



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:41 am GMT

PDB ID : 3J9U  
EMDB ID: : EMD-6285  
Title : Yeast V-ATPase state 2  
Authors : Zhao, J.; Benlekbir, S.; Rubinstein, J.L.  
Deposited on : 2015-02-23  
Resolution : 7.60 Å(reported)  
Based on PDB ID : 4DL0, 4RND, 1HO8, 1U7L

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

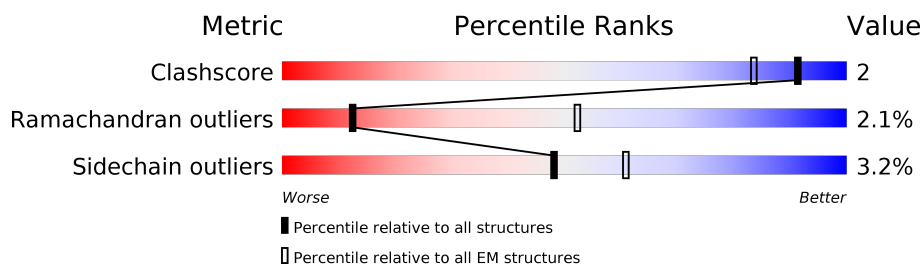
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.60 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	58% 20% . . 18%
2	N	118	69% 24% . .
3	A	616	69% 23% . . .
3	C	616	73% 19% . .
3	E	616	71% 20% 5% .
4	B	517	63% 22% . 12%
4	D	517	64% 21% . 12%
4	F	517	64% 21% . 12%
5	Q	345	76% 21% .

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Mol	Chain	Length	Quality of chain
6	H	114	
6	J	114	
6	L	114	
7	G	233	
7	I	233	
7	K	233	
8	P	478	
9	b	840	
10	O	392	
11	R	160	
11	S	160	
11	T	160	
11	U	160	
11	V	160	
11	W	160	
11	X	160	
11	Y	160	
11	Z	160	
11	a	160	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 57659 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	S	0	0
			1691	1061	305	321	4		

- 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
			928	589	157	182		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	E	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	A	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	F	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	B	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	345	Total	C	N	O	S	0	0
			2802	1779	454	555	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	105	Total	C	N	O		0	0
			824	517	144	163			
6	H	105	Total	C	N	O		0	0
			824	517	144	163			
6	J	105	Total	C	N	O		0	0
			824	517	144	163			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	G	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	I	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	461	Total	C	N	O	S	0	0
			3712	2373	623	704	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	312	Total	C	N	O	S	0	0
			2540	1614	434	489	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	392	Total	C	N	O	S	0	0
			3122	2005	516	596	5		

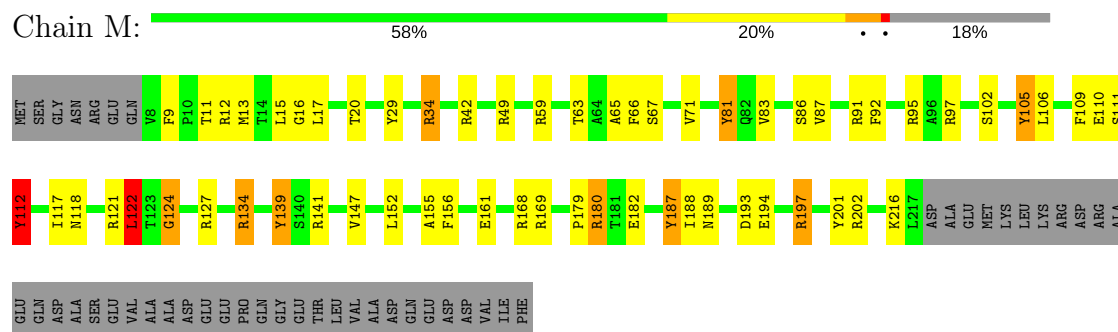
- Molecule 11 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	X	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	a	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	R	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Z	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	S	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Y	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	T	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	V	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	W	150	Total 1071	C 704	N 173	O 187	S 7	0	0

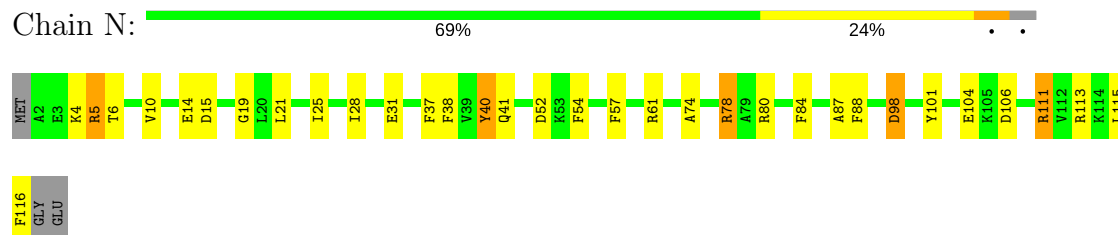
### 3 Residue-property plots

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.

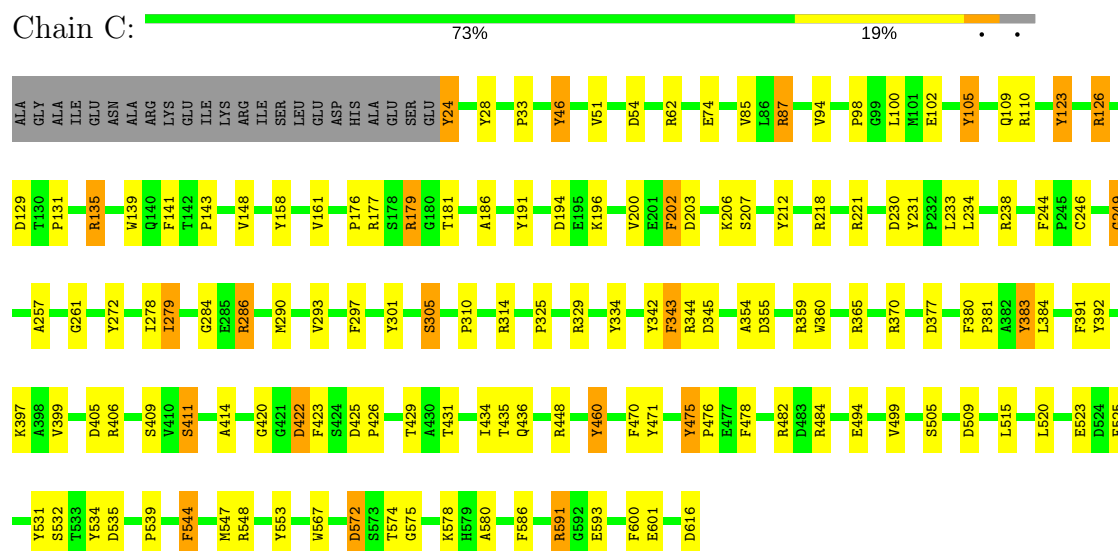
#### • Molecule 1: V-type proton ATPase subunit D



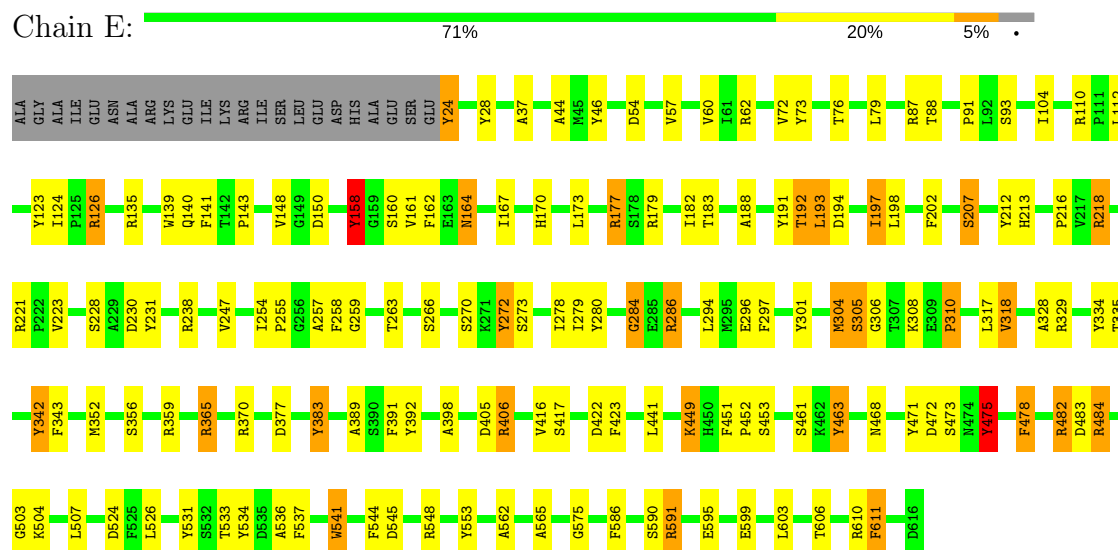
#### • Molecule 2: V-type proton ATPase subunit F



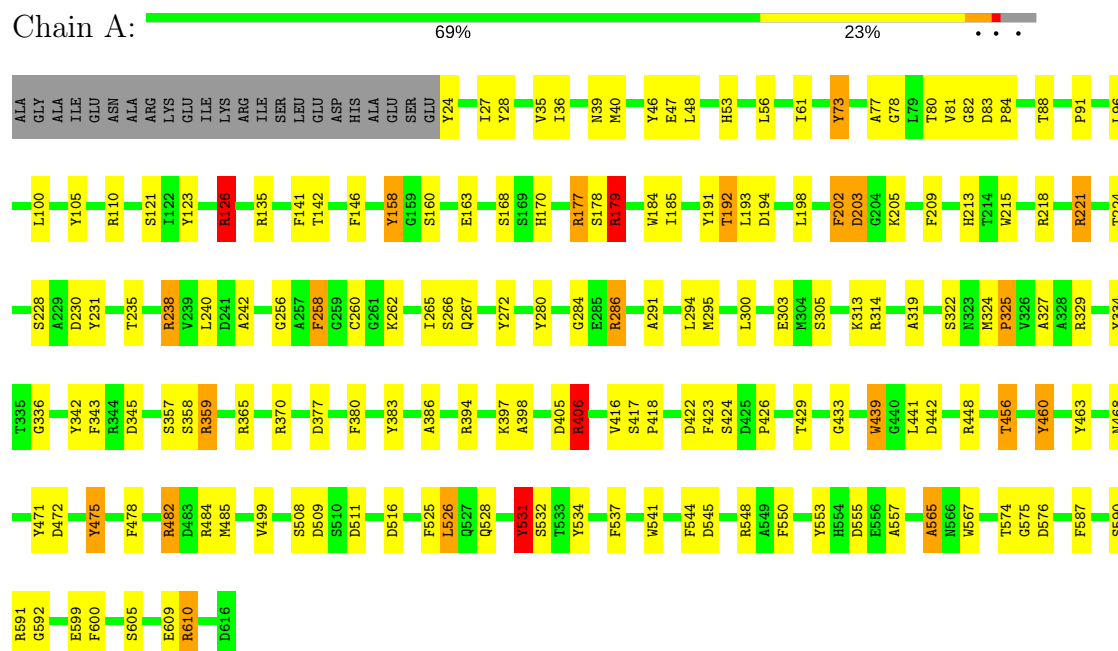
#### • Molecule 3: V-type proton ATPase catalytic subunit A



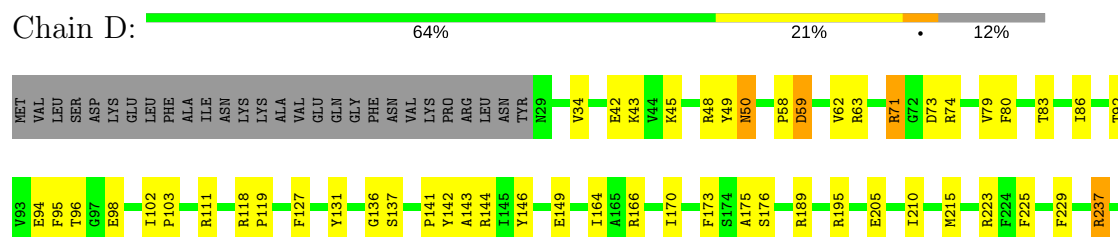
• Molecule 3: V-type proton ATPase catalytic subunit A



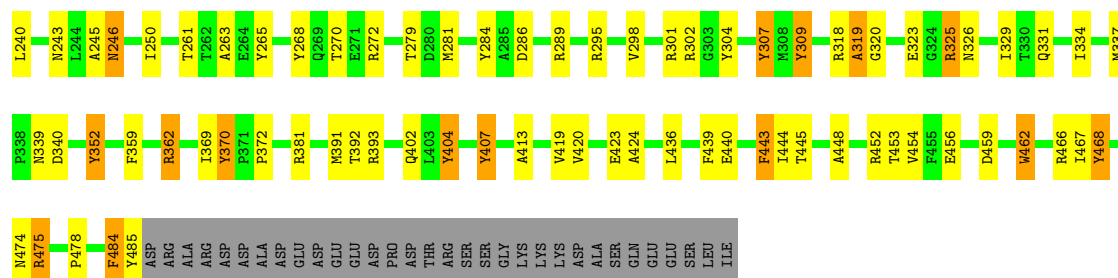
• Molecule 3: V-type proton ATPase catalytic subunit A



• Molecule 4: V-type proton ATPase subunit B

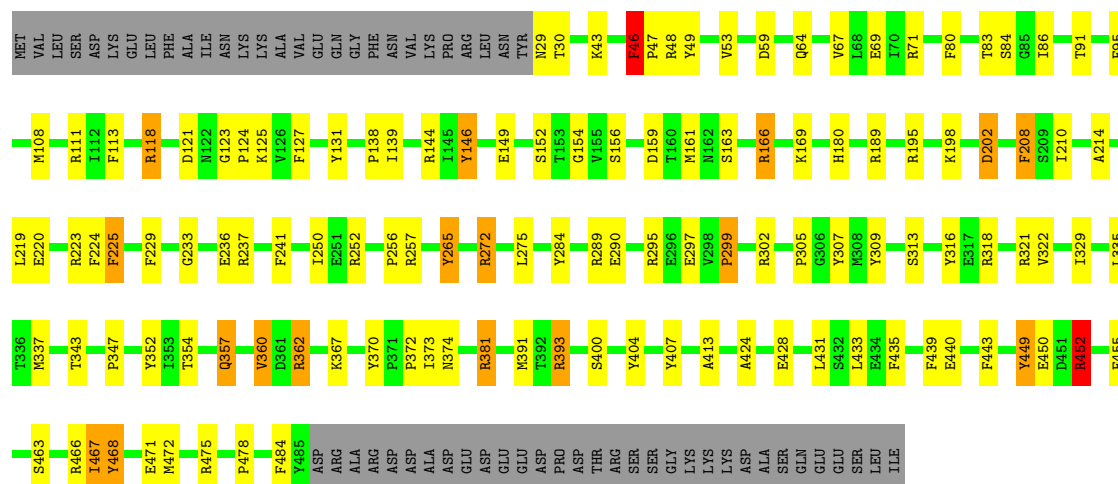






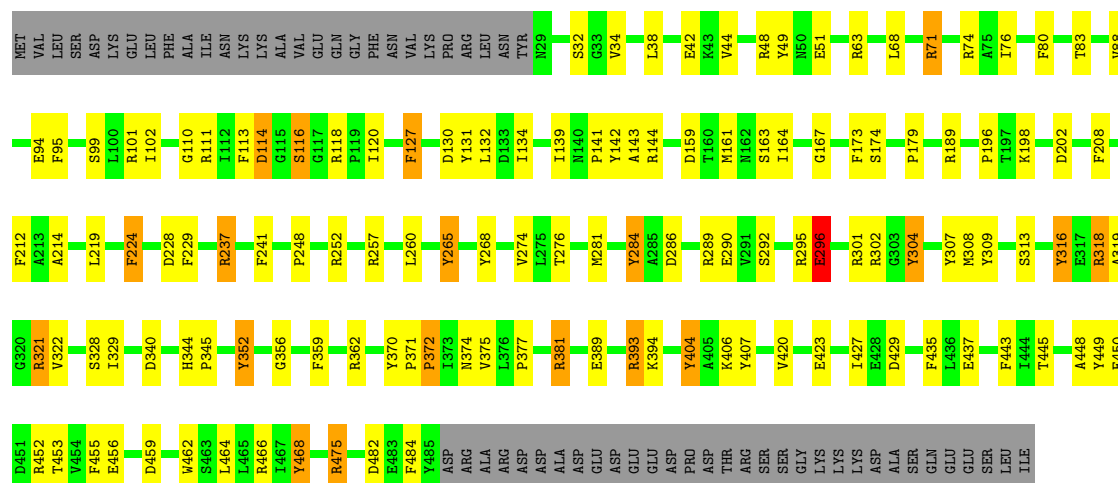
• Molecule 4: V-type proton ATPase subunit B

Chain F: 64% 21% 12%



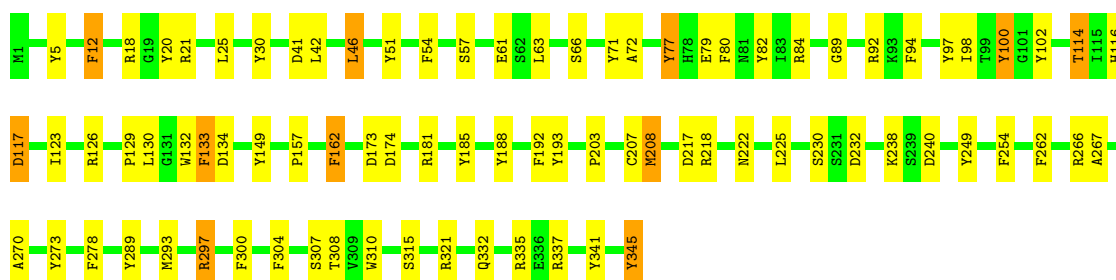
• Molecule 4: V-type proton ATPase subunit B

Chain B: 63% 22% 12%



• Molecule 5: V-type proton ATPase subunit d

Chain Q: 76% 21% 12%



- Molecule 6: V-type proton ATPase subunit G

Chain L: 76% 16% 8%



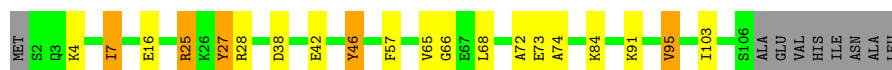
- Molecule 6: V-type proton ATPase subunit G

Chain H: 81% 11% 8%



- Molecule 6: V-type proton ATPase subunit G

Chain J: 75% 13% 8%



- Molecule 7: V-type proton ATPase subunit E

Chain K: 74% 15% 7%



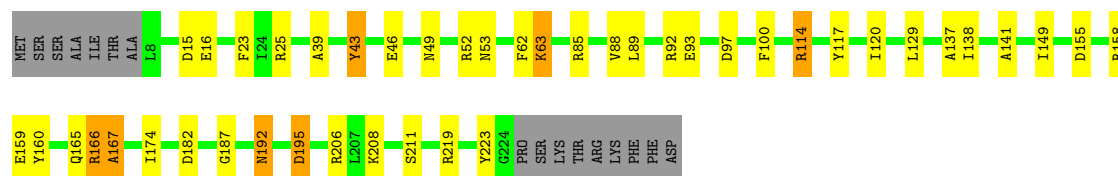
- Molecule 7: V-type proton ATPase subunit E

Chain G: 78% 13% 7%



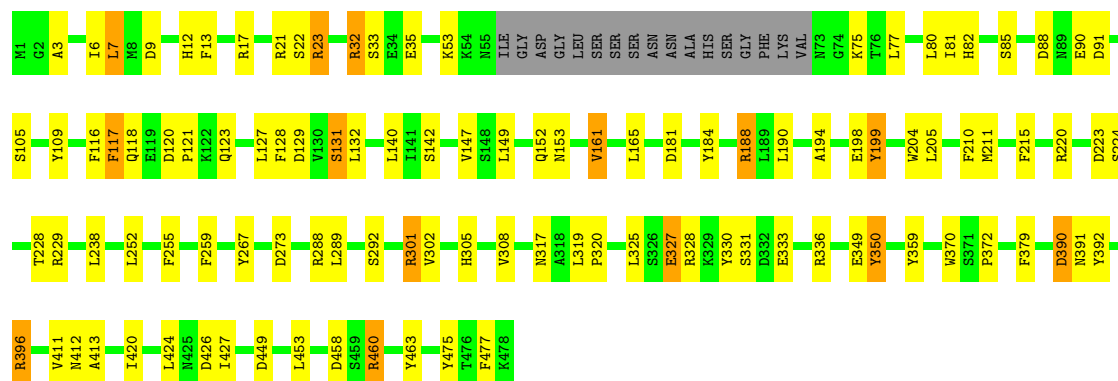
- Molecule 7: V-type proton ATPase subunit E

Chain I: 



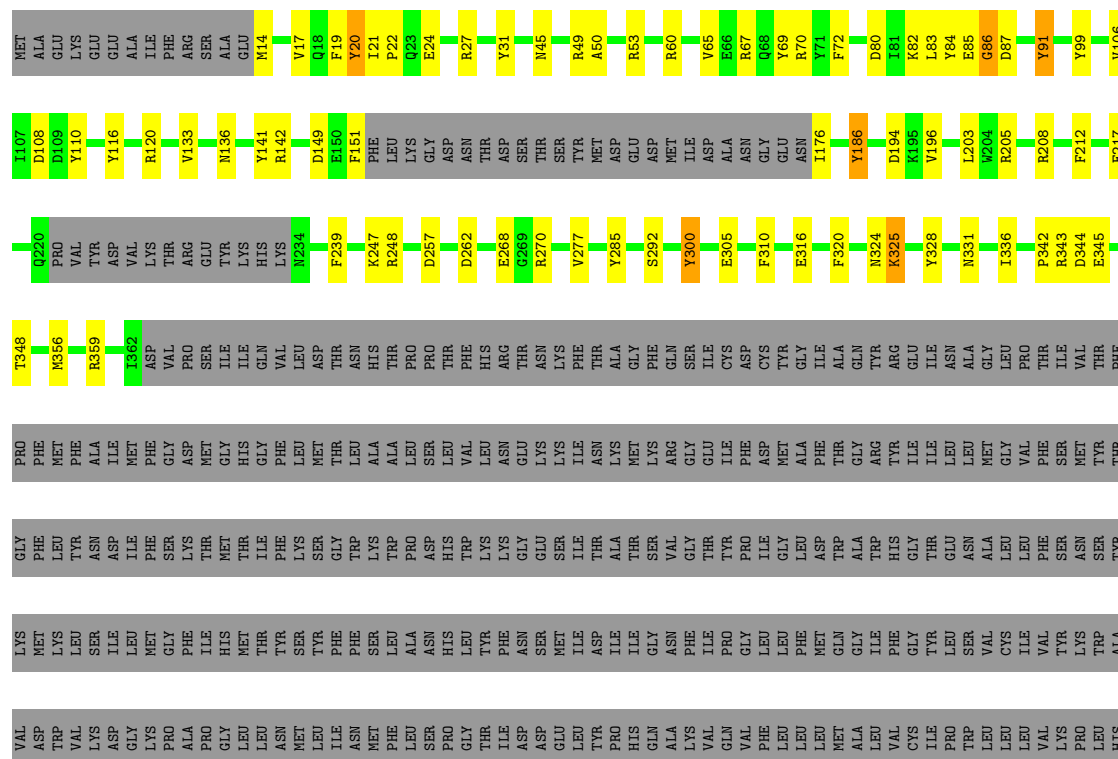
• Molecule 8: V-type proton ATPase subunit H

Chain P: 



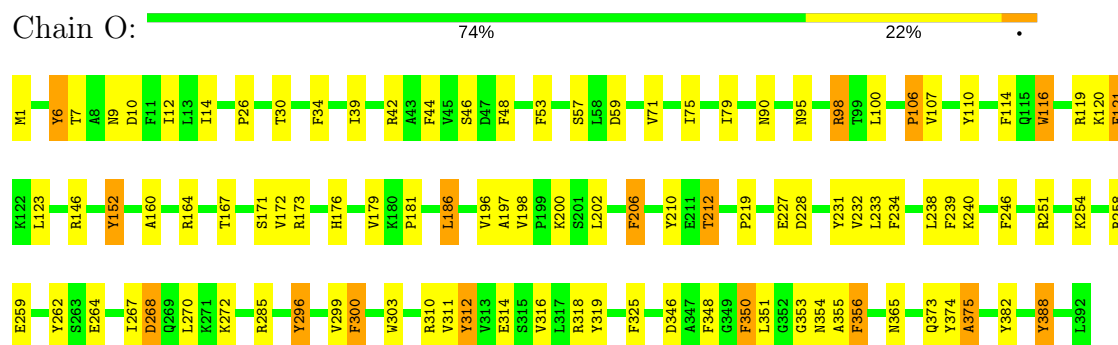
• Molecule 9: V-type proton ATPase subunit a, vacuolar isoform

Chain b: 

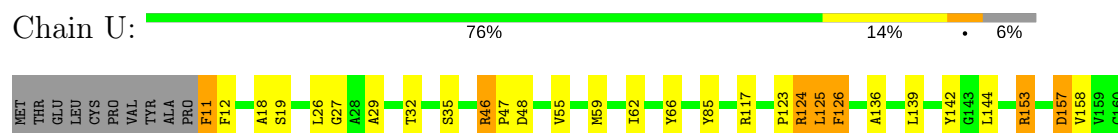


PHE	VAL	MET
LYS	ILE	TRP
THR	HIS	PHE
THR	THR	ALA
HIS	ILE	LEU
LYS	GLU	THR
LYS	PHE	CYS
LYS	CYS	ALA
SER	LEU	VAL
HIS	ASN	LEU
GLU	CYS	VAL
PRO	VAL	LEU
LEU	SER	MET
PRO	HIS	GLU
SER	THR	GLY
THR	ALA	THR
GLU	SER	ALA
ALA	TYR	LEU
ASP	ARG	ASP
ALA	LEU	ALA
SER	LEU	SER
GLU	ALA	LEU
ASP	TRP	ASP
LEU	LEU	SER
GLU	LEU	LEU
ALA	ALA	GLU
GLN	HIS	ALA
GLN	ALA	GLN
LEU	GLN	LEU
ILE	LEU	ILE
SER	SER	SER
ALA	SER	LYS
MET	VAL	PHE
ASP	TRP	ASP
ALA	THR	ASP
ASP	MET	ASP
ALA	GLY	ASP
GLU	THR	GLU
GLU	ILE	GLU
GLU	GLN	GLU
GLU	ILE	GLU
VAL	ALA	GLU
VAL	PHE	VAL
GLY	GLY	GLY
SER	PHE	SER
GLY	ARG	GLY
SER	GLY	SER
HIS	PHE	HIS
GLY	VAL	GLY
ASP	GLY	ASP
PHE	VAL	PHE
GLY	MET	GLY
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MET	ALA	MET
ILE	ALA	ILE
HIS	PHE	HIS
GLN	ALA	GLN

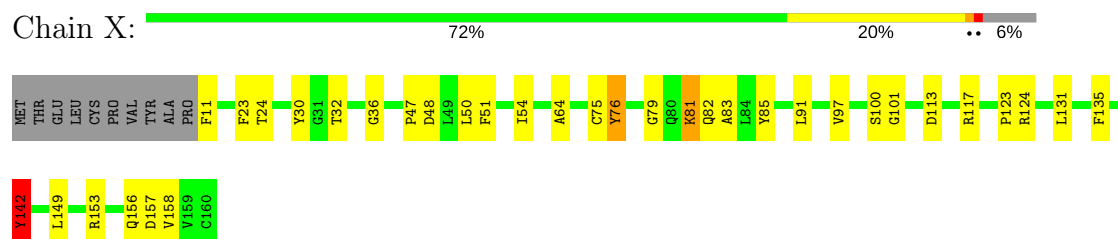
• Molecule 10: V-type proton ATPase subunit C



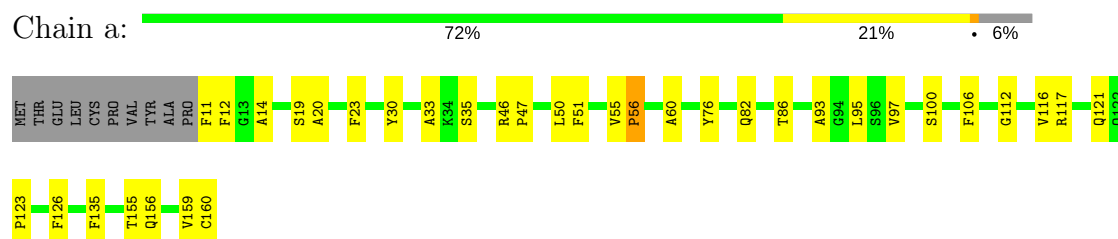
• Molecule 11: V-type proton ATPase subunit c



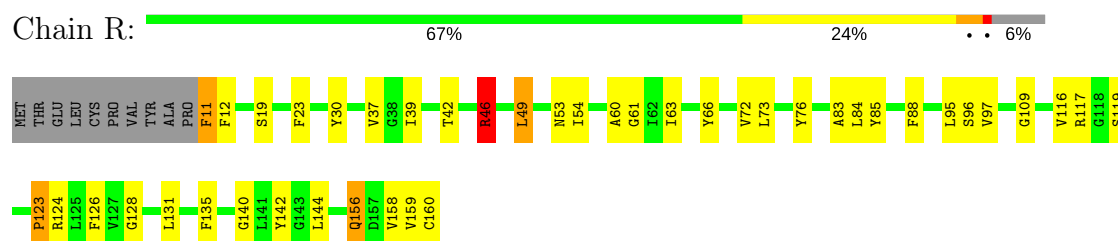
• Molecule 11: V-type proton ATPase subunit c



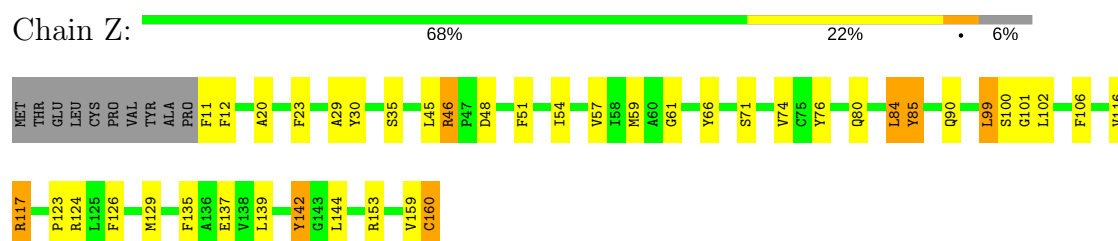
• Molecule 11: V-type proton ATPase subunit c



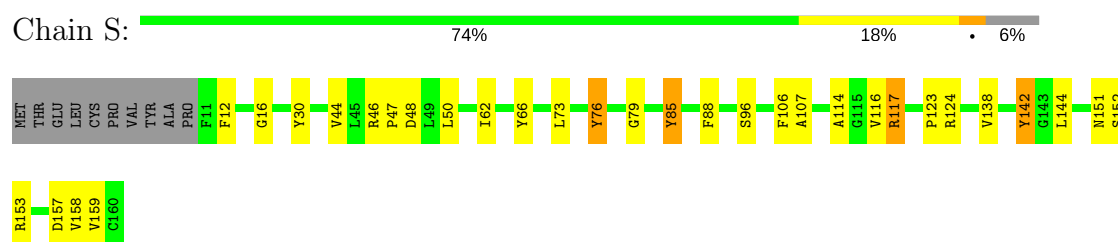
- Molecule 11: V-type proton ATPase subunit c



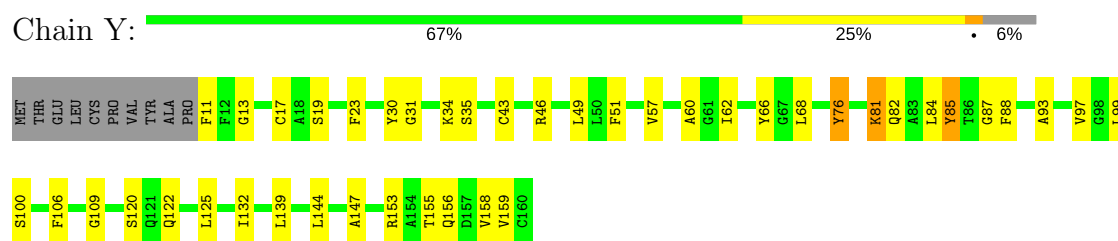
- Molecule 11: V-type proton ATPase subunit c



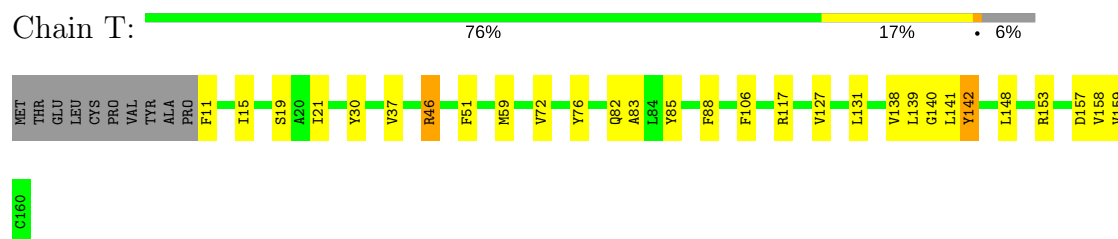
- Molecule 11: V-type proton ATPase subunit c



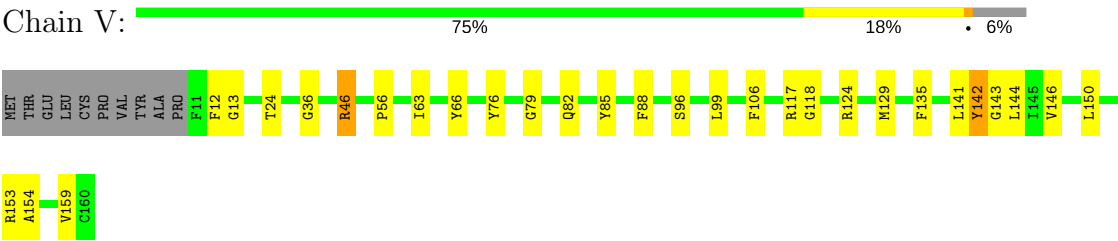
- Molecule 11: V-type proton ATPase subunit c



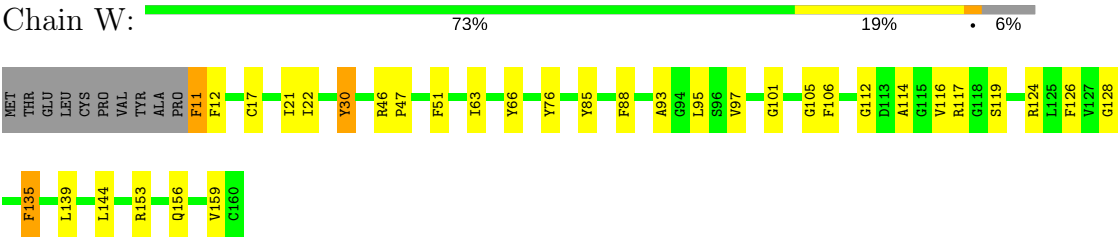
- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c



● Molecule 11: V-type proton ATPase subunit c



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	38347	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 (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	1.80	24/1710 (1.4%)	2.05	49/2295 (2.1%)
10	O	1.69	27/3185 (0.8%)	1.94	77/4314 (1.8%)
11	R	1.71	12/1086 (1.1%)	1.93	28/1472 (1.9%)
11	S	1.65	7/1086 (0.6%)	1.87	18/1472 (1.2%)
11	T	1.65	5/1086 (0.5%)	1.90	21/1472 (1.4%)
11	U	1.67	7/1086 (0.6%)	1.91	22/1472 (1.5%)
11	V	1.65	7/1086 (0.6%)	1.87	21/1472 (1.4%)
11	W	1.67	9/1086 (0.8%)	1.88	23/1472 (1.6%)
11	X	1.63	9/1086 (0.8%)	1.94	28/1472 (1.9%)
11	Y	1.69	9/1086 (0.8%)	1.80	23/1472 (1.6%)
11	Z	1.77	15/1086 (1.4%)	1.97	32/1472 (2.2%)
11	a	1.75	9/1086 (0.8%)	1.93	27/1472 (1.8%)
2	N	1.77	11/944 (1.2%)	1.88	23/1277 (1.8%)
3	A	1.72	45/4677 (1.0%)	2.01	130/6339 (2.1%)
3	C	1.70	33/4677 (0.7%)	1.96	121/6339 (1.9%)
3	E	1.72	41/4677 (0.9%)	1.92	112/6339 (1.8%)
4	B	1.71	40/3654 (1.1%)	1.97	93/4953 (1.9%)
4	D	1.74	34/3654 (0.9%)	1.96	80/4953 (1.6%)
4	F	1.78	49/3654 (1.3%)	1.99	91/4953 (1.8%)
5	Q	1.71	23/2861 (0.8%)	2.02	73/3880 (1.9%)
6	H	1.55	2/828 (0.2%)	1.76	10/1098 (0.9%)
6	J	1.63	7/828 (0.8%)	1.70	9/1098 (0.8%)
6	L	1.64	4/828 (0.5%)	1.75	13/1098 (1.2%)
7	G	1.66	13/1743 (0.7%)	1.84	27/2338 (1.2%)
7	I	1.68	13/1743 (0.7%)	1.87	36/2338 (1.5%)
7	K	1.71	14/1743 (0.8%)	1.83	34/2338 (1.5%)
8	P	1.66	22/3766 (0.6%)	1.86	76/5087 (1.5%)
9	b	1.74	22/2578 (0.9%)	1.98	66/3479 (1.9%)
All	All	1.71	513/58610 (0.9%)	1.93	1363/79236 (1.7%)

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



Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	9
10	O	0	8
11	R	0	1
11	S	0	2
11	T	0	4
11	U	0	4
11	V	0	3
11	W	0	2
11	X	0	2
11	Y	0	2
11	Z	0	3
11	a	0	2
2	N	0	4
3	A	0	12
3	C	0	13
3	E	0	15
4	B	0	17
4	D	0	13
4	F	0	14
5	Q	0	8
6	J	0	3
6	L	0	1
7	G	0	1
7	I	0	3
7	K	0	6
8	P	0	5
9	b	0	6
All	All	0	163

The worst 5 of 513 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	43	CYS	CB-SG	8.32	1.96	1.82
4	F	118	ARG	CZ-NH1	8.24	1.43	1.33
11	Z	101	GLY	CA-C	-8.09	1.39	1.51
3	E	365	ARG	CZ-NH2	7.91	1.43	1.33
1	M	97	ARG	CZ-NH2	7.89	1.43	1.33

The worst 5 of 1363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	82	TYR	CB-CG-CD1	20.73	133.44	121.00
5	Q	82	TYR	CB-CG-CD2	-18.34	110.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	TYR	CB-CG-CD2	-16.36	111.19	121.00
3	A	272	TYR	CB-CG-CD2	-16.22	111.27	121.00
1	M	34	ARG	NE-CZ-NH1	15.89	128.25	120.30

There are no chirality outliers.

5 of 163 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	105	TYR	Sidechain
1	M	112	TYR	Sidechain
1	M	127	ARG	Sidechain
1	M	34	ARG	Sidechain
1	M	81	TYR	Sidechain

## 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	1691	0	1740	5	0
2	N	928	0	926	2	0
3	A	4578	0	4519	16	0
3	C	4578	0	4518	4	0
3	E	4578	0	4519	19	0
4	B	3585	0	3567	11	0
4	D	3585	0	3567	11	0
4	F	3585	0	3567	11	0
5	Q	2802	0	2689	5	0
6	H	824	0	877	0	0
6	J	824	0	877	4	0
6	L	824	0	877	2	0
7	G	1731	0	1797	2	0
7	I	1731	0	1797	4	0
7	K	1731	0	1797	6	0
8	P	3712	0	3829	17	0
9	b	2540	0	2537	0	0
10	O	3122	0	3155	7	0
11	R	1071	0	1141	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	S	1071	0	1141	8	0
11	T	1071	0	1141	2	0
11	U	1071	0	1141	4	0
11	V	1071	0	1141	9	0
11	W	1071	0	1141	10	0
11	X	1071	0	1141	5	0
11	Y	1071	0	1141	6	0
11	Z	1071	0	1141	5	0
11	a	1071	0	1141	0	0
All	All	57659	0	58565	178	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 2.

The worst 5 of 178 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)
11:R:97:VAL:CG1	11:R:144:LEU:CD2	1.93	1.47
11:R:97:VAL:HG11	11:R:144:LEU:CD2	1.54	1.31
11:R:97:VAL:CG1	11:R:144:LEU:HD23	1.53	1.27
11:R:97:VAL:HG13	11:R:144:LEU:HD23	1.17	1.16
11:R:97:VAL:CG1	11:R:144:LEU:HD21	1.64	1.13

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%)	32	74
2	N	113/118 (96%)	102 (90%)	7 (6%)	4 (4%)	4	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	591/616 (96%)	551 (93%)	23 (4%)	17 (3%)	5	38
3	C	591/616 (96%)	545 (92%)	31 (5%)	15 (2%)	6	41
3	E	591/616 (96%)	544 (92%)	31 (5%)	16 (3%)	6	40
4	B	455/517 (88%)	415 (91%)	26 (6%)	14 (3%)	5	36
4	D	455/517 (88%)	410 (90%)	32 (7%)	13 (3%)	5	38
4	F	455/517 (88%)	425 (93%)	20 (4%)	10 (2%)	8	44
5	Q	343/345 (99%)	317 (92%)	18 (5%)	8 (2%)	7	43
6	H	103/114 (90%)	102 (99%)	0	1 (1%)	18	61
6	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
6	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	18	61
7	G	215/233 (92%)	206 (96%)	7 (3%)	2 (1%)	20	63
7	I	215/233 (92%)	207 (96%)	6 (3%)	2 (1%)	20	63
7	K	215/233 (92%)	206 (96%)	8 (4%)	1 (0%)	32	74
8	P	457/478 (96%)	434 (95%)	18 (4%)	5 (1%)	17	60
9	b	306/840 (36%)	289 (94%)	11 (4%)	6 (2%)	9	46
10	O	390/392 (100%)	350 (90%)	26 (7%)	14 (4%)	4	33
11	R	148/160 (92%)	137 (93%)	7 (5%)	4 (3%)	6	40
11	S	148/160 (92%)	136 (92%)	9 (6%)	3 (2%)	9	46
11	T	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	9	46
11	U	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	9	46
11	V	148/160 (92%)	141 (95%)	6 (4%)	1 (1%)	25	68
11	W	148/160 (92%)	137 (93%)	9 (6%)	2 (1%)	13	54
11	X	148/160 (92%)	138 (93%)	5 (3%)	5 (3%)	4	35
11	Y	148/160 (92%)	139 (94%)	6 (4%)	3 (2%)	9	46
11	Z	148/160 (92%)	145 (98%)	2 (1%)	1 (1%)	25	68
11	a	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	9	46
All	All	7389/8469 (87%)	6890 (93%)	341 (5%)	158 (2%)	12	45

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	475	TYR
4	D	45	LYS

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Mol	Chain	Res	Type
4	D	59	ASP
4	D	143	ALA
3	E	475	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	183/221 (83%)	176 (96%)	7 (4%)	38	67
2	N	102/104 (98%)	99 (97%)	3 (3%)	48	73
3	A	497/515 (96%)	479 (96%)	18 (4%)	40	68
3	C	497/515 (96%)	481 (97%)	16 (3%)	44	71
3	E	497/515 (96%)	475 (96%)	22 (4%)	33	63
4	B	391/444 (88%)	377 (96%)	14 (4%)	40	68
4	D	391/444 (88%)	377 (96%)	14 (4%)	40	68
4	F	391/444 (88%)	375 (96%)	16 (4%)	35	65
5	Q	309/309 (100%)	300 (97%)	9 (3%)	48	73
6	H	87/94 (93%)	86 (99%)	1 (1%)	78	89
6	J	87/94 (93%)	84 (97%)	3 (3%)	42	69
6	L	87/94 (93%)	87 (100%)	0	100	100
7	G	194/208 (93%)	187 (96%)	7 (4%)	40	68
7	I	194/208 (93%)	190 (98%)	4 (2%)	59	80
7	K	194/208 (93%)	187 (96%)	7 (4%)	40	68
8	P	426/439 (97%)	416 (98%)	10 (2%)	56	79
9	b	275/728 (38%)	266 (97%)	9 (3%)	43	70
10	O	348/348 (100%)	337 (97%)	11 (3%)	44	71
11	R	110/119 (92%)	107 (97%)	3 (3%)	50	74
11	S	110/119 (92%)	108 (98%)	2 (2%)	64	84
11	T	110/119 (92%)	109 (99%)	1 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	U	110/119 (92%)	107 (97%)	3 (3%)	50	74
11	V	110/119 (92%)	108 (98%)	2 (2%)	64	84
11	W	110/119 (92%)	109 (99%)	1 (1%)	82	91
11	X	110/119 (92%)	105 (96%)	5 (4%)	32	63
11	Y	110/119 (92%)	104 (94%)	6 (6%)	25	58
11	Z	110/119 (92%)	104 (94%)	6 (6%)	25	58
11	a	110/119 (92%)	107 (97%)	3 (3%)	50	74
All	All	6250/7122 (88%)	6047 (97%)	203 (3%)	48	71

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	416	VAL
5	Q	114	THR
11	Z	117	ARG
3	A	599	GLU
4	B	296	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
5	Q	287	HIS
8	P	425	ASN
11	Z	80	GLN
6	L	3	GLN
7	K	200	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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.