



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Apr 13, 2019 – 12:41 PM EDT

PDB ID : 6O7V  
EMDB ID: : EMD-0646  
Title : Saccharomyces cerevisiae V-ATPase Stv1-V1VO State 1  
Authors : Vasanthakumar, T.; Bueler, S.A.; Wu, D.; Beilsten-Edmands, V.; Robinson, C.V.; Rubinstein, J.L.  
Deposited on : 2019-03-08  
Resolution : 6.60 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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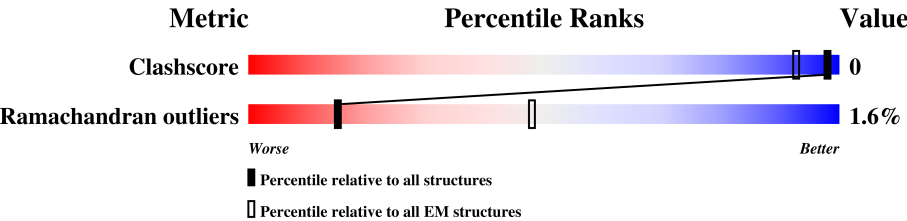
MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

# 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 6.60 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.











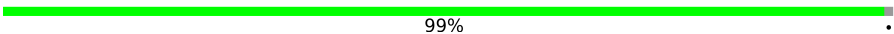
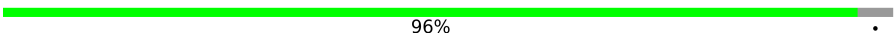
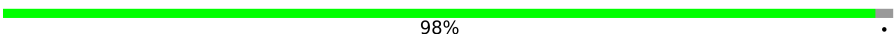
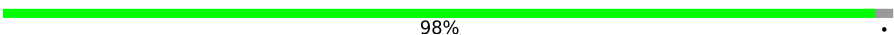
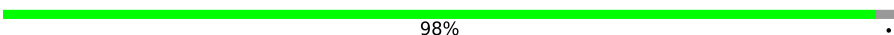

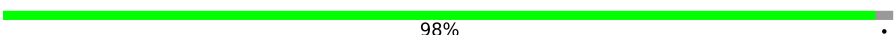
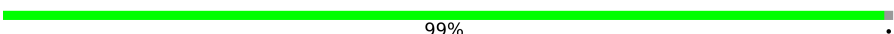
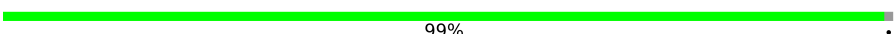
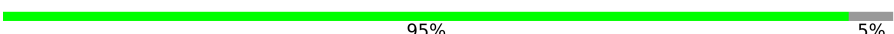


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	M	256	<div><div style="width: 77%; background-color: green;"></div><div style="width: 5%; background-color: yellow;"></div><div style="width: 18%; background-color: grey;"></div></div>
2	N	118	<div><div style="width: 92%; background-color: green;"></div><div style="width: 5%; background-color: yellow;"></div><div style="width: 3%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
3	A	639	<div><div style="width: 85%; background-color: green;"></div><div style="width: 8%; background-color: yellow;"></div><div style="width: 7%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
3	C	639	<div><div style="width: 87%; background-color: green;"></div><div style="width: 5%; background-color: yellow;"></div><div style="width: 7%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
3	E	639	<div><div style="width: 84%; background-color: green;"></div><div style="width: 8%; background-color: yellow;"></div><div style="width: 7%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
4	B	517	<div><div style="width: 80%; background-color: green;"></div><div style="width: 8%; background-color: yellow;"></div><div style="width: 12%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
4	D	517	<div><div style="width: 82%; background-color: green;"></div><div style="width: 6%; background-color: yellow;"></div><div style="width: 12%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
4	F	517	<div><div style="width: 80%; background-color: green;"></div><div style="width: 7%; background-color: yellow;"></div><div style="width: 12%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
5	H	114	<div><div style="width: 89%; background-color: green;"></div><div style="width: 8%; background-color: yellow;"></div><div style="width: 3%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
5	J	114	<div><div style="width: 86%; background-color: green;"></div><div style="width: 6%; background-color: yellow;"></div><div style="width: 8%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>
5	L	114	<div><div style="width: 89%; background-color: green;"></div><div style="width: 8%; background-color: yellow;"></div><div style="width: 3%; background-color: orange;"></div><div style="width: 1%; background-color: red;"></div><div style="width: 1%; background-color: grey;"></div></div>

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Mol	Chain	Length	Quality of chain
6	G	233	 87% 6% 7%
6	I	233	 89% 7%
6	K	233	 88% 5% 7%
7	P	478	 92% . . .
8	O	392	 91% 7% .
9	a	890	 70% 30%
10	b	265	 17% 83%
11	c	213	 92% 8%
12	d	345	 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 D.

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

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

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

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

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

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

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

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

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

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

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

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

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

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

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

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

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

- 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		
13	h	157	Total	C	N	O	0	0
			763	449	157	157		
13	i	157	Total	C	N	O	0	0
			763	449	157	157		
13	j	156	Total	C	N	O	0	0
			758	446	156	156		
13	k	158	Total	C	N	O	0	0
			768	452	158	158		
13	l	157	Total	C	N	O	0	0
			763	449	157	157		
13	m	158	Total	C	N	O	0	0
			768	452	158	158		
13	n	158	Total	C	N	O	0	0
			768	452	158	158		

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

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

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

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

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

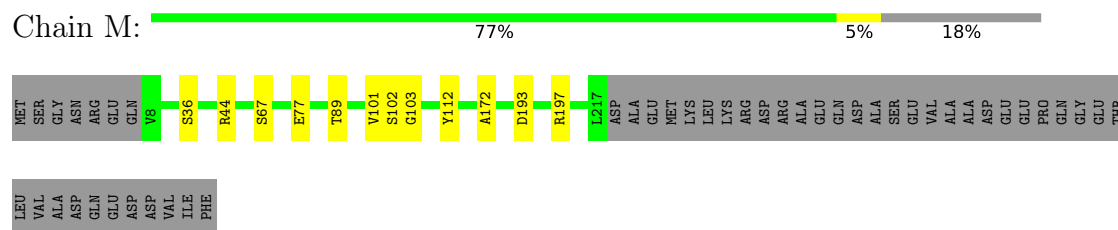
Mol	Chain	Residues	Atoms				AltConf	Trace
16	f	61	Total	C	N	O	0	0
			301	179	61	61		



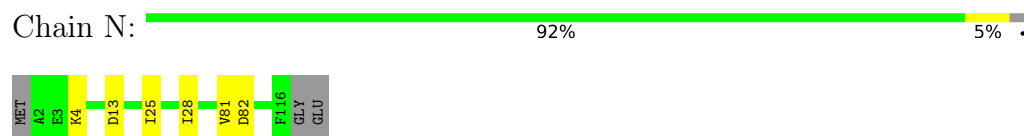
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

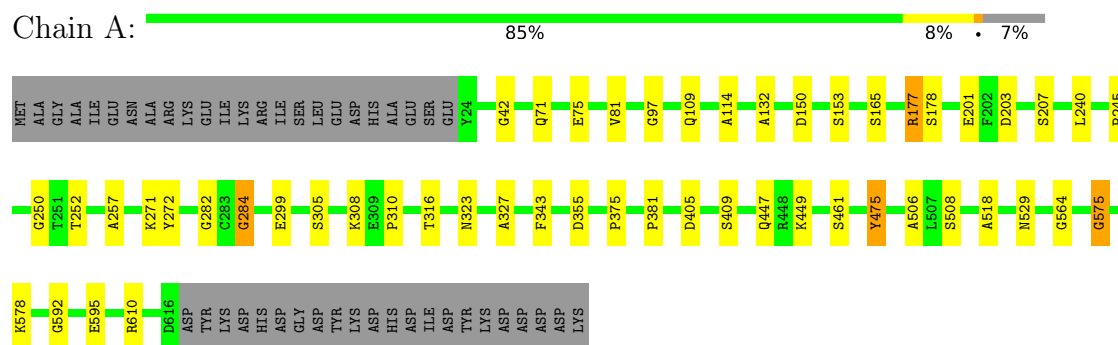
- Molecule 1: V-type proton ATPase subunit D



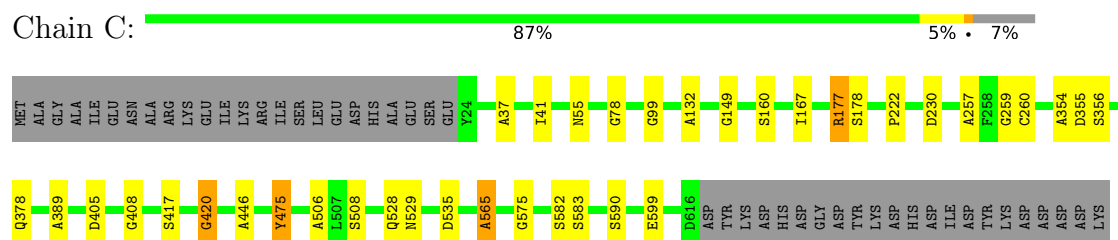
- Molecule 2: V-type proton ATPase subunit F



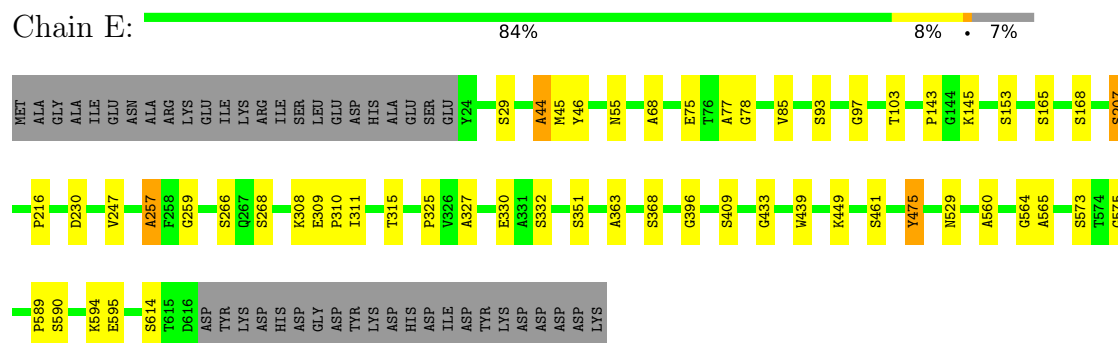
- Molecule 3: Vacuolar ATP synthase catalytic subunit A



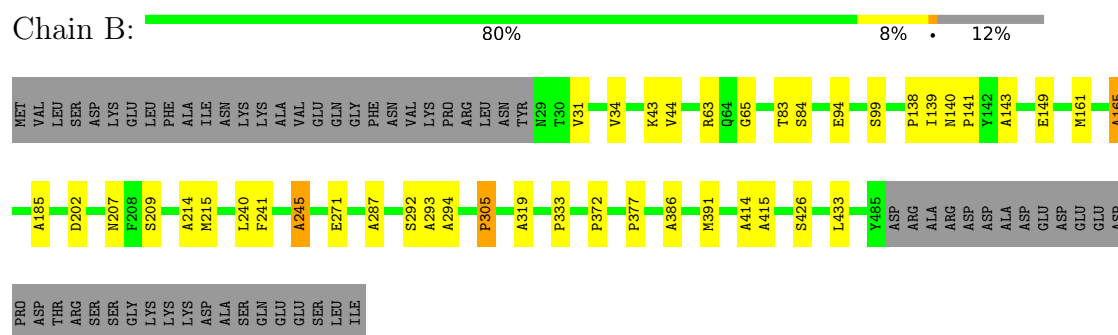
- Molecule 3: Vacuolar ATP synthase catalytic subunit A



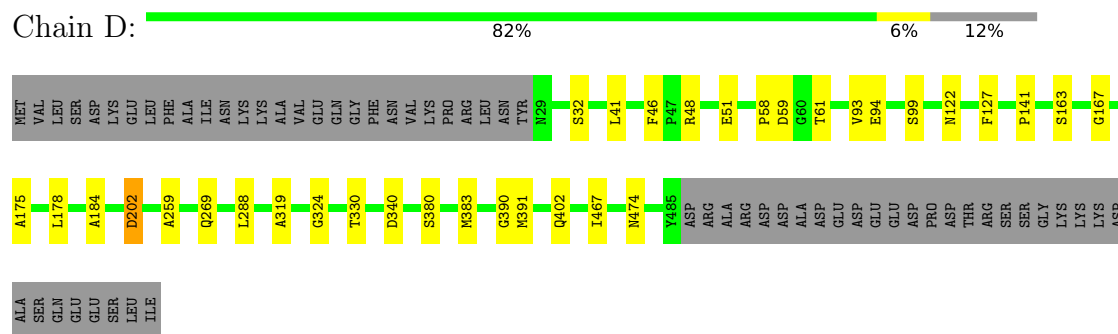
- Molecule 3: Vacuolar ATP synthase catalytic subunit A



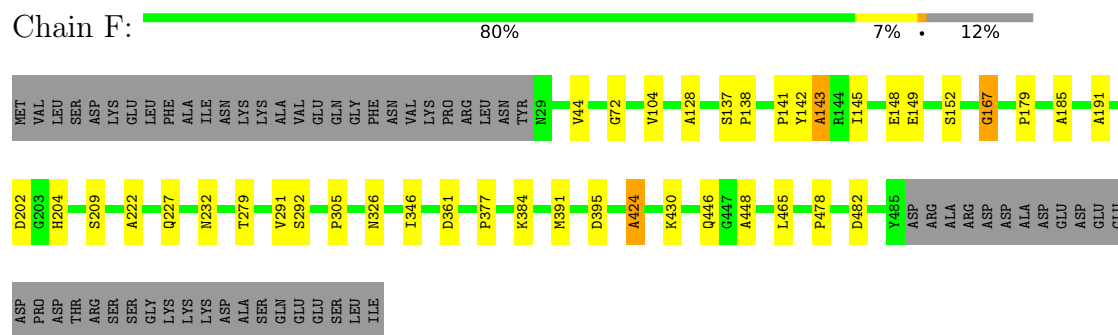
• Molecule 4: V-type proton ATPase subunit B




• Molecule 4: V-type proton ATPase subunit B

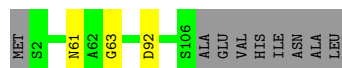


• Molecule 4: V-type proton ATPase subunit B




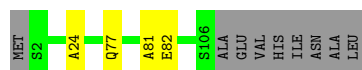
• Molecule 5: V-type proton ATPase subunit G

Chain L:  89% 8%




- Molecule 5: V-type proton ATPase subunit G

Chain H:  89% 8%



- Molecule 5: V-type proton ATPase subunit G

Chain J:  86% 6% 8%




- Molecule 6: V-type proton ATPase subunit E

Chain K:  88% 5% 7%



- Molecule 6: V-type proton ATPase subunit E

Chain G:  87% 6% 7%



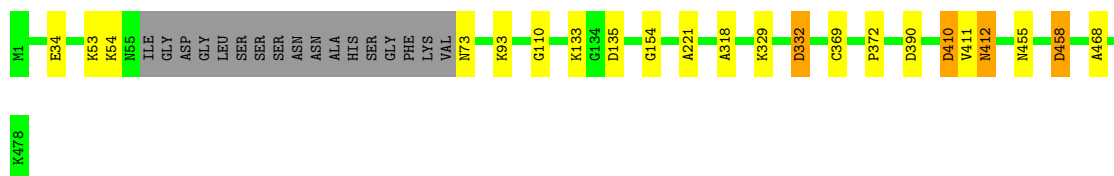
- Molecule 6: V-type proton ATPase subunit E

Chain I:  89% 7%



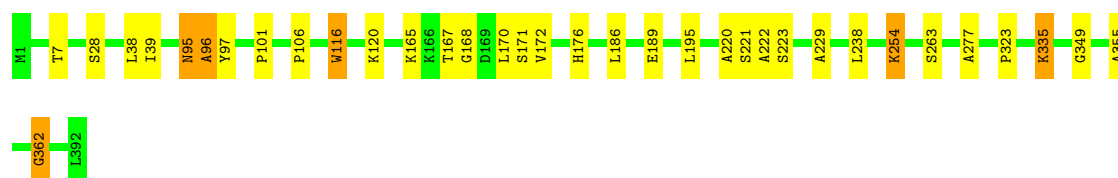
- Molecule 7: V-type proton ATPase subunit H

Chain P:  92%



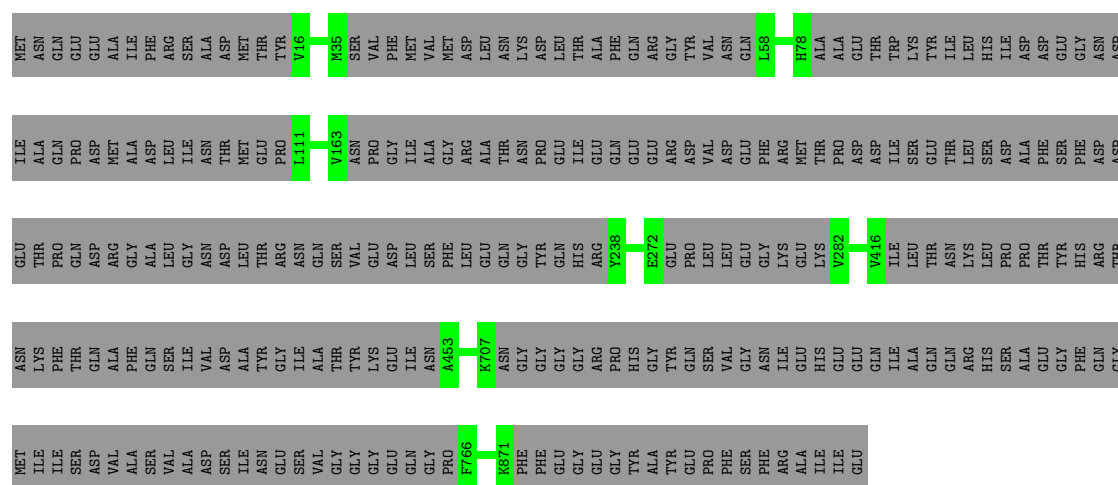
- Molecule 8: V-type proton ATPase subunit C

Chain O:  91% 7%



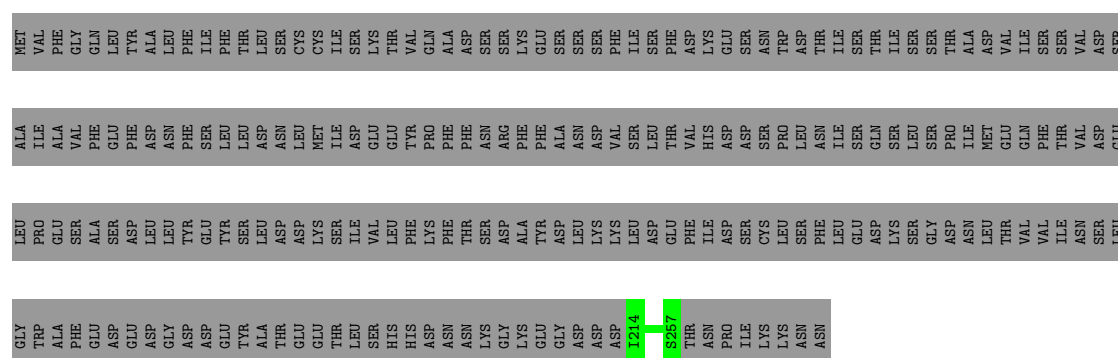
- Molecule 9: V-type proton ATPase subunit a, Golgi isoform

Chain a:  70% 30%



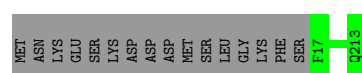
- Molecule 10: V0 assembly protein 1

Chain b:  17% 83%



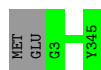
- Molecule 11: V-type proton ATPase subunit c''

Chain c:  92% 8%



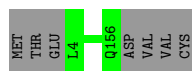
- Molecule 12: V-type proton ATPase subunit d

Chain d:  99% .



- Molecule 13: V-type proton ATPase subunit c

Chain g:  96% .



- Molecule 13: V-type proton ATPase subunit c

Chain h:  98% .



- Molecule 13: V-type proton ATPase subunit c

Chain i:  98% .



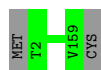
- Molecule 13: V-type proton ATPase subunit c

Chain j:  98% .



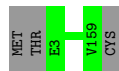
- Molecule 13: V-type proton ATPase subunit c

Chain k:  99% .



- Molecule 13: V-type proton ATPase subunit c

Chain l:  98% .



- Molecule 13: V-type proton ATPase subunit c

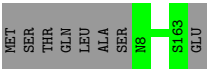
Chain m:  99% .



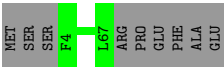
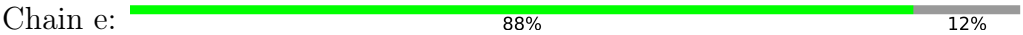
● Molecule 13: V-type proton ATPase subunit c



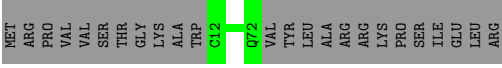
● Molecule 14: V-type proton ATPase subunit c'



● Molecule 15: V-type proton ATPase subunit e



● Molecule 16: Putative protein YPR170W-B



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	25045	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 ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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  >2	RMSZ	# Z  >2
1	M	1.57	3/1038 (0.3%)	1.66	10/1445 (0.7%)
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
2	N	1.54	0/570	1.68	5/794 (0.6%)
3	A	1.59	9/2914 (0.3%)	1.74	28/4048 (0.7%)
3	C	1.58	6/2914 (0.2%)	1.66	17/4048 (0.4%)
3	E	1.63	16/2914 (0.5%)	1.73	26/4048 (0.6%)
4	B	1.59	8/2249 (0.4%)	1.74	21/3126 (0.7%)
4	D	1.55	6/2249 (0.3%)	1.74	13/3126 (0.4%)
4	F	1.57	7/2249 (0.3%)	1.71	22/3126 (0.7%)
5	H	1.51	0/518	1.59	3/720 (0.4%)
5	J	1.56	1/518 (0.2%)	1.61	7/720 (1.0%)
5	L	1.54	0/518	1.56	2/720 (0.3%)
6	G	1.58	5/1077 (0.5%)	1.65	8/1502 (0.5%)
6	I	1.54	3/1077 (0.3%)	1.57	5/1502 (0.3%)
6	K	1.54	4/1077 (0.4%)	1.65	7/1502 (0.5%)
7	P	1.55	6/2290 (0.3%)	1.64	12/3195 (0.4%)
8	O	1.56	5/1946 (0.3%)	1.72	18/2715 (0.7%)
9	a	0.25	0/3085	0.49	0/4288
All	All	1.29	79/39540 (0.2%)	1.40	204/54928 (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
3	A	0	1
4	F	0	1
All	All	0	2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	268	SER	CA-CB	8.94	1.66	1.52
3	E	461	SER	CA-CB	8.09	1.65	1.52
4	B	426	SER	CA-CB	7.65	1.64	1.52
6	G	211	SER	CA-CB	6.95	1.63	1.52
3	A	592	GLY	CA-C	-6.84	1.41	1.51
3	A	409	SER	CA-CB	6.72	1.63	1.52
6	I	114	ARG	N-CA	-6.64	1.33	1.46
1	M	36	SER	CA-CB	6.43	1.62	1.52
6	I	72	SER	CA-CB	6.41	1.62	1.52
8	O	223	SER	CA-CB	6.40	1.62	1.52
6	G	160	TYR	C-N	6.32	1.44	1.33
4	F	137	SER	CA-CB	6.25	1.62	1.52
3	E	529	ASN	C-N	6.19	1.44	1.33
3	C	417	SER	CA-CB	6.17	1.62	1.52
6	I	8	LEU	N-CA	6.08	1.58	1.46
3	E	332	SER	CA-CB	6.07	1.62	1.52
8	O	238	LEU	N-CA	-6.04	1.34	1.46
4	F	232	ASN	C-N	5.95	1.43	1.33
3	E	145	LYS	N-CA	-5.87	1.34	1.46
7	P	455	ASN	CA-CB	5.84	1.68	1.53
1	M	67	SER	CA-CB	5.80	1.61	1.52
6	K	151	SER	CA-CB	5.77	1.61	1.52
4	B	215	MET	C-N	5.74	1.43	1.33
3	E	97	GLY	N-CA	5.74	1.54	1.46
4	B	99	SER	CA-CB	5.70	1.61	1.52
6	G	182	ASP	CA-C	-5.68	1.38	1.52
3	A	250	GLY	CA-C	-5.65	1.42	1.51
8	O	28	SER	CA-CB	5.65	1.61	1.52
6	G	143	GLU	N-CA	-5.64	1.35	1.46
7	P	73	ASN	C-N	5.62	1.43	1.33
3	E	351	SER	CA-CB	5.61	1.61	1.52
4	B	333	PRO	CA-C	5.57	1.64	1.52
3	E	165	SER	CA-CB	5.57	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	465	LEU	N-CA	-5.56	1.35	1.46
6	G	163	LYS	CA-CB	5.53	1.66	1.53
6	K	194	SER	CA-CB	5.45	1.61	1.52
3	E	363	ALA	CA-CB	5.44	1.63	1.52
4	F	167	GLY	CA-C	-5.43	1.43	1.51
3	C	599	GLU	CA-CB	5.42	1.65	1.53
7	P	110	GLY	CA-C	-5.42	1.43	1.51
3	E	396	GLY	CA-C	-5.40	1.43	1.51
3	E	46	TYR	CA-CB	5.37	1.65	1.53
3	A	610	ARG	N-CA	-5.34	1.35	1.46
4	F	395	ASP	CA-CB	5.33	1.65	1.53
3	A	564	GLY	CA-C	-5.32	1.43	1.51
3	E	29	SER	CA-CB	5.31	1.60	1.52
3	A	575	GLY	CA-C	-5.29	1.43	1.51
3	E	475	TYR	CA-CB	5.28	1.65	1.53
4	D	61	THR	N-CA	-5.28	1.35	1.46
5	J	12	GLN	N-CA	5.27	1.56	1.46
3	E	433	GLY	N-CA	-5.24	1.38	1.46
4	B	433	LEU	N-CA	-5.24	1.35	1.46
8	O	362	GLY	CA-C	-5.23	1.43	1.51
7	P	154	GLY	N-CA	-5.23	1.38	1.46
3	A	97	GLY	N-CA	-5.23	1.38	1.46
4	D	167	GLY	N-CA	-5.21	1.38	1.46
3	A	518	ALA	CA-CB	5.21	1.63	1.52
3	C	167	ILE	N-CA	-5.21	1.35	1.46
4	D	402	GLN	CA-CB	-5.20	1.42	1.53
4	F	227	GLN	CA-CB	5.19	1.65	1.53
7	P	332	ASP	CA-CB	5.19	1.65	1.53
3	E	325	PRO	N-CA	-5.19	1.38	1.47
4	F	152	SER	CA-CB	5.18	1.60	1.52
1	M	103	GLY	N-CA	5.13	1.53	1.46
4	B	305	PRO	C-N	5.11	1.42	1.33
3	C	149	GLY	CA-C	5.11	1.60	1.51
3	C	99	GLY	CA-C	-5.08	1.43	1.51
4	D	32	SER	C-N	5.08	1.42	1.33
4	D	163	SER	CA-CB	5.08	1.60	1.52
6	K	108	SER	CA-CB	5.08	1.60	1.52
6	K	109	GLY	CA-C	-5.07	1.43	1.51
4	B	94	GLU	CA-C	-5.06	1.39	1.52
3	E	573	SER	CA-CB	5.04	1.60	1.52
8	O	349	GLY	CA-C	-5.04	1.43	1.51
4	B	207	ASN	N-CA	-5.03	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	160	SER	CA-CB	5.02	1.60	1.52
7	P	329	LYS	N-CA	-5.01	1.36	1.46
4	D	41	LEU	CA-CB	5.01	1.65	1.53
3	A	272	TYR	N-CA	-5.00	1.36	1.46

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	116	TRP	N-CA-CB	8.64	126.16	110.60
4	F	424	ALA	N-CA-CB	8.62	122.17	110.10
3	E	257	ALA	N-CA-CB	8.44	121.91	110.10
8	O	96	ALA	N-CA-CB	8.06	121.38	110.10
4	B	165	ALA	CB-CA-C	-7.75	98.48	110.10
3	E	614	SER	N-CA-CB	7.73	122.09	110.50
3	E	257	ALA	CB-CA-C	-7.67	98.59	110.10
4	B	414	ALA	N-CA-CB	7.52	120.63	110.10
4	F	478	PRO	N-CA-CB	7.51	112.31	103.30
4	B	245	ALA	CB-CA-C	-7.47	98.89	110.10
3	E	75	GLU	N-CA-CB	7.16	123.50	110.60
3	A	132	ALA	N-CA-CB	7.05	119.97	110.10
2	N	82	ASP	N-CA-CB	7.01	123.22	110.60
4	F	104	VAL	N-CA-C	-7.01	92.07	111.00
4	F	430	LYS	N-CA-CB	6.98	123.16	110.60
3	A	355	ASP	N-CA-C	-6.93	92.28	111.00
4	B	140	ASN	N-CA-CB	6.92	123.06	110.60
8	O	222	ALA	N-CA-CB	6.89	119.75	110.10
8	O	335	LYS	N-CA-CB	6.81	122.86	110.60
4	B	161	MET	CB-CA-C	-6.72	96.96	110.40
7	P	468	ALA	CB-CA-C	-6.71	100.04	110.10
3	E	449	LYS	N-CA-CB	6.65	122.57	110.60
3	A	178	SER	N-CA-CB	6.53	120.29	110.50
3	A	150	ASP	CB-CA-C	-6.48	97.44	110.40
3	E	565	ALA	N-CA-CB	6.48	119.17	110.10
8	O	277	ALA	CB-CA-C	-6.46	100.41	110.10
3	C	408	GLY	N-CA-C	-6.42	97.05	113.10
3	A	271	LYS	N-CA-CB	-6.41	99.06	110.60
1	M	172	ALA	CB-CA-C	-6.40	100.50	110.10
4	D	175	ALA	N-CA-C	-6.40	93.72	111.00
3	E	309	GLU	N-CA-CB	6.38	122.08	110.60
4	F	191	ALA	N-CA-CB	6.34	118.97	110.10
3	A	201	GLU	N-CA-CB	6.32	121.97	110.60
7	P	34	GLU	N-CA-CB	6.25	121.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	178	LEU	CB-CA-C	-6.24	98.34	110.20
3	A	327	ALA	CB-CA-C	-6.24	100.74	110.10
7	P	412	ASN	N-CA-CB	6.20	121.75	110.60
3	E	44	ALA	CB-CA-C	6.14	119.31	110.10
3	E	153	SER	N-CA-C	-6.14	94.43	111.00
6	G	191	SER	N-CA-CB	6.12	119.68	110.50
4	F	482	ASP	N-CA-CB	6.11	121.60	110.60
4	B	241	PHE	CB-CA-C	-6.11	98.19	110.40
4	D	383	MET	CB-CA-C	-6.10	98.20	110.40
6	G	178	TYR	N-CA-CB	6.10	121.58	110.60
1	M	44	ARG	CB-CA-C	-6.08	98.23	110.40
1	M	172	ALA	N-CA-CB	6.03	118.55	110.10
6	K	130	LEU	N-CA-CB	-6.02	98.36	110.40
7	P	410	ASP	CB-CA-C	6.02	122.43	110.40
2	N	13	ASP	N-CA-CB	6.01	121.41	110.60
7	P	369	CYS	N-CA-CB	6.01	121.41	110.60
3	A	177	ARG	N-CA-CB	6.00	121.40	110.60
3	A	447	GLN	CB-CA-C	-5.98	98.43	110.40
4	D	184	ALA	N-CA-CB	5.95	118.43	110.10
1	M	112	TYR	N-CA-CB	5.94	121.30	110.60
8	O	323	PRO	O-C-N	5.92	132.17	122.70
6	I	12	GLN	N-CA-CB	5.91	121.24	110.60
8	O	95	ASN	N-CA-CB	5.89	121.20	110.60
3	A	506	ALA	N-CA-CB	5.88	118.33	110.10
6	I	216	PRO	N-CA-CB	5.86	110.33	103.30
3	E	327	ALA	CB-CA-C	-5.86	101.32	110.10
3	C	55	ASN	N-CA-CB	5.83	121.09	110.60
5	H	82	GLU	N-CA-CB	5.82	121.08	110.60
6	K	70	MET	N-CA-CB	5.81	121.06	110.60
1	M	101	VAL	N-CA-C	-5.80	95.35	111.00
3	E	409	SER	CB-CA-C	-5.79	99.10	110.10
3	A	461	SER	N-CA-CB	5.78	119.17	110.50
3	A	240	LEU	O-C-N	5.76	131.91	122.70
3	C	475	TYR	N-CA-CB	5.75	120.94	110.60
5	H	24	ALA	O-C-N	-5.74	113.52	122.70
8	O	165	LYS	N-CA-CB	5.71	120.89	110.60
6	G	212	GLU	N-CA-CB	5.70	120.86	110.60
2	N	25	ILE	N-CA-CB	5.70	123.90	110.80
1	M	89	THR	N-CA-CB	5.69	121.11	110.30
4	F	279	THR	O-C-N	-5.69	113.60	122.70
8	O	229	ALA	CB-CA-C	-5.68	101.57	110.10
4	B	34	VAL	N-CA-C	-5.68	95.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	209	SER	N-CA-CB	5.68	119.02	110.50
6	G	72	SER	N-CA-CB	5.67	119.00	110.50
4	D	94	GLU	N-CA-C	-5.66	95.73	111.00
4	F	222	ALA	CB-CA-C	-5.65	101.62	110.10
6	K	15	ASP	CB-CA-C	-5.64	99.13	110.40
3	C	222	PRO	N-CA-CB	5.63	110.06	103.30
3	E	330	GLU	N-CA-CB	5.63	120.74	110.60
5	J	72	ALA	CB-CA-C	-5.63	101.66	110.10
1	M	102	SER	N-CA-CB	5.63	118.94	110.50
8	O	254	LYS	N-CA-CB	5.62	120.72	110.60
3	A	284	GLY	N-CA-C	-5.62	99.05	113.10
3	A	316	THR	N-CA-C	-5.61	95.86	111.00
3	E	207	SER	N-CA-CB	5.60	118.91	110.50
7	P	318	ALA	CB-CA-C	-5.60	101.70	110.10
4	F	142	TYR	C-N-CA	5.59	135.68	121.70
6	K	113	ASN	N-CA-CB	5.59	120.66	110.60
3	A	252	THR	N-CA-C	-5.57	95.96	111.00
7	P	411	VAL	CB-CA-C	5.57	121.98	111.40
3	A	327	ALA	N-CA-CB	5.55	117.86	110.10
3	C	41	ILE	C-N-CA	5.54	133.93	122.30
6	G	56	ASN	CB-CA-C	-5.53	99.34	110.40
2	N	28	ILE	N-CA-C	-5.52	96.09	111.00
3	C	582	SER	N-CA-CB	5.52	118.78	110.50
7	P	372	PRO	N-CA-CB	5.51	109.92	103.30
3	C	132	ALA	N-CA-CB	5.50	117.80	110.10
3	A	282	GLY	N-CA-C	-5.49	99.36	113.10
3	A	299	GLU	O-C-N	5.49	131.49	122.70
7	P	221	ALA	N-CA-CB	5.48	117.77	110.10
6	K	33	LYS	N-CA-CB	5.47	120.45	110.60
6	K	111	ALA	CB-CA-C	-5.47	101.89	110.10
4	B	185	ALA	CB-CA-C	-5.47	101.89	110.10
5	J	103	ILE	CB-CA-C	-5.47	100.67	111.60
6	I	76	THR	N-CA-CB	5.47	120.69	110.30
3	C	354	ALA	N-CA-C	-5.46	96.25	111.00
5	J	68	LEU	CB-CA-C	5.46	120.57	110.20
4	B	165	ALA	N-CA-CB	5.45	117.72	110.10
1	M	197	ARG	N-CA-CB	5.44	120.39	110.60
8	O	170	LEU	CB-CA-C	-5.44	99.87	110.20
8	O	263	SER	N-CA-CB	5.43	118.65	110.50
3	E	311	ILE	C-N-CA	5.42	135.26	121.70
3	C	583	SER	CB-CA-C	-5.42	99.81	110.10
4	B	65	GLY	N-CA-C	-5.41	99.57	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	93	LYS	CB-CA-C	-5.41	99.58	110.40
3	E	368	SER	N-CA-CB	5.40	118.61	110.50
8	O	116	TRP	N-CA-C	-5.40	96.42	111.00
7	P	458	ASP	N-CA-CB	5.40	120.31	110.60
3	C	178	SER	N-CA-CB	5.39	118.59	110.50
3	A	81	VAL	CB-CA-C	-5.38	101.17	111.40
3	E	259	GLY	C-N-CA	5.37	135.13	121.70
2	N	81	VAL	N-CA-CB	5.37	123.31	111.50
6	G	105	GLU	CB-CA-C	-5.37	99.66	110.40
3	C	37	ALA	N-CA-CB	5.37	117.61	110.10
4	B	214	ALA	CB-CA-C	-5.37	102.05	110.10
4	D	324	GLY	N-CA-C	-5.36	99.69	113.10
3	C	405	ASP	N-CA-CB	5.36	120.24	110.60
5	J	39	ALA	N-CA-CB	5.36	117.60	110.10
3	A	343	PHE	O-C-N	-5.34	114.15	122.70
3	C	177	ARG	N-CA-CB	5.34	120.21	110.60
3	A	475	TYR	N-CA-CB	5.34	120.21	110.60
8	O	38	LEU	C-N-CA	5.34	135.04	121.70
3	A	114	ALA	N-CA-CB	5.33	117.56	110.10
3	E	68	ALA	CB-CA-C	-5.32	102.12	110.10
4	F	448	ALA	CB-CA-C	-5.32	102.12	110.10
4	F	209	SER	N-CA-CB	5.32	118.47	110.50
4	F	149	GLU	N-CA-CB	5.29	120.13	110.60
4	F	346	ILE	CA-C-O	-5.29	108.99	120.10
3	C	565	ALA	N-CA-CB	5.29	117.50	110.10
3	E	266	SER	N-CA-CB	5.28	118.41	110.50
3	A	578	LYS	O-C-N	-5.25	114.29	122.70
6	I	10	PRO	N-CA-CB	5.24	109.59	103.30
4	F	143	ALA	CB-CA-C	-5.24	102.24	110.10
5	J	104	LYS	N-CA-C	-5.22	96.90	111.00
3	C	446	ALA	N-CA-CB	5.22	117.40	110.10
4	B	287	ALA	N-CA-CB	5.21	117.40	110.10
3	C	506	ALA	N-CA-CB	5.21	117.39	110.10
4	D	380	SER	N-CA-C	-5.21	96.94	111.00
4	D	259	ALA	O-C-N	5.21	131.03	122.70
8	O	221	SER	N-CA-CB	5.21	118.31	110.50
5	J	44	ASP	CB-CA-C	-5.21	99.99	110.40
3	A	109	GLN	N-CA-CB	5.20	119.97	110.60
4	B	143	ALA	CB-CA-C	-5.20	102.29	110.10
4	D	269	GLN	CB-CA-C	-5.19	100.03	110.40
8	O	220	ALA	N-CA-CB	5.19	117.36	110.10
1	M	193	ASP	N-CA-CB	5.18	119.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	439	TRP	C-N-CA	5.18	133.18	122.30
5	L	61	ASN	N-CA-CB	5.18	119.92	110.60
6	K	119	PRO	N-CA-CB	5.17	109.51	103.30
3	A	71	GLN	N-CA-C	-5.16	97.06	111.00
5	H	81	ALA	CB-CA-C	-5.16	102.37	110.10
3	C	420	GLY	N-CA-C	-5.15	100.22	113.10
7	P	133	LYS	N-CA-C	-5.15	97.09	111.00
4	B	84	SER	N-CA-CB	5.12	118.18	110.50
5	J	39	ALA	O-C-N	5.11	130.88	122.70
3	E	103	THR	N-CA-C	-5.11	97.21	111.00
3	E	560	ALA	CB-CA-C	-5.11	102.44	110.10
4	B	31	VAL	O-C-N	5.10	130.86	122.70
4	D	202	ASP	C-N-CA	5.10	133.01	122.30
4	F	291	VAL	O-C-N	-5.10	114.54	122.70
4	F	145	ILE	N-CA-C	-5.09	97.25	111.00
8	O	195	LEU	O-C-N	5.09	130.85	122.70
4	B	415	ALA	N-CA-CB	5.08	117.21	110.10
3	A	165	SER	CB-CA-C	-5.08	100.45	110.10
4	B	294	ALA	N-CA-CB	5.08	117.21	110.10
5	L	92	ASP	CB-CA-C	-5.08	100.25	110.40
8	O	97	TYR	N-CA-CB	5.08	119.74	110.60
4	B	63	ARG	N-CA-C	-5.08	97.30	111.00
3	E	77	ALA	C-N-CA	-5.07	111.65	122.30
6	I	86	LEU	CB-CA-C	-5.07	100.57	110.20
4	B	43	LYS	C-N-CA	5.07	134.36	121.70
3	A	508	SER	N-CA-CB	5.06	118.09	110.50
4	F	361	ASP	C-N-CA	5.06	134.34	121.70
3	A	323	ASN	CB-CA-C	-5.05	100.29	110.40
6	G	145	ASP	C-N-CA	5.05	134.31	121.70
3	E	85	VAL	N-CA-C	-5.04	97.38	111.00
3	E	315	THR	N-CA-CB	5.04	119.88	110.30
4	F	185	ALA	CB-CA-C	-5.04	102.54	110.10
4	D	288	LEU	CB-CA-C	-5.04	100.63	110.20
6	G	111	ALA	N-CA-CB	5.03	117.14	110.10
4	D	330	THR	CA-C-N	-5.03	106.14	117.20
4	B	240	LEU	CB-CA-C	-5.03	100.65	110.20
3	E	247	VAL	O-C-N	-5.02	114.67	122.70
4	F	305	PRO	N-CA-CB	5.02	109.32	103.30
4	D	93	VAL	N-CA-C	-5.02	97.46	111.00
4	F	204	HIS	N-CA-CB	5.01	119.62	110.60
1	M	77	GLU	N-CA-CB	5.01	119.62	110.60
4	F	446	GLN	N-CA-C	-5.01	97.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	384	LYS	CA-C-N	-5.00	106.19	117.20
3	E	168	SER	N-CA-CB	5.00	118.00	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	153	SER	Mainchain
4	F	44	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1039	0	475	0	0
2	N	571	0	255	0	0
3	A	2915	0	1343	0	0
3	C	2915	0	1343	2	0
3	E	2915	0	1343	1	0
4	B	2250	0	1016	3	0
4	D	2250	0	1016	1	0
4	F	2250	0	1016	0	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	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	18305	6	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 (6) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:165:ALA:HB2	4:B:386:ALA:CB	2.38	0.54
4:B:165:ALA:HB2	4:B:386:ALA:HB2	1.92	0.51
3:E:93:SER:HA	3:E:216:PRO:HA	1.98	0.45
4:D:51:GLU:HA	4:D:99:SER:HA	2.03	0.41
3:C:355:ASP:HA	3:C:356:SER:HA	1.91	0.41
4:B:245:ALA:HB1	3:C:389:ALA:HB1	2.02	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%)	206 (99%)	2 (1%)	0	100	100
2	N	113/118 (96%)	102 (90%)	10 (9%)	1 (1%)	19	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	591/639 (92%)	541 (92%)	31 (5%)	19 (3%)	4	34
3	C	591/639 (92%)	538 (91%)	37 (6%)	16 (3%)	5	38
3	E	591/639 (92%)	542 (92%)	32 (5%)	17 (3%)	5	36
4	B	455/517 (88%)	413 (91%)	27 (6%)	15 (3%)	4	33
4	D	455/517 (88%)	416 (91%)	25 (6%)	14 (3%)	4	34
4	F	455/517 (88%)	411 (90%)	30 (7%)	14 (3%)	4	34
5	H	103/114 (90%)	99 (96%)	3 (3%)	1 (1%)	17	59
5	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
5	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	17	59
6	G	215/233 (92%)	207 (96%)	7 (3%)	1 (0%)	31	74
6	I	215/233 (92%)	208 (97%)	6 (3%)	1 (0%)	31	74
6	K	215/233 (92%)	205 (95%)	9 (4%)	1 (0%)	31	74
7	P	457/478 (96%)	431 (94%)	18 (4%)	8 (2%)	9	47
8	O	390/392 (100%)	350 (90%)	21 (5%)	19 (5%)	2	26
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%)	7509 (94%)	325 (4%)	128 (2%)	15	50

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	257	ALA
3	A	475	TYR
4	B	292	SER
3	C	475	TYR
3	C	529	ASN
3	C	565	ALA
4	D	46	PHE
4	D	467	ILE
3	E	257	ALA
3	E	308	LYS
3	E	475	TYR
4	F	143	ALA
4	F	377	PRO
7	P	53	LYS
7	P	390	ASP
8	O	116	TRP
8	O	254	LYS
2	N	4	LYS
3	A	529	ASN
3	A	575	GLY
4	B	83	THR
4	B	141	PRO
4	B	391	MET
3	C	259	GLY
3	C	378	GLN
3	C	528	GLN
3	C	535	ASP
3	C	575	GLY
4	D	59	ASP
4	D	127	PHE
3	E	230	ASP
3	E	575	GLY
3	E	590	SER
4	F	141	PRO
4	F	179	PRO
4	F	391	MET
7	P	54	LYS
7	P	332	ASP
7	P	410	ASP
7	P	412	ASN
7	P	458	ASP
8	O	39	ILE
8	O	172	VAL

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Mol	Chain	Res	Type
5	H	77	GLN
6	G	144	ARG
3	A	42	GLY
3	A	207	SER
3	A	245	PRO
3	A	308	LYS
3	A	405	ASP
3	A	449	LYS
3	A	595	GLU
4	B	44	VAL
4	B	293	ALA
4	B	305	PRO
4	B	319	ALA
4	B	372	PRO
4	B	377	PRO
3	C	508	SER
4	D	48	ARG
4	D	122	ASN
4	D	141	PRO
4	D	319	ALA
4	D	474	ASN
3	E	44	ALA
3	E	78	GLY
3	E	589	PRO
3	E	594	LYS
3	E	595	GLU
4	F	128	ALA
4	F	167	GLY
4	F	202	ASP
4	F	424	ALA
5	L	63	GLY
8	O	7	THR
8	O	96	ALA
8	O	167	THR
8	O	171	SER
8	O	176	HIS
8	O	186	LEU
8	O	335	LYS
3	A	203	ASP
3	C	78	GLY
3	C	257	ALA
3	C	260	CYS

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Mol	Chain	Res	Type
4	D	202	ASP
4	D	340	ASP
4	D	390	GLY
3	E	45	MET
3	E	207	SER
3	E	310	PRO
4	F	148	GLU
4	F	326	ASN
8	O	95	ASN
3	A	75	GLU
3	A	177	ARG
3	A	305	SER
3	A	381	PRO
4	B	138	PRO
4	B	149	GLU
4	B	202	ASP
4	B	271	GLU
3	C	177	ARG
3	C	230	ASP
3	C	590	SER
3	E	55	ASN
4	F	292	SER
7	P	135	ASP
8	O	106	PRO
8	O	355	ALA
4	D	391	MET
8	O	120	LYS
8	O	189	GLU
8	O	101	PRO
3	A	310	PRO
3	A	375	PRO
4	D	58	PRO
4	F	72	GLY
6	K	168	PRO
3	A	284	GLY
4	B	139	ILE
3	C	420	GLY
3	E	143	PRO
3	E	564	GLY
8	O	362	GLY
6	I	168	PRO
4	F	138	PRO

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Mol	Chain	Res	Type
8	O	168	GLY

### 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 carbohydrates 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.