



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 11:38 AM EDT

PDB ID : 5D80  
Title : Crystal Structure of Yeast V1-ATPase in the Autoinhibited Form  
Authors : Oot, R.A.; Kane, P.M.; Berry, E.A.; Wilkens, S.  
Deposited on : 2015-08-14  
Resolution : 6.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

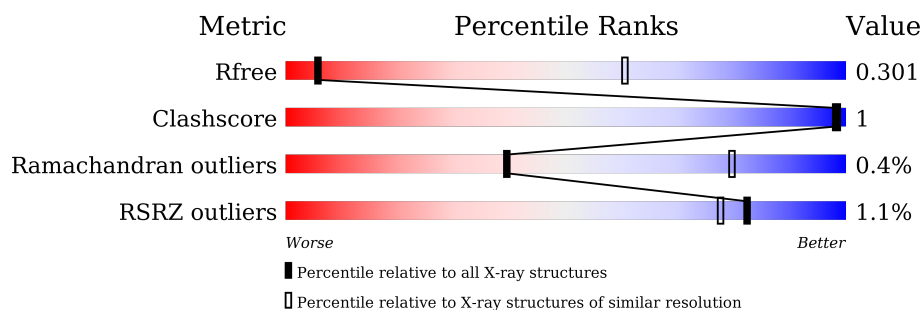
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.20 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.







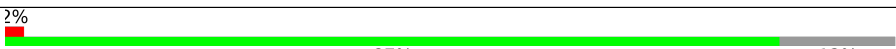
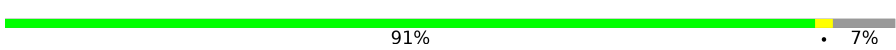


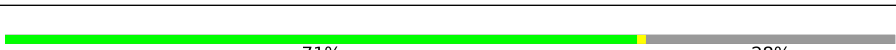
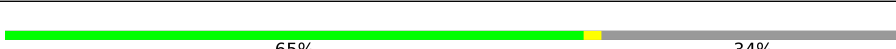



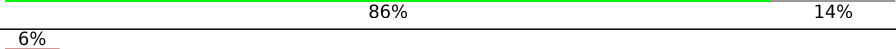
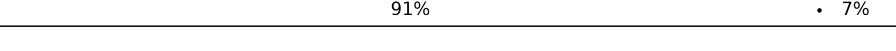
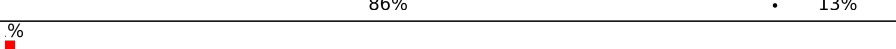

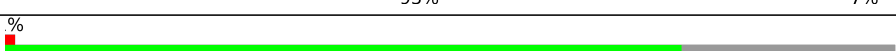
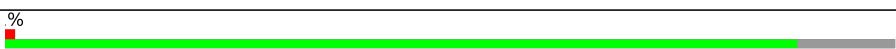

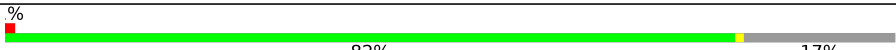
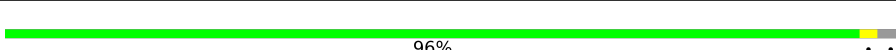
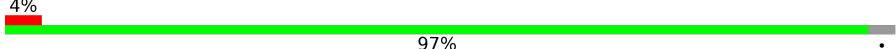
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1007 (8.70-3.66)
Clashscore	102246	1055 (8.70-3.70)
Ramachandran outliers	100387	1028 (8.70-3.66)
RSRZ outliers	91569	1006 (8.70-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	617	
1	B	617	
1	C	617	
1	a	617	
1	b	617	
1	c	617	
2	D	517	

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Mol	Chain	Length	Quality of chain
2	E	517	
2	F	517	
2	d	517	
2	e	517	
2	f	517	
3	H	478	
3	h	478	
4	J	122	
4	L	122	
4	N	122	
4	j	122	
4	l	122	
4	n	122	
5	I	233	
5	K	233	
5	M	233	
5	i	233	
5	k	233	
5	m	233	
6	G	256	
6	g	256	
7	O	118	
7	o	118	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 47363 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 catalytic subunit A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	0	0	0
			2905	1723	591	591			
1	B	598	Total	C	N	O	0	0	0
			2940	1744	598	598			
1	C	589	Total	C	N	O	0	0	0
			2895	1717	589	589			
1	a	591	Total	C	N	O	0	0	0
			2905	1723	591	591			
1	b	598	Total	C	N	O	0	0	0
			2940	1744	598	598			
1	c	589	Total	C	N	O	0	0	0
			2895	1717	589	589			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	457	Total	C	N	O	0	0	0
			2250	1336	457	457			
2	E	453	Total	C	N	O	0	0	0
			2231	1325	453	453			
2	F	447	Total	C	N	O	0	0	0
			2201	1307	447	447			
2	d	456	Total	C	N	O	0	0	0
			2245	1333	456	456			
2	e	453	Total	C	N	O	0	0	0
			2231	1325	453	453			
2	f	449	Total	C	N	O	0	0	0
			2211	1313	449	449			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	445	Total	C	N	O	0	0	0
			2212	1322	445	445			
3	h	445	Total	C	N	O	0	0	0
			2212	1322	445	445			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	104	Total	C	N	O	0	0	0
			514	306	104	104			
4	L	88	Total	C	N	O	0	0	0
			435	259	88	88			
4	N	81	Total	C	N	O	0	0	0
			400	238	81	81			
4	j	104	Total	C	N	O	0	0	0
			514	306	104	104			
4	l	68	Total	C	N	O	0	0	0
			335	199	68	68			
4	n	105	Total	C	N	O	0	0	0
			519	309	105	105			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-7	MET	-	initiating methionine	UNP P48836
J	-6	ASP	-	expression tag	UNP P48836
J	-5	TYR	-	expression tag	UNP P48836
J	-4	LYS	-	expression tag	UNP P48836
J	-3	ASP	-	expression tag	UNP P48836
J	-2	ASP	-	expression tag	UNP P48836
J	-1	ASP	-	expression tag	UNP P48836
J	0	ASP	-	expression tag	UNP P48836
J	1	LYS	-	expression tag	UNP P48836
L	-7	MET	-	initiating methionine	UNP P48836
L	-6	ASP	-	expression tag	UNP P48836
L	-5	TYR	-	expression tag	UNP P48836
L	-4	LYS	-	expression tag	UNP P48836
L	-3	ASP	-	expression tag	UNP P48836
L	-2	ASP	-	expression tag	UNP P48836
L	-1	ASP	-	expression tag	UNP P48836
L	0	ASP	-	expression tag	UNP P48836
L	1	LYS	-	expression tag	UNP P48836
N	-7	MET	-	initiating methionine	UNP P48836

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-6	ASP	-	expression tag	UNP P48836
N	-5	TYR	-	expression tag	UNP P48836
N	-4	LYS	-	expression tag	UNP P48836
N	-3	ASP	-	expression tag	UNP P48836
N	-2	ASP	-	expression tag	UNP P48836
N	-1	ASP	-	expression tag	UNP P48836
N	0	ASP	-	expression tag	UNP P48836
N	1	LYS	-	expression tag	UNP P48836
j	-7	MET	-	initiating methionine	UNP P48836
j	-6	ASP	-	expression tag	UNP P48836
j	-5	TYR	-	expression tag	UNP P48836
j	-4	LYS	-	expression tag	UNP P48836
j	-3	ASP	-	expression tag	UNP P48836
j	-2	ASP	-	expression tag	UNP P48836
j	-1	ASP	-	expression tag	UNP P48836
j	0	ASP	-	expression tag	UNP P48836
j	1	LYS	-	expression tag	UNP P48836
l	-7	MET	-	initiating methionine	UNP P48836
l	-6	ASP	-	expression tag	UNP P48836
l	-5	TYR	-	expression tag	UNP P48836
l	-4	LYS	-	expression tag	UNP P48836
l	-3	ASP	-	expression tag	UNP P48836
l	-2	ASP	-	expression tag	UNP P48836
l	-1	ASP	-	expression tag	UNP P48836
l	0	ASP	-	expression tag	UNP P48836
l	1	LYS	-	expression tag	UNP P48836
n	-7	MET	-	initiating methionine	UNP P48836
n	-6	ASP	-	expression tag	UNP P48836
n	-5	TYR	-	expression tag	UNP P48836
n	-4	LYS	-	expression tag	UNP P48836
n	-3	ASP	-	expression tag	UNP P48836
n	-2	ASP	-	expression tag	UNP P48836
n	-1	ASP	-	expression tag	UNP P48836
n	0	ASP	-	expression tag	UNP P48836
n	1	LYS	-	expression tag	UNP P48836

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	216	Total	C	N	O	0	0	0
			1073	641	216	216			
5	K	203	Total	C	N	O	0	0	0
			1008	602	203	203			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	203	Total	C	N	O	0	0	0
			1008	602	203	203			
5	i	216	Total	C	N	O	0	0	0
			1073	641	216	216			
5	k	178	Total	C	N	O	0	0	0
			883	527	178	178			
5	m	208	Total	C	N	O	0	0	0
			1033	617	208	208			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	223	Total	C	N	O	0	0	0
			1104	658	223	223			
6	g	212	Total	C	N	O	0	0	0
			1049	625	212	212			

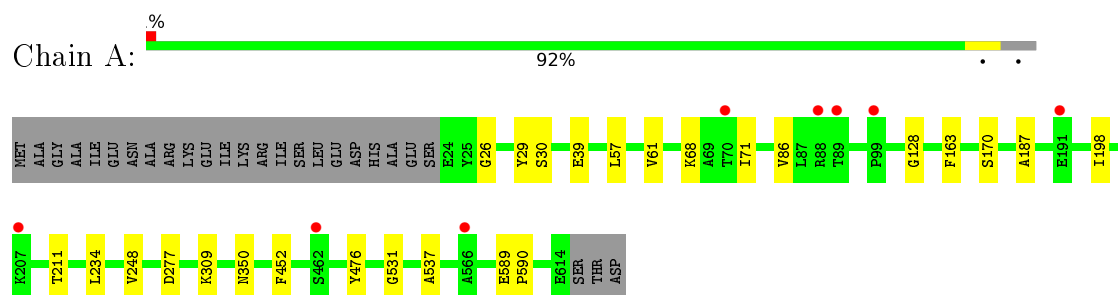
- Molecule 7 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	o	115	Total	C	N	O	0	0	0
			571	341	115	115			
7	O	115	Total	C	N	O	0	0	0
			571	341	115	115			

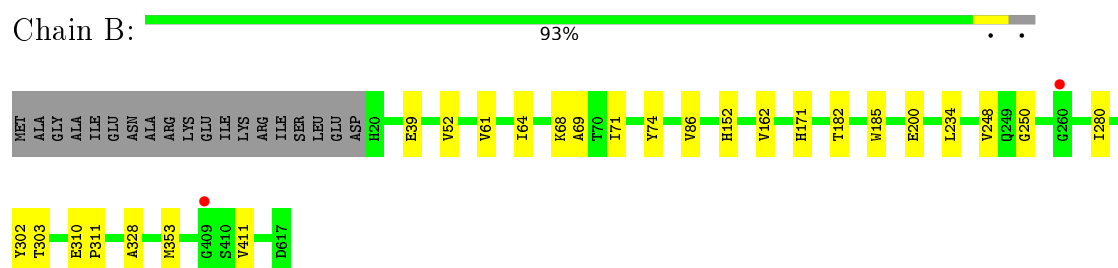
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

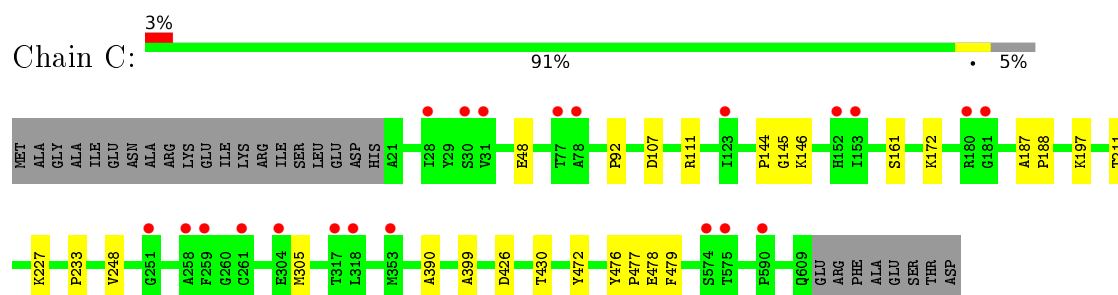
- Molecule 1: V-type proton ATPase catalytic subunit A



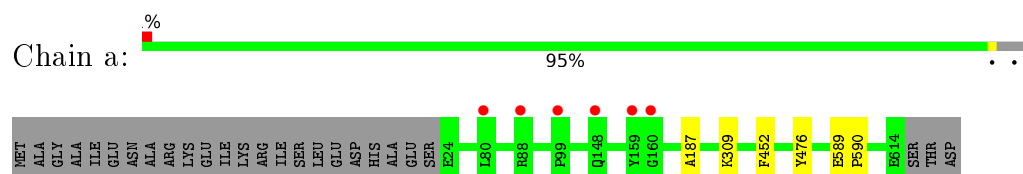
- Molecule 1: V-type proton ATPase catalytic subunit A



- Molecule 1: V-type proton ATPase catalytic subunit A



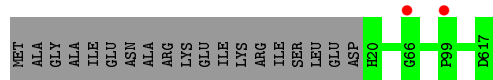
- Molecule 1: V-type proton ATPase catalytic subunit A





- Molecule 1: V-type proton ATPase catalytic subunit A

Chain b:  97%




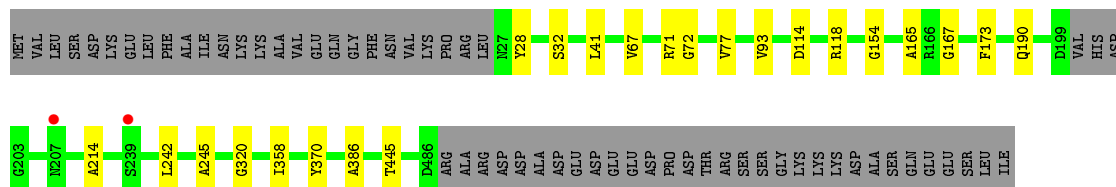
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain c:  94% 5%




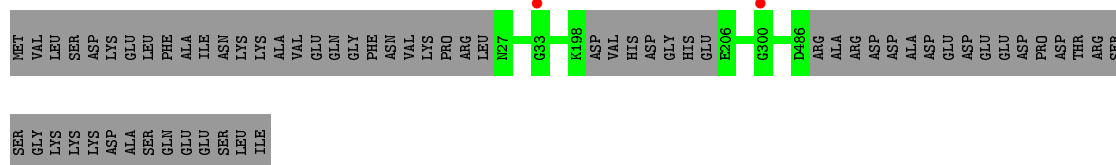
- Molecule 2: V-type proton ATPase subunit B

Chain D:  84% 12%




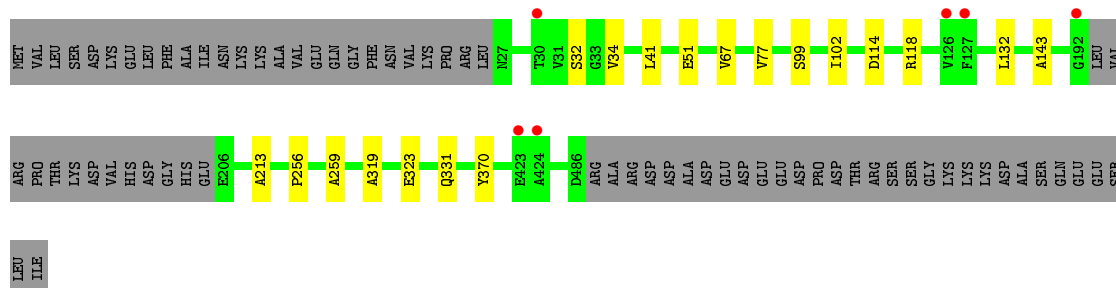
- Molecule 2: V-type proton ATPase subunit B

Chain E:  88% 12%




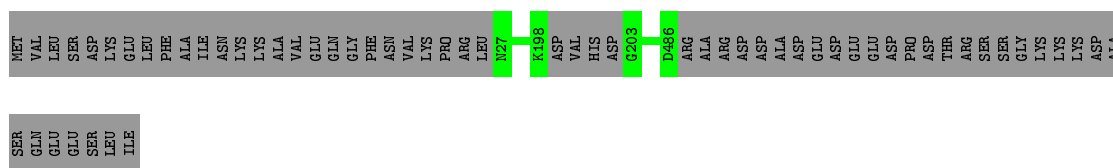
- Molecule 2: V-type proton ATPase subunit B

Chain F:  83% 14%




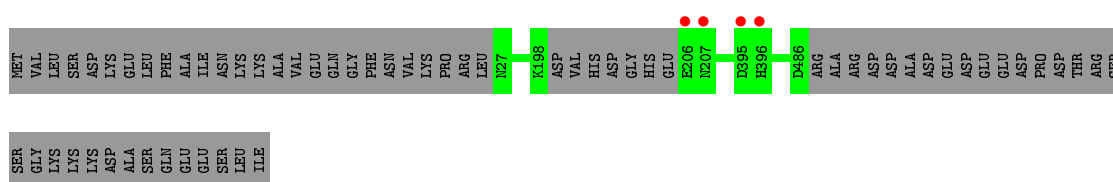
- Molecule 2: V-type proton ATPase subunit B

Chain d:  88% 12%




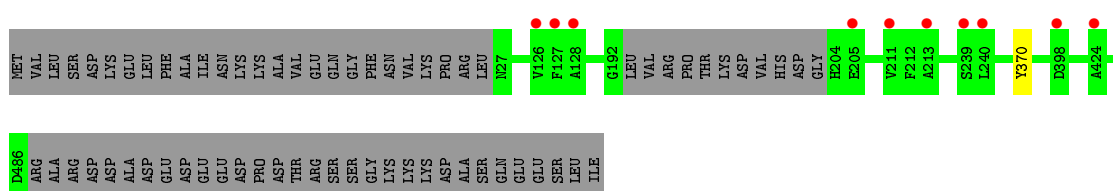
- Molecule 2: V-type proton ATPase subunit B

Chain e:  88% 12%



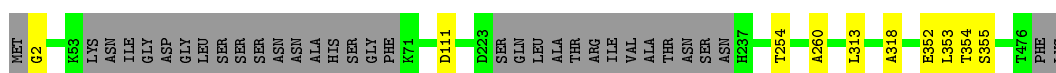
- Molecule 2: V-type proton ATPase subunit B

Chain f:  87% 13% 2%



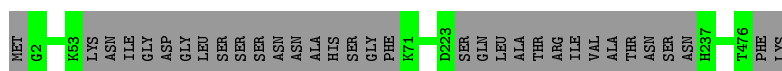
- Molecule 3: V-type proton ATPase subunit H

Chain H:  91% 7%




- Molecule 3: V-type proton ATPase subunit H

Chain h:  93% 7%



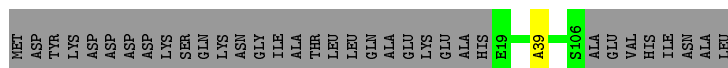
- Molecule 4: V-type proton ATPase subunit G

Chain J:  84% 15%



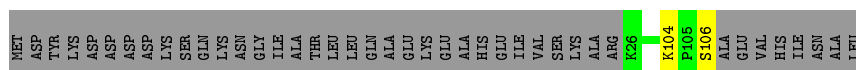
- Molecule 4: V-type proton ATPase subunit G

Chain L:  71% 28%




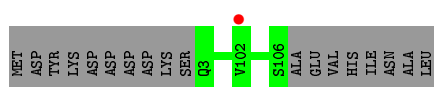
- Molecule 4: V-type proton ATPase subunit G

Chain N:  65% 34%



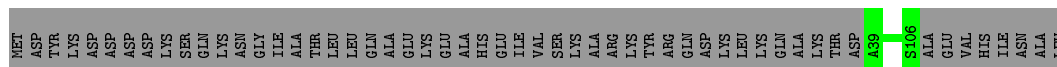
- Molecule 4: V-type proton ATPase subunit G

Chain j:  85% 15%




- Molecule 4: V-type proton ATPase subunit G

Chain l:  56% 44%



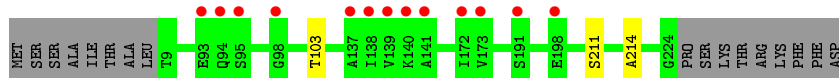
- Molecule 4: V-type proton ATPase subunit G

Chain n:  86% 14%



- Molecule 5: V-type proton ATPase subunit E

Chain I:  91% 7%




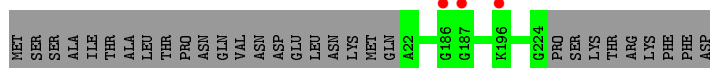
- Molecule 5: V-type proton ATPase subunit E

Chain K:  86% 13%

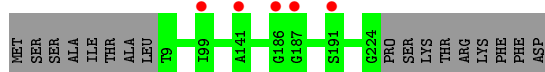
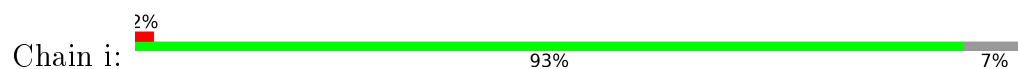


- Molecule 5: V-type proton ATPase subunit E

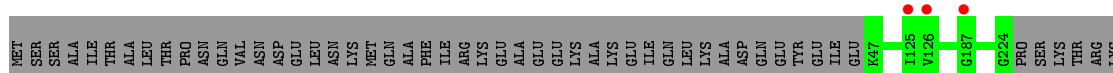
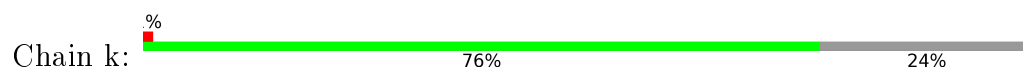
Chain M:  87% 13%



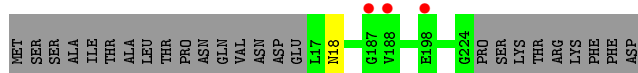
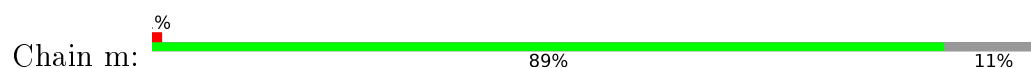
- Molecule 5: V-type proton ATPase subunit E



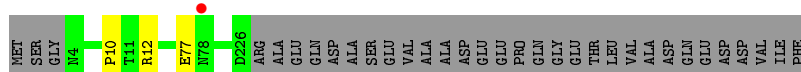
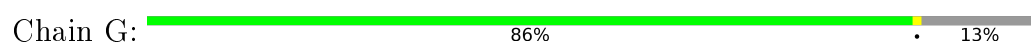
- Molecule 5: V-type proton ATPase subunit E



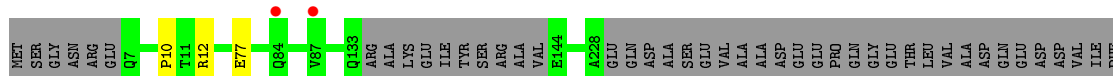
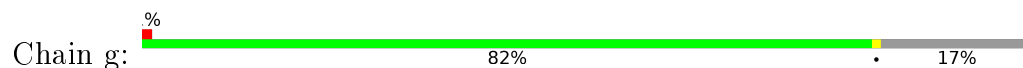
- Molecule 5: V-type proton ATPase subunit E



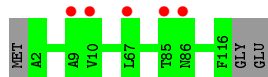
- Molecule 6: V-type proton ATPase subunit D



- Molecule 6: V-type proton ATPase subunit D



- Molecule 7: V-type proton ATPase subunit F



- Molecule 7: V-type proton ATPase subunit F



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	468.02Å 159.65Å 248.27Å 90.00° 113.75° 90.00°	Depositor
Resolution (Å)	39.72 – 6.20 39.72 – 6.20	Depositor EDS
% Data completeness (in resolution range)	87.6 (39.72-6.20) 87.7 (39.72-6.20)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 6.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.255 , 0.302 0.240 , 0.301	Depositor DCC
$R_{free}$ test set	1997 reflections (5.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	422.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 814.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	47363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	320.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.19	0/2904	0.34	0/4034
1	B	0.19	0/2939	0.35	0/4083
1	C	0.20	0/2894	0.37	0/4020
1	a	0.19	0/2904	0.34	0/4034
1	b	0.19	0/2939	0.35	0/4083
1	c	0.20	0/2894	0.37	0/4020
2	D	0.20	0/2248	0.36	0/3123
2	E	0.20	0/2229	0.35	0/3097
2	F	0.19	0/2199	0.34	0/3055
2	d	0.20	0/2243	0.36	0/3116
2	e	0.20	0/2229	0.35	0/3097
2	f	0.19	0/2209	0.34	0/3069
3	H	0.20	0/2209	0.37	0/3080
3	h	0.21	0/2209	0.37	0/3080
4	J	0.20	0/513	0.33	0/713
4	L	0.21	0/434	0.34	0/603
4	N	0.19	0/399	0.33	0/554
4	j	0.20	0/513	0.33	0/713
4	l	0.21	0/334	0.33	0/463
4	n	0.19	0/518	0.33	0/720
5	I	0.20	0/1072	0.31	0/1495
5	K	0.19	0/1007	0.32	0/1404
5	M	0.18	0/1007	0.30	0/1404
5	i	0.20	0/1072	0.31	0/1495
5	k	0.19	0/882	0.32	0/1229
5	m	0.19	0/1032	0.30	0/1439
6	G	0.21	0/1103	0.37	0/1536
6	g	0.21	0/1047	0.37	0/1456
7	O	0.19	0/570	0.36	0/794
7	o	0.19	0/570	0.36	0/794
All	All	0.20	0/47322	0.35	0/65803

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2905	0	1339	11	0
1	B	2940	0	1356	14	0
1	C	2895	0	1335	10	0
1	a	2905	0	1339	0	0
1	b	2940	0	1356	0	0
1	c	2895	0	1335	0	0
2	D	2250	0	1015	14	0
2	E	2231	0	1006	0	0
2	F	2201	0	995	10	0
2	d	2245	0	1013	0	0
2	e	2231	0	1006	0	0
2	f	2211	0	999	0	0
3	H	2212	0	951	6	0
3	h	2212	0	951	0	0
4	J	514	0	248	1	0
4	L	435	0	206	1	0
4	N	400	0	189	1	0
4	j	514	0	248	0	0
4	l	335	0	160	0	0
4	n	519	0	250	0	0
5	I	1073	0	481	2	0
5	K	1008	0	456	2	0
5	M	1008	0	456	0	0
5	i	1073	0	481	0	0
5	k	883	0	394	0	0
5	m	1033	0	466	0	0
6	G	1104	0	504	0	0
6	g	1049	0	478	0	0
7	O	571	0	255	1	0
7	o	571	0	255	0	0
All	All	47363	0	21523	67	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 1.

All (67) 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)
1:B:74:TYR:HA	1:B:328:ALA:HB3	1.69	0.74
1:A:531:GLY:HA2	1:A:537:ALA:HA	1.75	0.69
3:H:353:LEU:H	3:H:354:THR:C	1.96	0.69
2:F:213:ALA:HB1	2:F:256:PRO:HA	1.77	0.67
3:H:352:GLU:HA	3:H:355:SER:HA	1.78	0.66
1:B:302:TYR:HA	1:B:311:PRO:HA	1.79	0.64
2:F:51:GLU:HA	2:F:99:SER:HA	1.81	0.62
2:F:319:ALA:HB2	2:F:331:GLN:H	1.64	0.62
1:B:64:ILE:HA	1:B:69:ALA:HA	1.84	0.59
2:F:67:VAL:HA	2:F:77:VAL:HA	1.83	0.59
1:C:233:PRO:HA	1:C:248:VAL:HA	1.85	0.58
2:F:102:ILE:N	2:F:132:LEU:O	2.36	0.58
2:D:214:ALA:HB3	2:D:242:LEU:HA	1.85	0.58
2:D:114:ASP:N	2:D:118:ARG:O	2.36	0.58
1:B:39:GLU:HA	1:B:68:LYS:HA	1.86	0.57
5:K:187:GLY:HA3	5:K:202:THR:HA	1.86	0.56
1:A:198:ILE:H	1:A:211:THR:HA	1.73	0.56
2:D:28:TYR:H	2:D:93:VAL:H	1.53	0.55
2:D:165:ALA:HB2	2:D:386:ALA:HB2	1.89	0.55
1:B:303:THR:N	1:B:310:GLU:O	2.33	0.54
1:A:39:GLU:HA	1:A:68:LYS:HA	1.90	0.53
1:B:64:ILE:O	2:F:34:VAL:N	2.41	0.53
2:D:67:VAL:HA	2:D:77:VAL:HA	1.91	0.53
1:C:390:ALA:HB1	2:D:245:ALA:HB1	1.91	0.52
2:D:167:GLY:HA2	2:D:320:GLY:HA2	1.91	0.52
2:D:28:TYR:N	2:D:93:VAL:O	2.43	0.52
1:B:61:VAL:HA	1:B:71:ILE:HA	1.92	0.51
1:B:52:VAL:HA	1:B:86:VAL:HA	1.92	0.51
1:C:48:GLU:HA	1:C:92:PRO:HA	1.93	0.51
1:B:185:TRP:O	1:B:200:GLU:N	2.45	0.50
1:B:162:VAL:O	1:B:171:HIS:N	2.34	0.50
2:F:114:ASP:N	2:F:118:ARG:O	2.43	0.49
1:A:30:SER:HA	2:D:71:ARG:HA	1.94	0.49
1:A:163:PHE:HA	1:A:170:SER:HA	1.94	0.49
1:A:29:TYR:O	2:D:72:GLY:N	2.47	0.48
2:D:173:PHE:N	2:D:358:ILE:O	2.33	0.48
1:B:250:GLY:HA2	1:B:411:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:GLY:HA3	2:D:190:GLN:CB	2.45	0.46
1:C:161:SER:HA	1:C:172:LYS:HA	1.97	0.46
5:I:211:SER:HA	5:I:214:ALA:HB3	1.98	0.46
1:A:234:LEU:H	1:A:248:VAL:HA	1.81	0.46
1:C:426:ASP:O	1:C:430:THR:N	2.46	0.45
1:C:472:TYR:O	1:C:476:TYR:N	2.50	0.45
2:D:370:TYR:CB	2:D:445:THR:HA	2.47	0.45
1:A:57:LEU:HA	1:A:128:GLY:HA2	1.99	0.45
2:F:143:ALA:O	2:F:323:GLU:N	2.50	0.44
3:H:254:THR:HA	3:H:260:ALA:HB2	2.00	0.44
1:C:197:LYS:HA	1:C:211:THR:HA	1.99	0.44
2:D:32:SER:H	2:D:41:LEU:HA	1.83	0.43
1:A:61:VAL:HA	1:A:71:ILE:HA	2.01	0.43
1:C:227:LYS:HA	1:C:399:ALA:HB2	1.99	0.43
1:A:277:ASP:N	1:A:350:ASN:O	2.43	0.43
1:B:234:LEU:H	1:B:248:VAL:HA	1.84	0.43
2:F:32:SER:H	2:F:41:LEU:HA	1.84	0.43
1:B:280:ILE:O	1:B:353:MET:HA	2.19	0.42
4:J:95:VAL:HA	5:I:103:THR:HA	2.02	0.42
1:C:478:GLU:HA	1:C:479:PHE:HA	1.74	0.42
3:H:2:GLY:HA3	3:H:111:ASP:H	1.85	0.42
3:H:313:LEU:HA	3:H:318:ALA:HB3	2.01	0.42
1:A:26:GLY:O	1:A:86:VAL:N	2.32	0.42
1:C:107:ASP:N	1:C:111:ARG:O	2.40	0.42
4:N:104:LYS:O	4:N:106:SER:N	2.53	0.41
1:B:152:HIS:HA	1:B:182:THR:HA	2.02	0.41
2:F:213:ALA:HB2	2:F:259:ALA:HB3	2.02	0.41
3:H:2:GLY:HA3	3:H:111:ASP:N	2.37	0.41
7:O:11:ILE:O	7:O:69:ILE:HA	2.21	0.41
5:K:51:VAL:CB	4:L:39:ALA:HB1	3.37	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	589/617 (96%)	551 (94%)	32 (5%)	6 (1%)	19	64
1	B	596/617 (97%)	557 (94%)	39 (6%)	0	100	100
1	C	587/617 (95%)	546 (93%)	34 (6%)	7 (1%)	16	61
1	a	589/617 (96%)	551 (94%)	32 (5%)	6 (1%)	19	64
1	b	596/617 (97%)	557 (94%)	39 (6%)	0	100	100
1	c	587/617 (95%)	546 (93%)	34 (6%)	7 (1%)	16	61
2	D	453/517 (88%)	424 (94%)	29 (6%)	0	100	100
2	E	449/517 (87%)	424 (94%)	25 (6%)	0	100	100
2	F	443/517 (86%)	416 (94%)	26 (6%)	1 (0%)	52	86
2	d	452/517 (87%)	423 (94%)	29 (6%)	0	100	100
2	e	449/517 (87%)	424 (94%)	25 (6%)	0	100	100
2	f	445/517 (86%)	418 (94%)	26 (6%)	1 (0%)	52	86
3	H	439/478 (92%)	412 (94%)	27 (6%)	0	100	100
3	h	439/478 (92%)	412 (94%)	27 (6%)	0	100	100
4	J	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
4	L	86/122 (70%)	85 (99%)	1 (1%)	0	100	100
4	N	79/122 (65%)	76 (96%)	3 (4%)	0	100	100
4	j	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
4	l	66/122 (54%)	65 (98%)	1 (2%)	0	100	100
4	n	103/122 (84%)	100 (97%)	3 (3%)	0	100	100
5	I	214/233 (92%)	214 (100%)	0	0	100	100
5	K	201/233 (86%)	200 (100%)	1 (0%)	0	100	100
5	M	201/233 (86%)	200 (100%)	1 (0%)	0	100	100
5	i	214/233 (92%)	214 (100%)	0	0	100	100
5	k	176/233 (76%)	175 (99%)	1 (1%)	0	100	100
5	m	206/233 (88%)	204 (99%)	1 (0%)	1 (0%)	34	76
6	G	221/256 (86%)	211 (96%)	7 (3%)	3 (1%)	14	58
6	g	208/256 (81%)	199 (96%)	6 (3%)	3 (1%)	14	58
7	O	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
7	o	113/118 (96%)	110 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9518/10638 (90%)	9024 (95%)	459 (5%)	35 (0%)	39	79

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	ALA
1	C	188	PRO
1	c	187	ALA
1	c	188	PRO
6	G	10	PRO
6	G	12	ARG
6	G	77	GLU
6	g	10	PRO
6	g	12	ARG
6	g	77	GLU
1	A	476	TYR
1	A	589	GLU
1	C	144	PRO
1	a	476	TYR
1	a	589	GLU
1	c	144	PRO
1	A	590	PRO
1	C	305	MET
1	a	590	PRO
1	c	305	MET
1	C	146	LYS
1	c	146	LYS
5	m	18	ASN
1	A	187	ALA
1	A	309	LYS
1	a	187	ALA
1	a	309	LYS
1	C	145	GLY
1	c	145	GLY
1	C	477	PRO
2	F	370	TYR
1	c	477	PRO
2	f	370	TYR
1	A	452	PHE
1	a	452	PHE

### 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	591/617 (95%)	-0.42	8 (1%) 78 71	153, 336, 460, 561	0
1	B	598/617 (96%)	-0.53	2 (0%) 94 92	112, 322, 468, 647	0
1	C	589/617 (95%)	-0.33	21 (3%) 46 44	148, 325, 484, 591	0
1	a	591/617 (95%)	-0.43	6 (1%) 84 79	155, 335, 460, 557	0
1	b	598/617 (96%)	-0.53	2 (0%) 94 92	109, 321, 465, 650	0
1	c	589/617 (95%)	-0.38	9 (1%) 76 70	146, 323, 481, 593	0
2	D	457/517 (88%)	-0.56	2 (0%) 93 90	93, 267, 414, 596	0
2	E	453/517 (87%)	-0.51	2 (0%) 93 90	149, 285, 407, 560	0
2	F	447/517 (86%)	-0.45	6 (1%) 79 73	138, 312, 463, 552	0
2	d	456/517 (88%)	-0.61	0 100 100	91, 265, 408, 553	0
2	e	453/517 (87%)	-0.46	4 (0%) 85 81	145, 285, 408, 566	0
2	f	449/517 (86%)	-0.38	10 (2%) 65 61	137, 313, 467, 570	0
3	H	445/478 (93%)	-0.82	0 100 100	85, 192, 339, 469	0
3	h	445/478 (93%)	-0.83	0 100 100	79, 193, 337, 470	0
4	J	104/122 (85%)	-0.72	0 100 100	140, 258, 401, 458	0
4	L	88/122 (72%)	-0.63	0 100 100	281, 427, 520, 540	0
4	N	81/122 (66%)	-0.51	0 100 100	244, 400, 519, 569	0
4	j	104/122 (85%)	-0.74	1 (0%) 84 79	140, 260, 398, 459	0
4	l	68/122 (55%)	-0.48	0 100 100	282, 414, 487, 535	0
4	n	105/122 (86%)	-0.31	0 100 100	229, 409, 525, 572	0
5	I	216/233 (92%)	-0.22	13 (6%) 25 26	103, 383, 522, 578	0
5	K	203/233 (87%)	-0.56	0 100 100	255, 380, 542, 600	0
5	M	203/233 (87%)	-0.20	3 (1%) 76 70	235, 422, 520, 578	0
5	i	216/233 (92%)	-0.35	5 (2%) 64 59	99, 382, 522, 573	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
5	k	178/233 (76%)	-0.29	3 (1%) 73 67	254, 366, 478, 548	0
5	m	208/233 (89%)	-0.33	3 (1%) 78 71	239, 415, 520, 577	0
6	G	223/256 (87%)	-0.58	1 (0%) 93 90	114, 325, 538, 586	0
6	g	212/256 (82%)	-0.65	2 (0%) 85 81	112, 316, 539, 581	0
7	O	115/118 (97%)	-0.40	0 100 100	260, 414, 524, 579	0
7	o	115/118 (97%)	-0.04	5 (4%) 39 37	260, 416, 526, 577	0
All	All	9600/10638 (90%)	-0.48	108 (1%) 82 77	79, 317, 487, 650	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	e	206	GLU	7.3
2	f	211	VAL	6.5
5	m	187	GLY	5.3
5	I	138	ILE	5.2
1	A	88	ARG	5.1
5	M	186	GLY	4.9
1	b	66	GLY	4.7
1	C	180	ARG	4.7
1	C	575	THR	4.6
5	M	187	GLY	4.6
1	C	181	GLY	4.6
5	I	137	ALA	4.2
1	a	148	GLN	3.8
1	c	259	PHE	3.7
5	I	95	SER	3.6
5	I	191	SER	3.6
5	i	187	GLY	3.5
1	C	153	ILE	3.3
2	e	207	ASN	3.3
2	f	127	PHE	3.2
2	F	424	ALA	3.2
1	C	30	SER	3.2
5	i	186	GLY	3.2
5	I	93	GLU	3.1
1	C	152	HIS	3.0
1	A	462	SER	3.0
5	I	139	VAL	3.0
2	e	395	ASP	3.0
2	f	240	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
7	o	9	ALA	3.0
1	a	88	ARG	3.0
2	F	192	GLY	3.0
2	e	396	HIS	3.0
5	k	187	GLY	3.0
2	f	213	ALA	2.9
7	o	67	LEU	2.9
2	f	239	SER	2.9
2	F	126	VAL	2.8
1	a	80	LEU	2.8
5	m	198	GLU	2.8
1	c	589	GLU	2.8
1	C	318	LEU	2.8
1	C	590	PRO	2.8
2	E	33	GLY	2.7
1	c	281	TYR	2.7
1	A	70	THR	2.7
6	g	87	VAL	2.7
1	C	258	ALA	2.7
1	a	99	PRO	2.7
1	C	574	SER	2.7
1	C	259	PHE	2.7
2	f	424	ALA	2.7
1	a	159	TYR	2.6
4	j	102	VAL	2.6
5	m	188	VAL	2.6
1	c	280	ILE	2.6
5	I	198	GLU	2.6
2	F	127	PHE	2.6
1	c	153	ILE	2.6
1	C	251	GLY	2.6
7	o	85	THR	2.5
1	c	590	PRO	2.5
2	f	128	ALA	2.5
2	F	30	THR	2.5
5	M	196	LYS	2.5
2	D	207	ASN	2.5
7	o	86	ASN	2.5
1	A	99	PRO	2.5
2	E	300	GLY	2.5
1	A	191	GLU	2.4
1	C	77	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	c	279	ILE	2.4
1	B	409	GLY	2.4
1	A	566	ALA	2.4
2	f	126	VAL	2.3
2	f	398	ASP	2.3
5	I	173	VAL	2.3
1	A	207	LYS	2.3
7	o	10	VAL	2.3
1	c	258	ALA	2.3
1	B	260	GLY	2.3
1	a	160	GLY	2.3
5	i	191	SER	2.3
1	C	78	ALA	2.3
1	b	99	PRO	2.3
5	I	94	GLN	2.3
1	C	28	ILE	2.2
5	k	126	VAL	2.2
5	i	141	ALA	2.2
2	f	205	GLU	2.2
6	g	84	GLN	2.2
1	C	353	MET	2.1
1	A	89	THR	2.1
1	C	261	CYS	2.1
1	C	317	THR	2.1
1	C	304	GLU	2.1
5	I	98	GLY	2.1
2	F	423	GLU	2.1
6	G	78	ASN	2.1
1	c	282	VAL	2.1
5	k	125	ILE	2.1
2	D	239	SER	2.1
5	I	141	ALA	2.1
5	i	99	ILE	2.1
5	I	140	LYS	2.1
1	C	31	VAL	2.0
1	C	123	ILE	2.0
5	I	172	ILE	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.