CA-C	-6.40	100.50	110.10
3	E	37	ALA	N-CA-CB	6.39	119.05	110.10
3	C	102	GLU	N-CA-CB	6.38	122.09	110.60
8	O	365	ASN	N-CA-CB	6.38	122.08	110.60
7	P	33	SER	N-CA-CB	6.36	120.03	110.50
7	P	152	GLN	N-CA-CB	6.33	122.00	110.60
6	I	165	GLN	C-N-CA	6.32	137.50	121.70
3	C	377	ASP	C-N-CA	6.30	137.46	121.70
4	D	448	ALA	CB-CA-C	6.27	119.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	452	PRO	N-CA-CB	6.22	110.76	103.30
6	G	53	ASN	C-N-CA	6.21	137.23	121.70
4	F	463	SER	N-CA-CB	6.20	119.80	110.50
4	B	374	ASN	N-CA-CB	6.20	121.76	110.60
6	G	165	GLN	C-N-CA	6.19	137.17	121.70
7	P	22	SER	N-CA-CB	6.14	119.71	110.50
6	K	83	LYS	CB-CA-C	-6.10	98.20	110.40
5	L	87	ALA	O-C-N	-6.09	112.95	122.70
4	D	261	THR	O-C-N	-6.08	112.97	122.70
4	B	196	PRO	N-CA-CB	6.06	110.57	103.30
3	C	305	SER	N-CA-CB	6.02	119.52	110.50
1	M	122	LEU	CB-CA-C	-6.01	98.78	110.20
4	F	357	GLN	N-CA-CB	6.01	121.41	110.60
4	D	339	ASN	N-CA-CB	6.00	121.41	110.60
6	K	214	ALA	CB-CA-C	-5.98	101.13	110.10
7	P	211	MET	CA-C-O	-5.98	107.54	120.10
3	A	511	ASP	O-C-N	-5.98	113.14	122.70
3	A	305	SER	N-CA-CB	5.97	119.45	110.50
2	N	74	ALA	CB-CA-C	-5.95	101.17	110.10
8	O	197	ALA	N-CA-CB	5.92	118.39	110.10
3	C	141	PHE	O-C-N	5.92	132.17	122.70
3	E	278	ILE	CB-CA-C	5.92	123.43	111.60
3	A	557	ALA	CB-CA-C	-5.89	101.26	110.10
7	P	7	LEU	N-CA-CB	5.87	122.15	110.40
2	N	98	ASP	N-CA-CB	5.87	121.17	110.60
3	C	448	ARG	N-CA-CB	5.85	121.12	110.60
4	D	240	LEU	CB-CA-C	-5.83	99.13	110.20
3	E	475	TYR	N-CA-CB	5.83	121.08	110.60
6	I	137	ALA	CB-CA-C	-5.82	101.37	110.10
3	E	273	SER	N-CA-CB	5.79	119.19	110.50
6	K	16	GLU	CB-CA-C	-5.79	98.82	110.40
4	B	113	PHE	O-C-N	-5.79	113.44	122.70
1	M	20	THR	N-CA-CB	-5.79	99.31	110.30
7	P	120	ASP	CB-CA-C	-5.78	98.83	110.40
5	J	74	ALA	N-CA-CB	5.77	118.18	110.10
7	P	413	ALA	N-CA-CB	5.76	118.16	110.10
6	I	141	ALA	N-CA-CB	5.75	118.15	110.10
4	B	144	ARG	N-CA-CB	5.74	120.94	110.60
4	D	246	ASN	N-CA-CB	5.72	120.89	110.60
6	I	16	GLU	N-CA-CB	5.71	120.88	110.60
4	F	347	PRO	N-CA-CB	5.66	110.10	103.30
3	C	181	THR	N-CA-C	-5.66	95.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	212	TYR	N-CA-CB	5.65	120.77	110.60
3	A	592	GLY	N-CA-C	-5.64	98.99	113.10
7	P	129	ASP	N-CA-CB	5.64	120.76	110.60
6	I	39	ALA	CB-CA-C	-5.63	101.65	110.10
3	A	508	SER	CB-CA-C	-5.62	99.42	110.10
7	P	411	VAL	CB-CA-C	5.61	122.06	111.40
3	C	110	ARG	N-CA-CB	5.61	120.70	110.60
6	K	34	GLU	N-CA-CB	5.59	120.66	110.60
5	L	50	LYS	N-CA-CB	5.58	120.65	110.60
3	A	160	SER	N-CA-CB	5.58	118.87	110.50
7	P	317	ASN	N-CA-CB	5.58	120.64	110.60
4	F	214	ALA	N-CA-CB	5.58	117.91	110.10
5	J	72	ALA	N-CA-CB	5.56	117.89	110.10
4	D	413	ALA	N-CA-CB	5.56	117.88	110.10
4	B	130	ASP	N-CA-C	-5.55	96.02	111.00
4	D	326	ASN	N-CA-CB	5.53	120.56	110.60
3	E	228	SER	CB-CA-C	-5.53	99.60	110.10
3	A	36	ILE	N-CA-C	-5.52	96.09	111.00
5	J	27	TYR	N-CA-CB	5.52	120.54	110.60
3	E	328	ALA	CB-CA-C	-5.52	101.82	110.10
7	P	142	SER	N-CA-CB	5.51	118.76	110.50
1	M	112	TYR	N-CA-CB	5.50	120.50	110.60
4	D	94	GLU	N-CA-C	-5.50	96.14	111.00
3	A	242	ALA	N-CA-CB	5.49	117.78	110.10
5	H	8	ALA	CB-CA-C	-5.49	101.87	110.10
3	E	461	SER	N-CA-CB	5.48	118.72	110.50
4	F	163	SER	N-CA-CB	5.47	118.71	110.50
7	P	390	ASP	N-CA-C	-5.47	96.22	111.00
4	D	334	ILE	N-CA-C	-5.47	96.23	111.00
3	A	398	ALA	CB-CA-C	-5.47	101.90	110.10
8	O	373	GLN	N-CA-CB	5.46	120.43	110.60
6	I	53	ASN	CB-CA-C	-5.46	99.48	110.40
3	A	286	ARG	CB-CA-C	-5.46	99.49	110.40
4	B	110	GLY	C-N-CA	5.46	135.34	121.70
3	C	601	GLU	CB-CA-C	-5.45	99.49	110.40
3	A	398	ALA	N-CA-CB	5.45	117.73	110.10
1	M	118	ASN	N-CA-CB	5.42	120.36	110.60
3	E	475	TYR	CA-C-N	5.42	132.28	117.10
3	C	100	LEU	CB-CA-C	-5.42	99.91	110.20
6	G	223	TYR	C-N-CA	-5.41	110.94	122.30
6	G	55	THR	O-C-N	-5.41	114.05	122.70
3	C	246	CYS	N-CA-C	-5.41	96.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	276	THR	N-CA-CB	5.40	120.55	110.30
3	C	580	ALA	N-CA-CB	5.39	117.65	110.10
3	E	44	ALA	N-CA-CB	5.39	117.65	110.10
4	B	214	ALA	CB-CA-C	-5.39	102.01	110.10
4	F	202	ASP	N-CA-CB	5.38	120.28	110.60
5	L	104	LYS	N-CA-CB	5.38	120.27	110.60
4	D	210	ILE	CB-CA-C	-5.37	100.85	111.60
3	E	562	ALA	N-CA-CB	5.37	117.62	110.10
8	O	116	TRP	N-CA-CB	5.37	120.26	110.60
4	D	142	TYR	C-N-CA	5.35	135.08	121.70
4	D	453	THR	N-CA-C	-5.35	96.55	111.00
4	B	42	GLU	N-CA-C	-5.35	96.56	111.00
4	B	322	VAL	N-CA-C	-5.35	96.56	111.00
3	E	545	ASP	CB-CA-C	-5.34	99.72	110.40
6	G	171	GLU	N-CA-CB	-5.34	100.99	110.60
4	F	478	PRO	N-CA-CB	5.34	109.70	103.30
4	F	374	ASN	N-CA-CB	5.33	120.19	110.60
8	O	57	SER	CB-CA-C	-5.33	99.97	110.10
3	C	399	VAL	N-CA-C	-5.33	96.62	111.00
6	K	81	ALA	CB-CA-C	-5.32	102.12	110.10
3	A	313	LYS	CB-CA-C	-5.32	99.77	110.40
5	L	53	GLU	O-C-N	-5.30	114.22	122.70
8	O	196	VAL	N-CA-C	-5.29	96.71	111.00
7	P	75	LYS	C-N-CA	5.29	134.93	121.70
3	E	305	SER	N-CA-CB	5.28	118.41	110.50
5	H	51	ASP	N-CA-CB	5.25	120.05	110.60
1	M	15	LEU	CA-C-N	5.25	126.70	116.20
3	E	468	ASN	N-CA-CB	5.25	120.04	110.60
2	N	28	ILE	N-CA-C	-5.24	96.85	111.00
7	P	121	PRO	N-CA-CB	5.24	109.59	103.30
4	D	50	ASN	N-CA-CB	5.24	120.02	110.60
4	D	281	MET	N-CA-CB	5.23	120.02	110.60
6	K	145	ASP	O-C-N	-5.22	114.34	122.70
7	P	413	ALA	N-CA-C	-5.22	96.89	111.00
2	N	37	PHE	N-CA-CB	5.22	120.00	110.60
8	O	351	LEU	CB-CA-C	-5.21	100.30	110.20
3	A	609	GLU	O-C-N	-5.20	114.39	122.70
4	F	156	SER	C-N-CA	5.19	134.68	121.70
3	C	434	ILE	C-N-CA	5.19	134.68	121.70
6	I	208	LYS	N-CA-CB	5.19	119.94	110.60
4	F	29	ASN	N-CA-C	-5.19	96.99	111.00
8	O	219	PRO	N-CA-CB	5.19	109.52	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	159	ASP	CB-CA-C	-5.19	100.03	110.40
7	P	390	ASP	N-CA-CB	5.18	119.93	110.60
4	D	279	THR	N-CA-C	-5.17	97.05	111.00
8	O	10	ASP	N-CA-C	-5.16	97.06	111.00
7	P	131	SER	N-CA-CB	5.16	118.24	110.50
3	C	176	PRO	N-CA-CB	5.15	109.48	103.30
2	N	41	GLN	O-C-N	5.15	130.93	122.70
6	I	49	ASN	CB-CA-C	-5.14	100.12	110.40
3	C	51	VAL	N-CA-CB	5.14	122.80	111.50
8	O	9	ASN	N-CA-CB	5.14	119.85	110.60
4	F	67	VAL	O-C-N	-5.13	114.48	122.70
4	D	420	VAL	C-N-CA	5.13	133.07	122.30
3	A	426	PRO	N-CA-CB	5.13	109.45	103.30
5	L	69	GLU	CB-CA-C	-5.12	100.15	110.40
3	E	294	LEU	O-C-N	-5.12	114.51	122.70
3	A	516	ASP	CB-CA-C	-5.11	100.19	110.40
3	C	616	ASP	N-CA-CB	5.09	119.77	110.60
3	E	308	LYS	N-CA-CB	5.09	119.77	110.60
8	O	316	VAL	O-C-N	-5.09	114.55	122.70
3	A	429	THR	N-CA-CB	5.08	119.95	110.30
3	E	453	SER	C-N-CA	5.08	134.39	121.70
6	I	85	ARG	N-CA-CB	5.08	119.73	110.60
3	C	494	GLU	CB-CA-C	-5.07	100.25	110.40
2	N	61	ARG	N-CA-CB	5.07	119.73	110.60
3	A	228	SER	N-CA-CB	5.07	118.10	110.50
3	A	163	GLU	N-CA-CB	-5.06	101.48	110.60
4	F	159	ASP	N-CA-CB	5.06	119.71	110.60
4	B	319	ALA	N-CA-CB	5.04	117.16	110.10
3	C	279	ILE	N-CA-C	-5.04	97.39	111.00
4	B	459	ASP	N-CA-CB	5.02	119.63	110.60
3	E	161	VAL	N-CA-C	-5.01	97.48	111.00
4	F	195	ARG	CA-C-N	5.01	131.12	117.10
3	A	224	THR	N-CA-CB	5.01	119.81	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	44	VAL	Peptide

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	M	1039	0	475	0	0
2	N	571	0	255	0	0
3	A	2915	0	1343	2	0
3	C	2915	0	1342	0	0
3	E	2915	0	1343	3	0
4	B	2250	0	1016	1	0
4	D	2250	0	1016	1	0
4	F	2250	0	1016	4	0
5	H	519	0	250	0	0
5	J	519	0	250	0	0
5	L	519	0	250	0	0
6	G	1078	0	483	0	0
6	I	1078	0	483	0	0
6	K	1078	0	483	1	0
7	P	2292	0	993	0	0
8	O	1947	0	876	0	0
9	a	3092	0	1352	0	0
10	b	218	0	98	0	0
11	c	962	0	477	0	0
12	d	1699	0	752	0	0
13	g	743	0	379	0	0
13	h	763	0	387	0	0
13	i	763	0	387	0	0
13	j	758	0	385	0	0
13	k	768	0	389	0	0
13	l	763	0	387	0	0
13	m	768	0	389	0	0
13	n	768	0	389	0	0
14	o	758	0	375	0	0
15	e	319	0	143	0	0
16	f	301	0	141	0	0
All	All	39578	0	18304	10	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (10) 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)
3:E:503:GLY:HA2	4:F:424:ALA:HB2	1.87	0.55
3:A:47:GLU:HA	3:A:91:PRO:HA	1.95	0.47
3:E:93:SER:HA	3:E:216:PRO:HA	1.99	0.45
4:B:51:GLU:HA	4:B:99:SER:HA	1.99	0.44
4:D:245:ALA:HB1	3:E:389:ALA:HB1	1.99	0.43
4:F:154:GLY:HA2	4:F:452:ARG:H	1.83	0.43
6:K:187:GLY:HA3	6:K:202:THR:HA	2.03	0.41
4:F:360:VAL:HA	4:F:373:ILE:HA	2.01	0.41
4:F:210:ILE:HA	4:F:275:LEU:O	2.21	0.41
3:A:355:ASP:HA	3:A:356:SER:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	208/256 (81%)	202 (97%)	5 (2%)	1 (0%)	29	69
2	N	113/118 (96%)	102 (90%)	7 (6%)	4 (4%)	3	25
3	A	591/639 (92%)	551 (93%)	23 (4%)	17 (3%)	4	29
3	C	591/639 (92%)	545 (92%)	31 (5%)	15 (2%)	5	32
3	E	591/639 (92%)	544 (92%)	31 (5%)	16 (3%)	5	31
4	B	455/517 (88%)	415 (91%)	26 (6%)	14 (3%)	4	27
4	D	455/517 (88%)	410 (90%)	32 (7%)	13 (3%)	4	29
4	F	455/517 (88%)	425 (93%)	20 (4%)	10 (2%)	6	35
5	H	103/114 (90%)	102 (99%)	0	1 (1%)	15	54
5	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
5	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	15	54
6	G	215/233 (92%)	206 (96%)	7 (3%)	2 (1%)	17	57
6	I	215/233 (92%)	207 (96%)	6 (3%)	2 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	215/233 (92%)	206 (96%)	8 (4%)	1 (0%)	29	69
7	P	457/478 (96%)	434 (95%)	18 (4%)	5 (1%)	14	52
8	O	390/392 (100%)	350 (90%)	26 (7%)	14 (4%)	3	25
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
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%)	7539 (95%)	307 (4%)	116 (2%)	14	46

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	475	TYR
4	D	45	LYS
4	D	59	ASP
4	D	143	ALA
3	E	475	TYR
3	E	565	ALA
3	E	575	GLY
4	F	46	PHE
3	A	202	PHE
3	A	475	TYR
4	B	141	PRO
4	B	372	PRO
8	O	120	LYS

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Mol	Chain	Res	Type
8	O	186	LEU
5	H	77	GLN
6	I	167	ALA
6	I	192	ASN
2	N	115	LEU
3	C	230	ASP
3	C	575	GLY
4	D	319	ALA
4	D	372	PRO
3	E	164	ASN
4	F	467	ILE
3	A	230	ASP
3	A	258	PHE
3	A	532	SER
3	A	575	GLY
4	B	139	ILE
4	B	377	PRO
7	P	3	ALA
8	O	39	ILE
8	O	172	VAL
8	O	375	ALA
1	M	124	GLY
2	N	98	ASP
3	C	261	GLY
3	C	310	PRO
4	D	58	PRO
4	D	141	PRO
4	D	149	GLU
3	E	405	ASP
3	E	449	LYS
3	E	536	ALA
4	F	299	PRO
3	A	39	ASN
3	A	203	ASP
3	A	284	GLY
3	A	441	LEU
3	A	565	ALA
5	L	63	GLY
7	P	35	GLU
8	O	90	ASN
8	O	167	THR
8	O	176	HIS

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Mol	Chain	Res	Type
3	C	257	ALA
3	C	305	SER
3	C	591	ARG
4	D	136	GLY
4	D	424	ALA
3	E	207	SER
3	E	257	ALA
4	F	83	THR
4	F	202	ASP
4	F	372	PRO
4	F	391	MET
3	A	325	PRO
3	A	405	ASP
3	A	531	TYR
3	A	590	SER
4	B	83	THR
4	B	116	SER
4	B	127	PHE
4	B	163	SER
4	B	167	GLY
4	B	292	SER
8	O	171	SER
6	G	195	ASP
3	C	207	SER
3	C	420	GLY
4	D	83	THR
3	E	230	ASP
3	E	305	SER
3	E	590	SER
4	F	123	GLY
4	F	125	LYS
4	F	360	VAL
4	B	143	ALA
4	B	202	ASP
6	K	152	MET
7	P	458	ASP
8	O	7	THR
8	O	95	ASN
8	O	100	LEU
8	O	116	TRP
6	G	135	PRO
2	N	4	LYS

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Mol	Chain	Res	Type
3	C	109	GLN
3	C	405	ASP
4	D	50	ASN
4	D	137	SER
3	E	259	GLY
3	A	456	THR
7	P	390	ASP
7	P	412	ASN
3	E	310	PRO
3	A	78	GLY
4	B	88	VAL
3	E	284	GLY
2	N	25	ILE
3	C	284	GLY
8	O	106	PRO
3	C	381	PRO
3	C	539	PRO
3	E	197	ILE
4	B	179	PRO

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

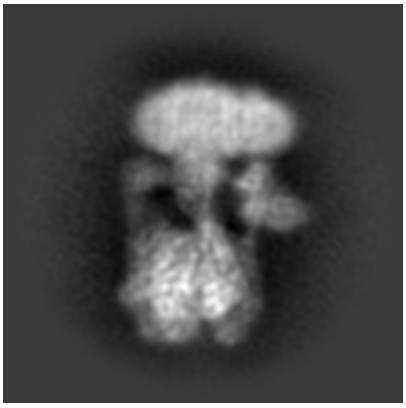
6 Map visualisation (i)

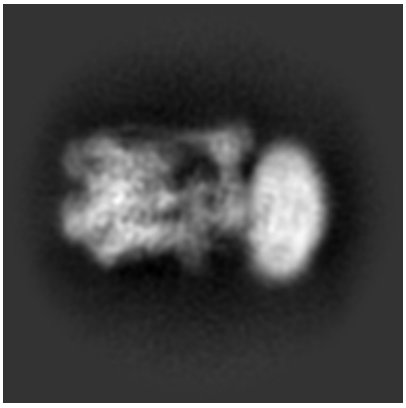
This section contains visualisations of the EMDB entry EMD-0647. These allow visual inspection of the internal detail of the map and identification of artifacts.

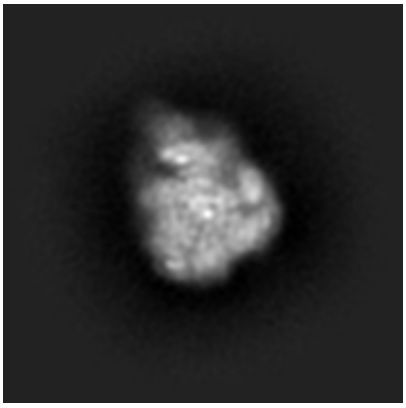
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

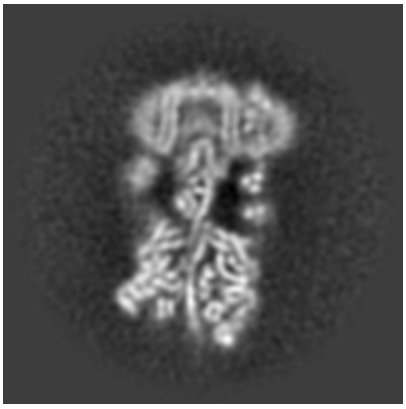

Y

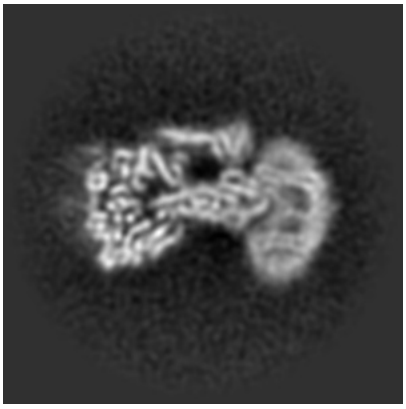

Z

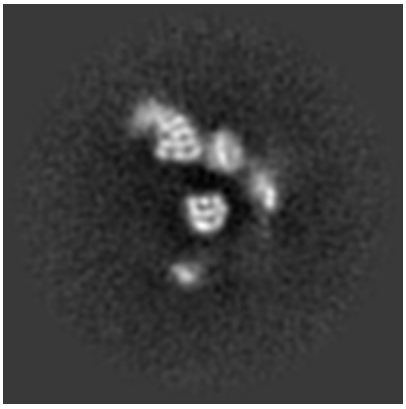
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 128


Y Index: 128

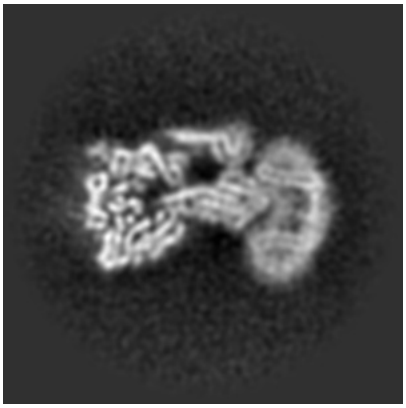

Z Index: 128

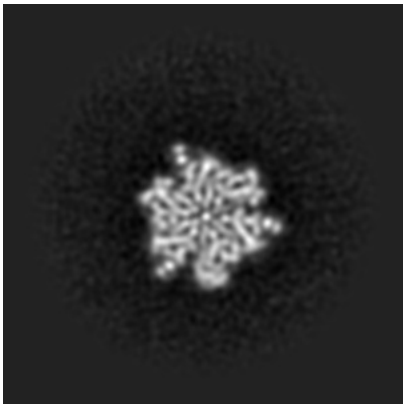
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 108


Y Index: 130


Z Index: 74

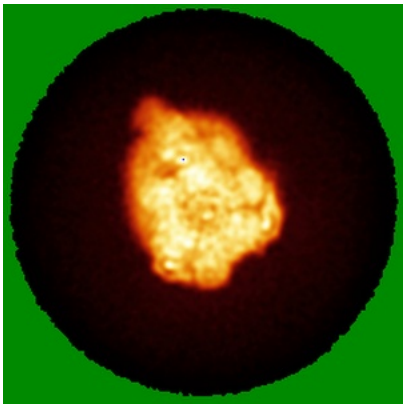
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

X

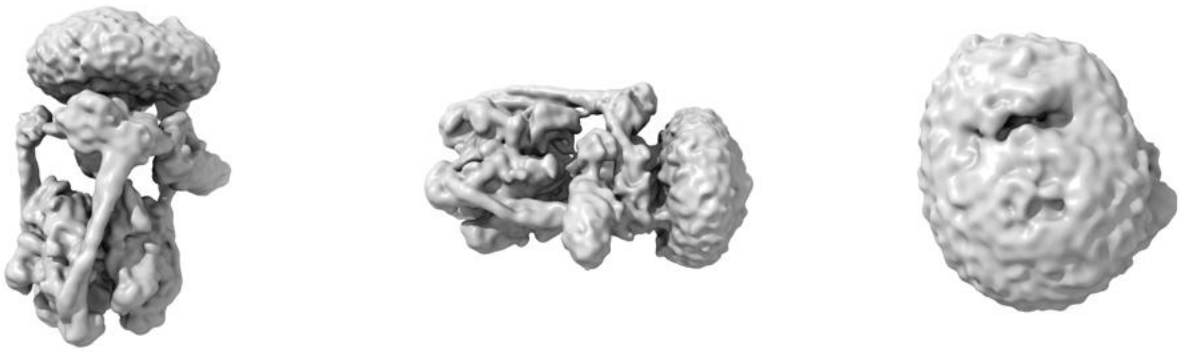
Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

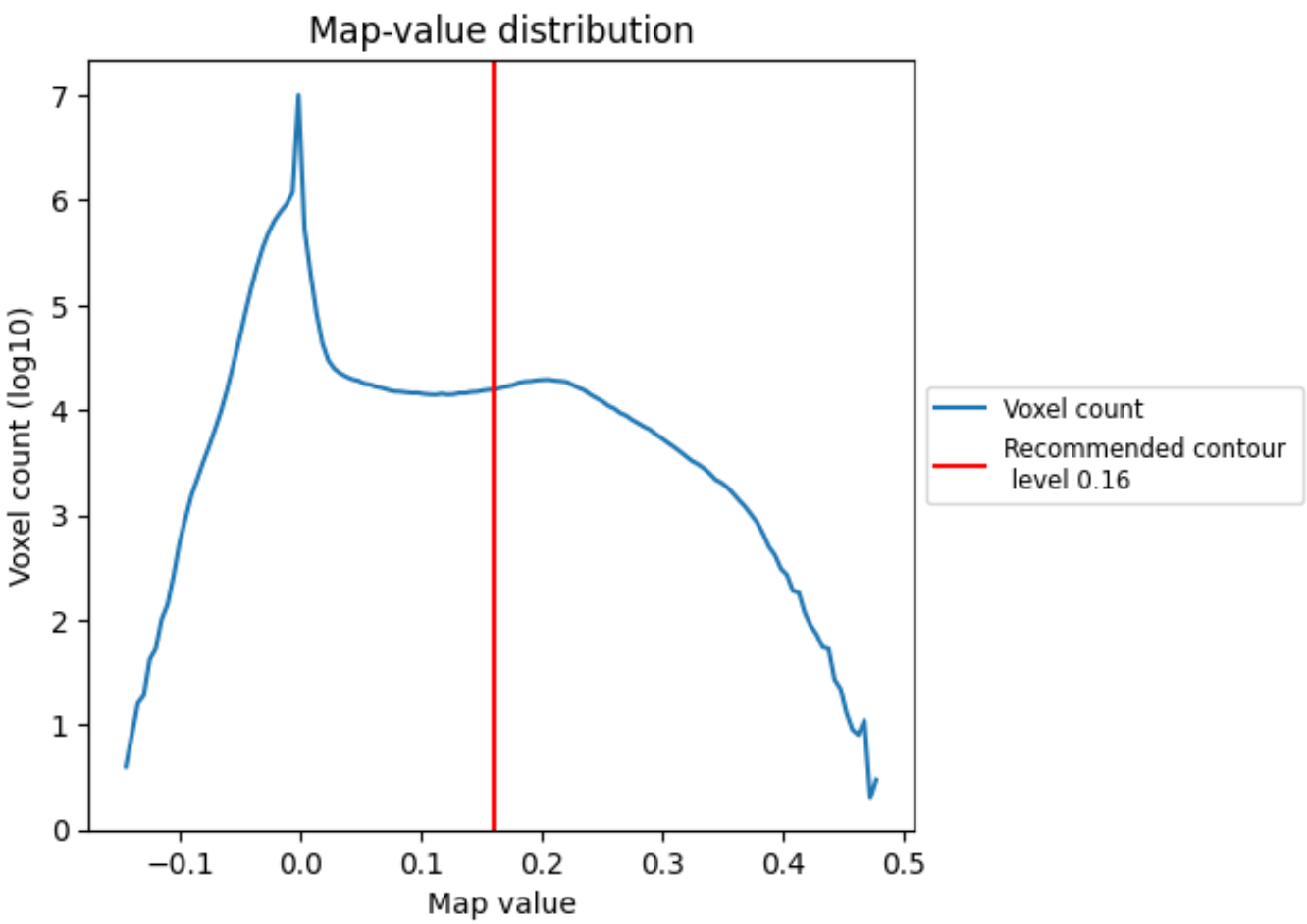
6.6 Mask visualisation (i)

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

7 Map analysis (i)

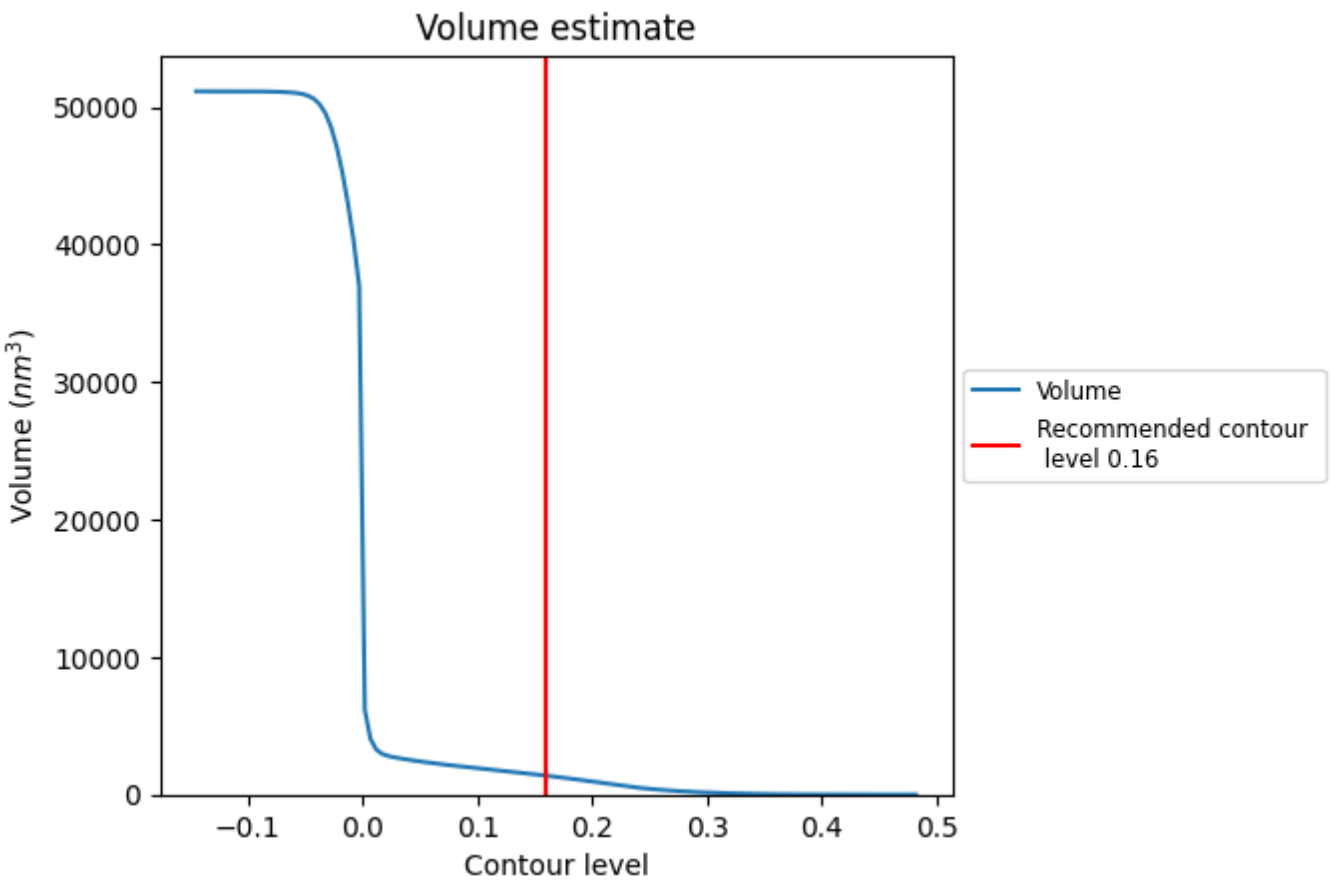
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

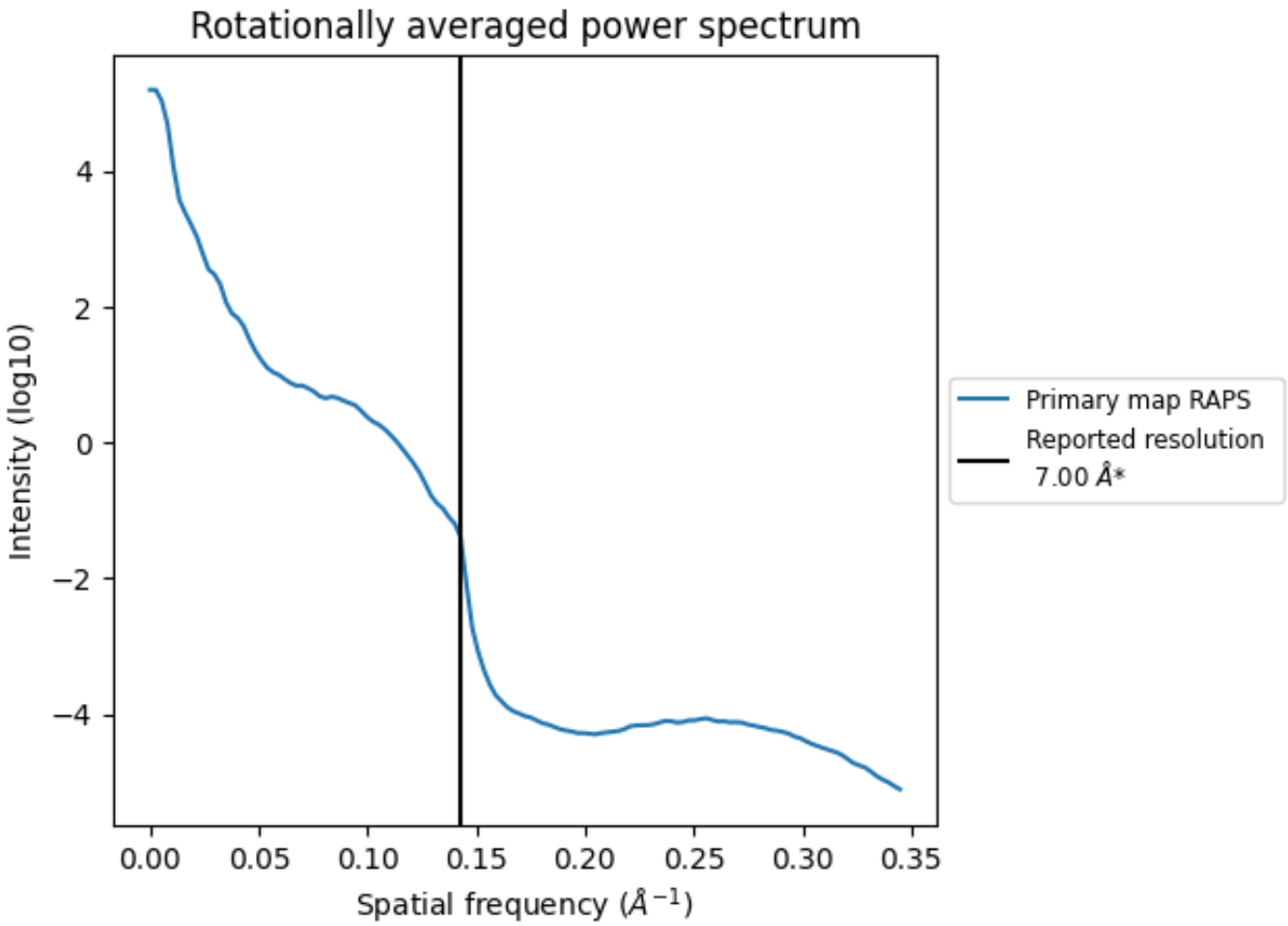
7.2 Volume estimate (i)



The volume at the recommended contour level is 1377 nm^3; this corresponds to an approximate mass of 1244 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 (i)



*Reported resolution corresponds to spatial frequency of 0.143 Å^{-1}

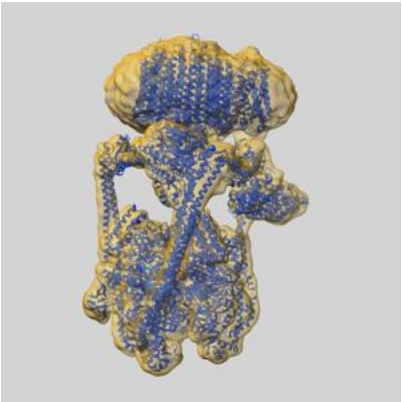
8 Fourier-Shell correlation (i)

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

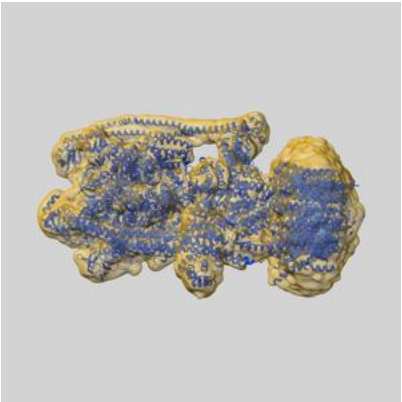
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0647 and PDB model 6O7W. Per-residue inclusion information can be found in section 3 on page 9.

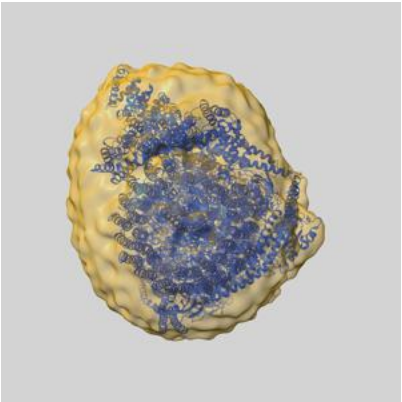
9.1 Map-model overlay (i)



X



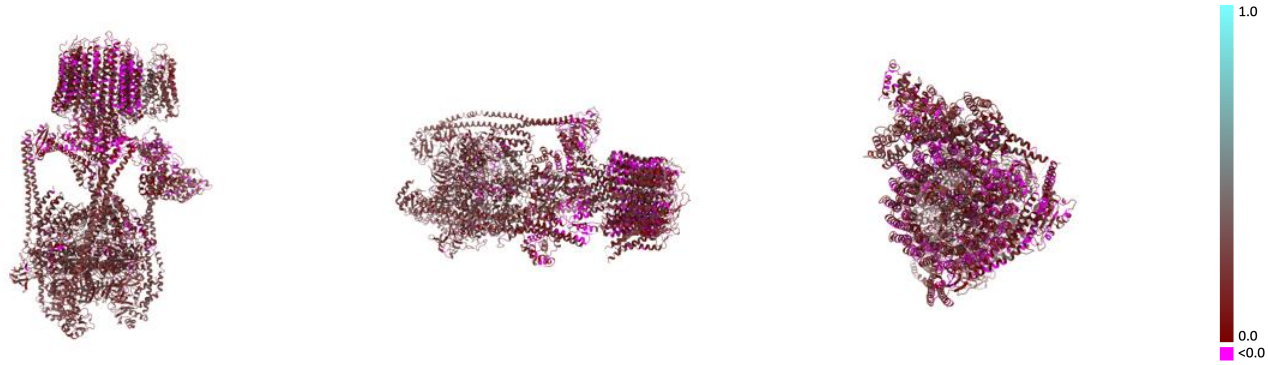
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

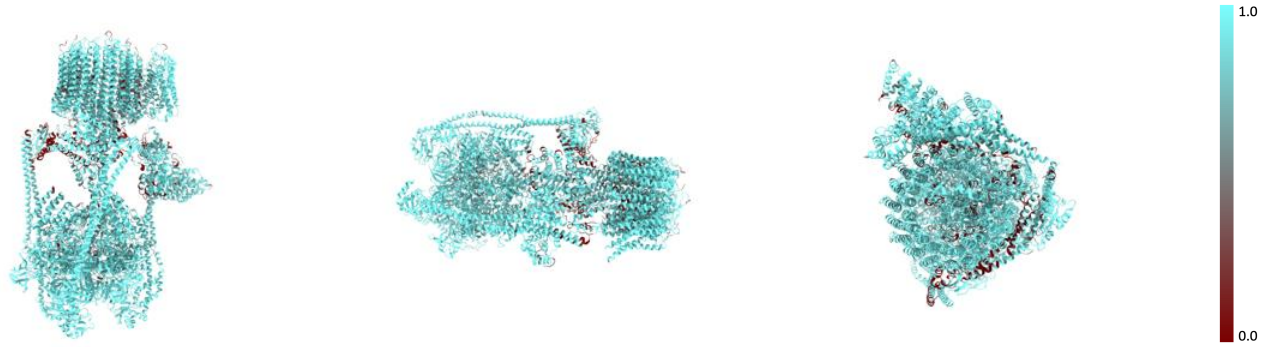
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

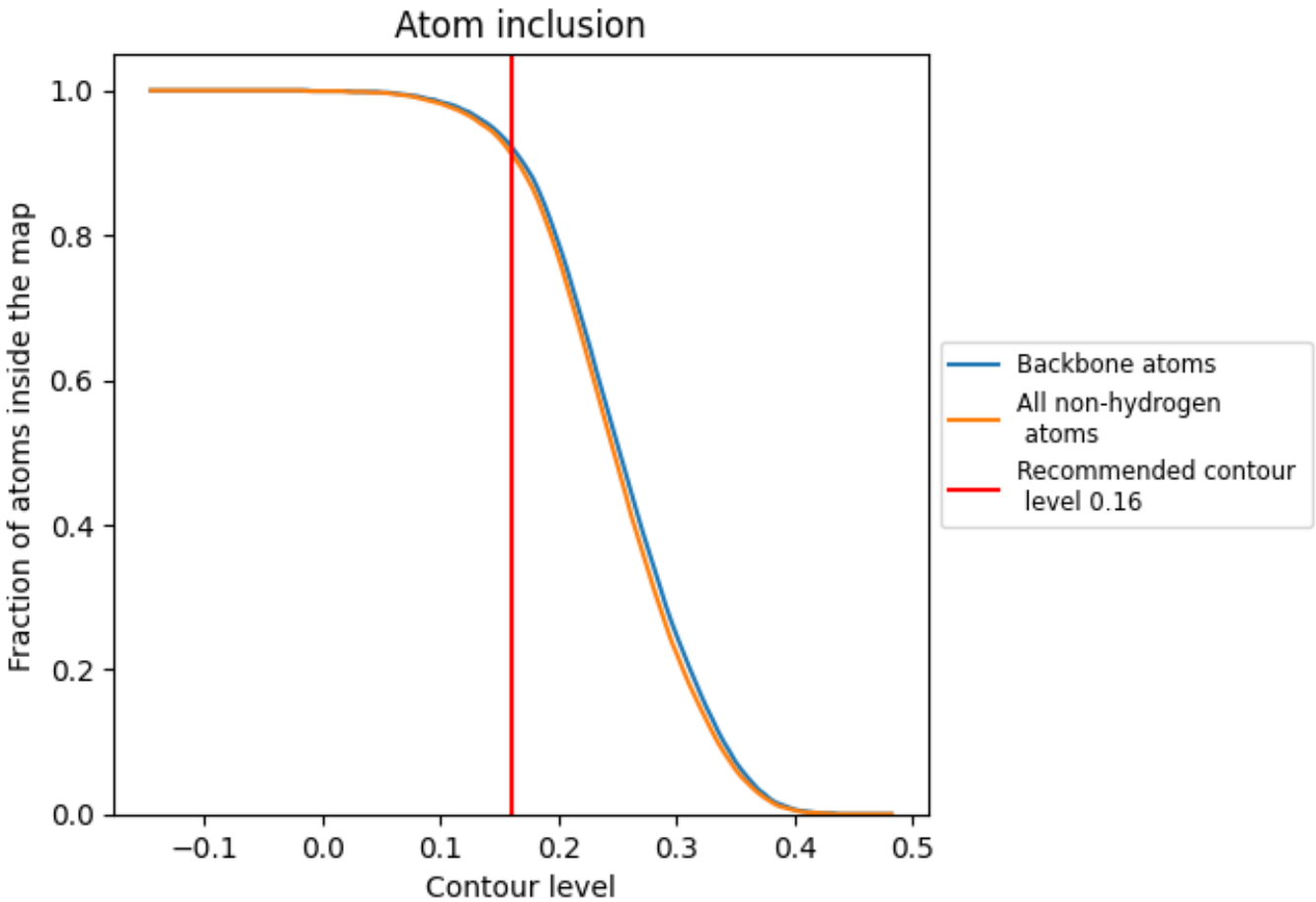
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.1630
A	0.9630	0.2060
B	0.9620	0.2130
C	0.9490	0.2010
D	0.9620	0.2000
E	0.9630	0.2030
F	0.9610	0.2110
G	0.9300	0.2090
H	0.9880	0.1990
I	0.9770	0.2260
J	0.9830	0.2170
K	0.9580	0.2150
L	0.9170	0.2060
M	0.9250	0.2000
N	0.8460	0.1930
O	0.6180	0.0800
P	0.8570	0.1310
a	0.8880	0.1460
b	0.7110	0.0980
c	0.9180	0.0670
d	0.7520	0.1440
e	0.9940	0.1760
f	0.9970	0.1910
g	0.9720	0.0820
h	0.9340	0.0760
i	0.9530	0.1230
j	0.9760	0.1140
k	0.9770	0.1070
l	0.9760	0.0890
m	0.8700	0.0390
n	0.8160	0.0510
o	0.9180	0.0600