



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 01:37 PM EDT

PDB ID : 5BW9  
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 : unknown  
Resolution : 7.00 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:

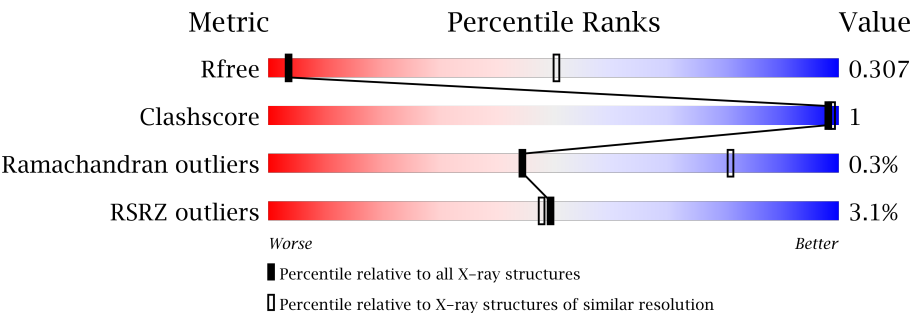
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.00 Å.

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






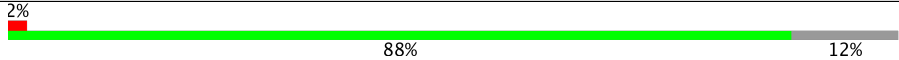
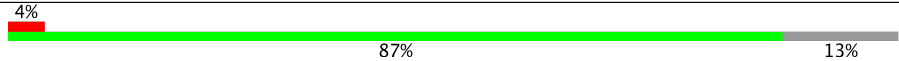
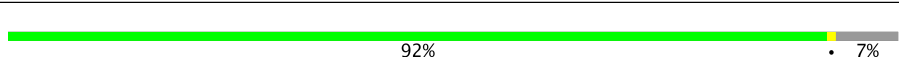
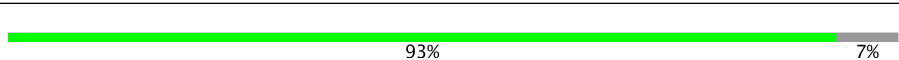
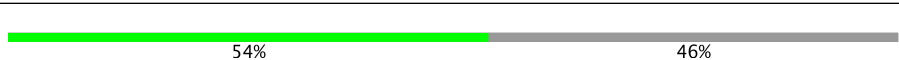
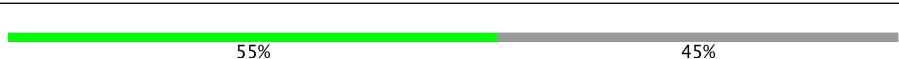
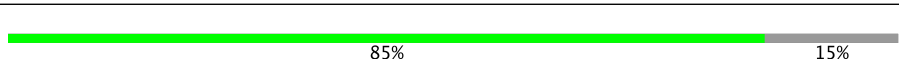



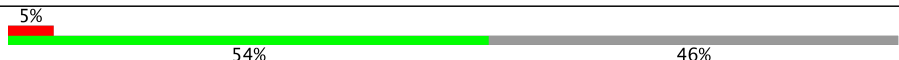
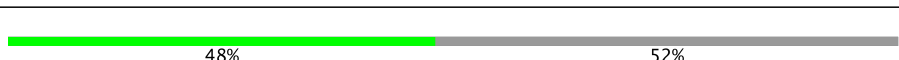
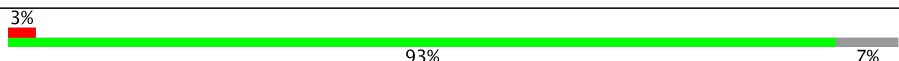
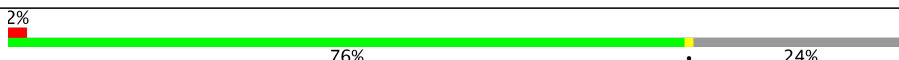
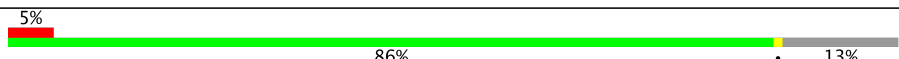
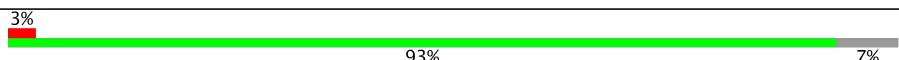
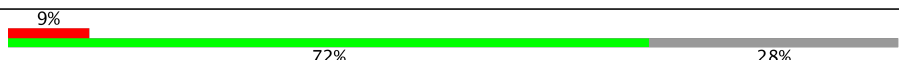
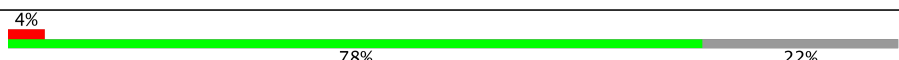
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	100719	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
RSRZ outliers	101464	1003 (10.00-3.72)

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	<div><div>6%</div><div>92%</div><div>• •</div></div>
1	B	617	<div><div>5%</div><div>93%</div><div>• •</div></div>
1	C	617	<div><div>2%</div><div>93%</div><div>• 5%</div></div>
1	a	617	<div><div>8%</div><div>95%</div><div>• •</div></div>
1	b	617	<div><div>3%</div><div>95%</div><div>5%</div></div>
1	c	617	<div><div>2%</div><div>94%</div><div>• 5%</div></div>
2	D	517	<div><div>•%</div><div>86%</div><div>• 12%</div></div>

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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	G	256	
4	g	256	
5	J	122	
5	L	122	
5	N	122	
5	j	122	
5	l	122	
5	n	122	
6	I	233	
6	K	233	
6	M	233	
6	i	233	
6	k	233	
6	m	233	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 44760 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	594	Total	C	N	O	0	0	0
			2920	1732	594	594			
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	589	Total	C	N	O	0	0	0
			2895	1717	589	589			
1	c	586	Total	C	N	O	0	0	0
			2880	1708	586	586			

- 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	449	Total	C	N	O	0	0	0
			2211	1313	449	449			
2	d	460	Total	C	N	O	0	0	0
			2265	1345	460	460			
2	e	456	Total	C	N	O	0	0	0
			2245	1333	456	456			
2	f	449	Total	C	N	O	0	0	0
			2212	1314	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	444	Total	C	N	O	0	0	0
			2208	1320	444	444			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	139	Total	C	N	O	0	0	0
			691	413	139	139			
4	g	141	Total	C	N	O	0	0	0
			701	419	141	141			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	104	Total	C	N	O	0	0	0
			514	306	104	104			
5	L	68	Total	C	N	O	0	0	0
			335	199	68	68			
5	N	81	Total	C	N	O	0	0	0
			400	238	81	81			
5	j	101	Total	C	N	O	0	0	0
			499	297	101	101			
5	l	66	Total	C	N	O	0	0	0
			325	193	66	66			
5	n	58	Total	C	N	O	0	0	0
			288	172	58	58			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
n	1	LYS	-	expression tag	UNP P48836

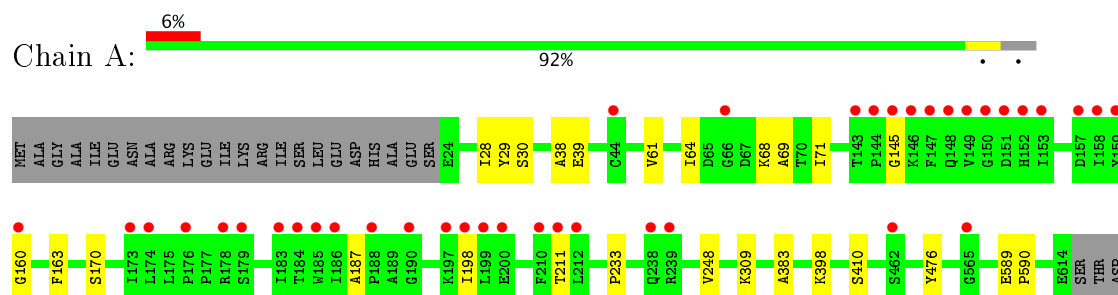
- Molecule 6 is a protein called V-type proton ATPase subunit E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	216	Total	C	N	O	0	0	0
			1073	641	216	216			
6	K	178	Total	C	N	O	0	0	0
			883	527	178	178			
6	M	203	Total	C	N	O	0	0	0
			1008	602	203	203			
6	i	217	Total	C	N	O	0	0	0
			1078	644	217	217			
6	k	168	Total	C	N	O	0	0	0
			833	497	168	168			
6	m	181	Total	C	N	O	0	0	0
			898	536	181	181			

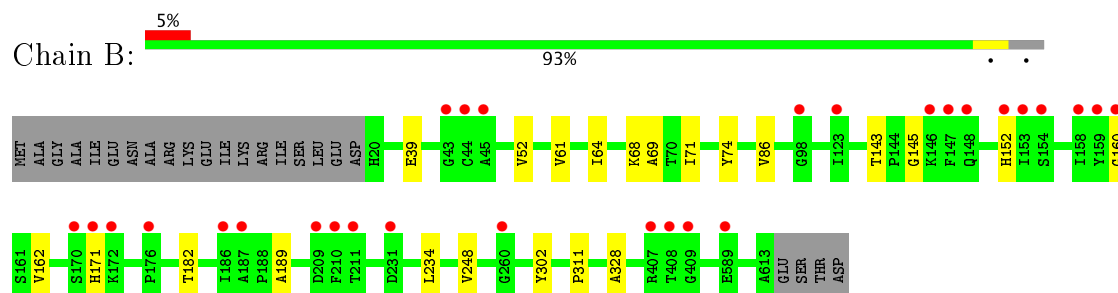
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

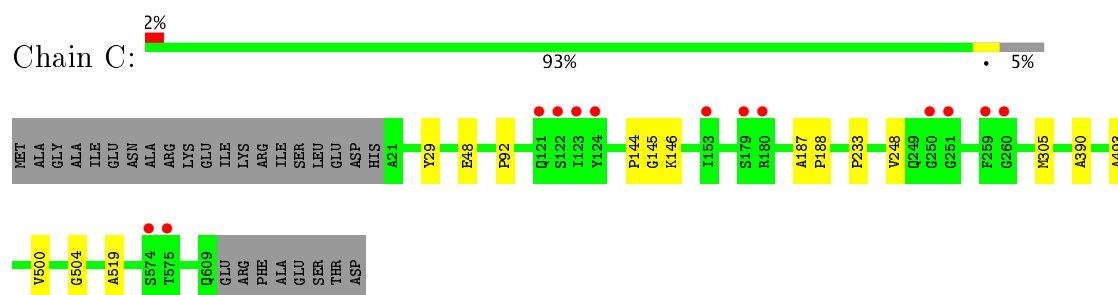
- Molecule 1: V-type proton ATPase catalytic subunit A



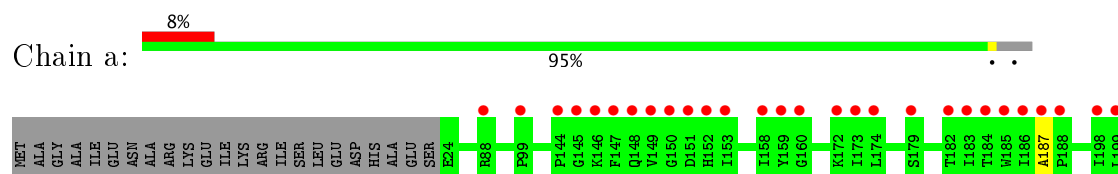
- Molecule 1: V-type proton ATPase catalytic subunit A

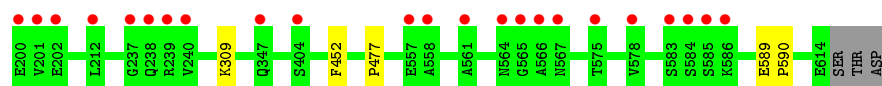


- Molecule 1: V-type proton ATPase catalytic subunit A

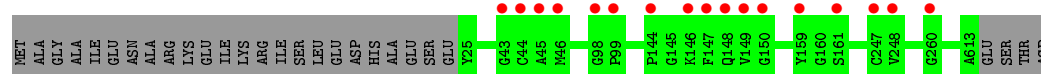


- Molecule 1: V-type proton ATPase catalytic subunit A

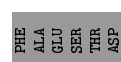
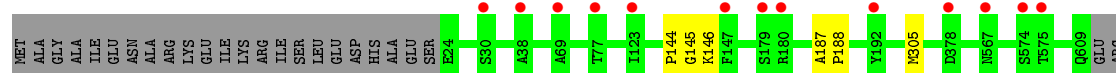




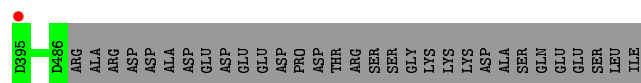
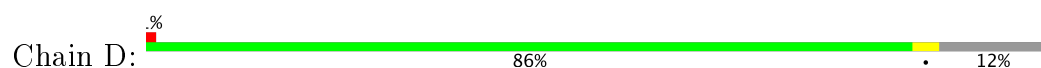
- Molecule 1: V-type proton ATPase catalytic subunit A



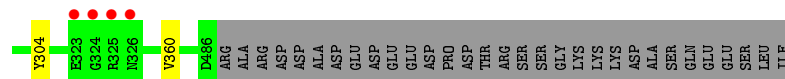
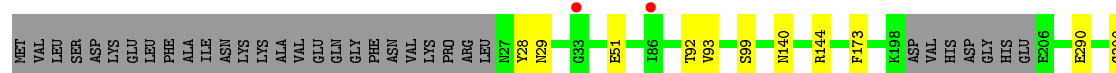
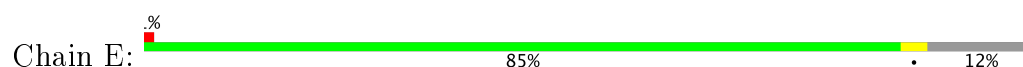
- Molecule 1: V-type proton ATPase catalytic subunit A



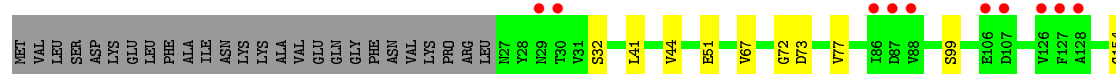
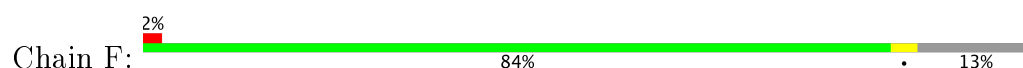
- Molecule 2: V-type proton ATPase subunit B

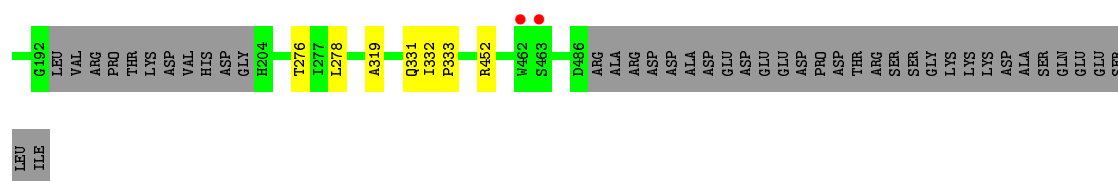


- Molecule 2: V-type proton ATPase subunit B

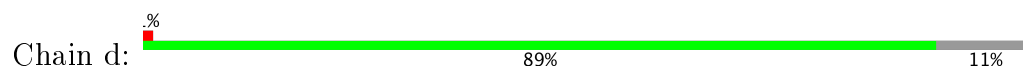


- Molecule 2: V-type proton ATPase subunit B

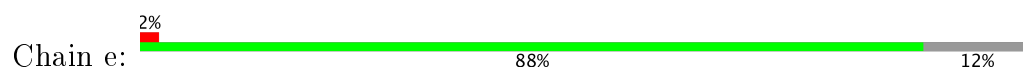




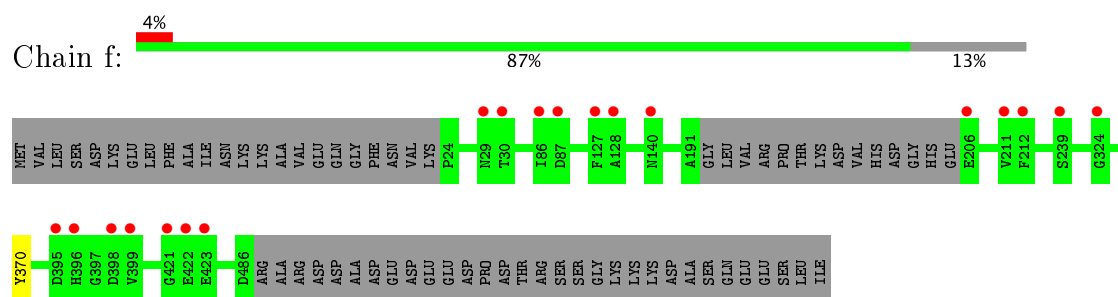
- Molecule 2: V-type proton ATPase subunit B



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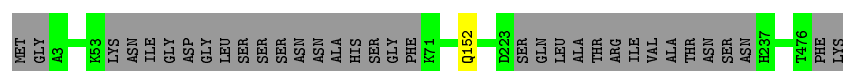
- Molecule 3: V-type proton ATPase subunit H



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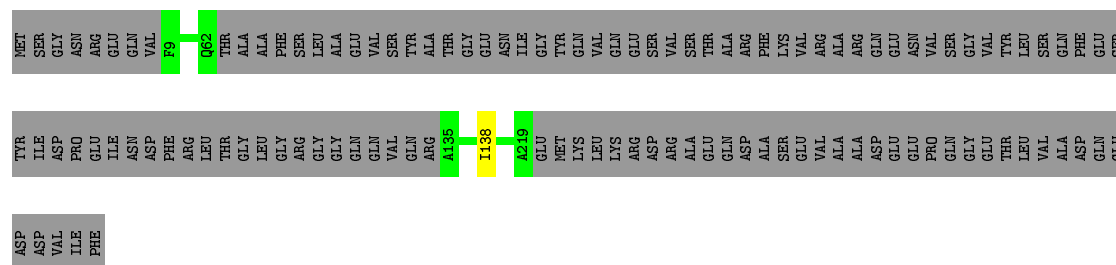


- Molecule 3: V-type proton ATPase subunit H



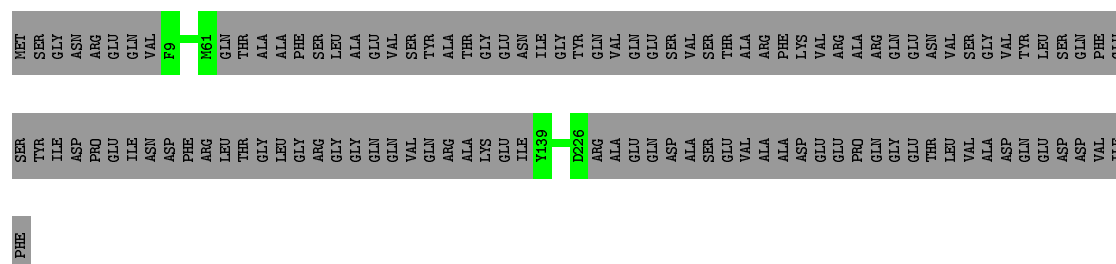
- Molecule 4: V-type proton ATPase subunit D

Chain G:  54% 46%



- Molecule 4: V-type proton ATPase subunit D

Chain g:  55% 45%



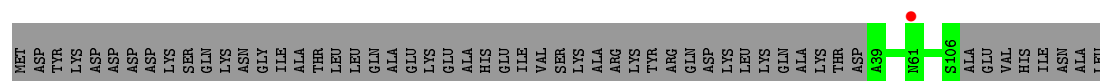
- Molecule 5: V-type proton ATPase subunit G

Chain J:  85% 15%



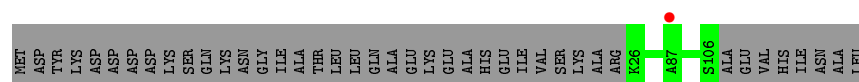
- Molecule 5: V-type proton ATPase subunit G

Chain L: 

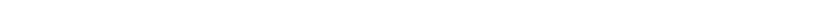


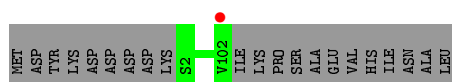
- Molecule 5: V-type proton ATPase subunit G

Chain N:  66% 34%

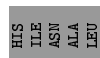
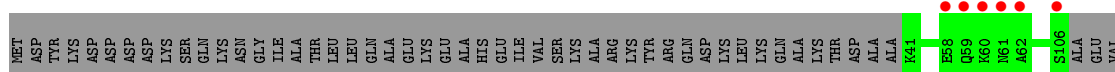


- Molecule 5: V-type proton ATPase subunit G

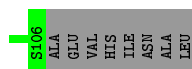
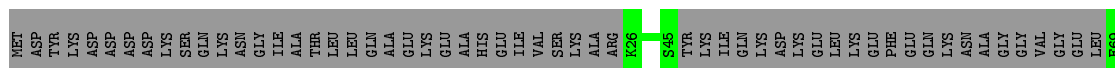
Chain j:  83% 17%



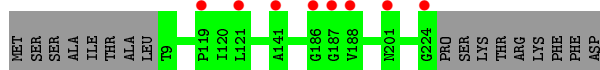
- Molecule 5: V-type proton ATPase subunit G



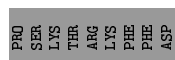
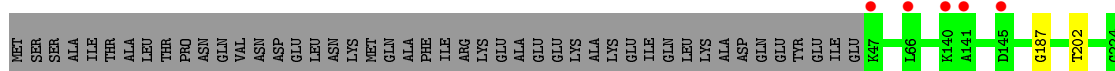
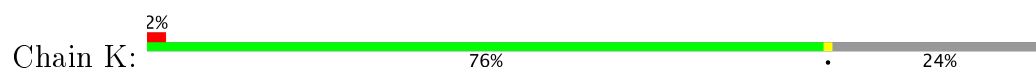
- Molecule 5: V-type proton ATPase subunit G



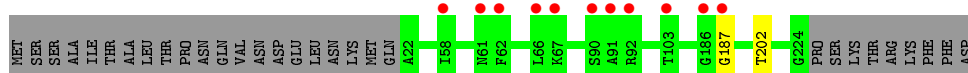
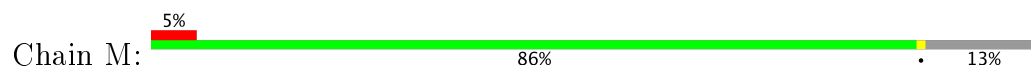
- Molecule 6: V-type proton ATPase subunit E



- Molecule 6: V-type proton ATPase subunit E

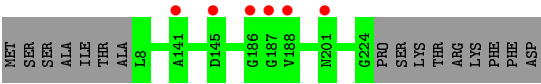


- Molecule 6: V-type proton ATPase subunit E

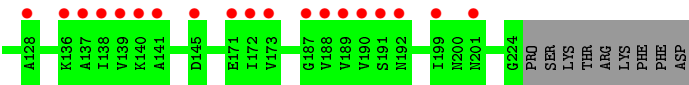
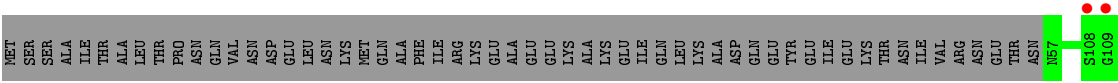


- Molecule 6: V-type proton ATPase subunit E

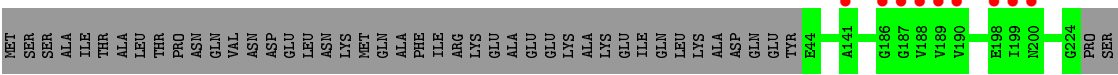
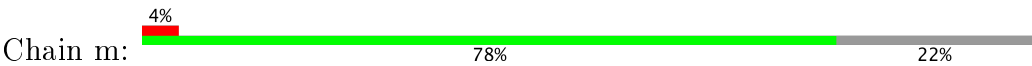




● Molecule 6: V-type proton ATPase subunit E



● Molecule 6: V-type proton ATPase subunit E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	468.48Å 159.74Å 245.04Å 90.00° 113.88° 90.00°	Depositor
Resolution (Å)	40.10 – 7.00 40.10 – 7.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.10-7.00) 90.4 (40.10-7.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 7.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1957)	Depositor
R, $R_{free}$	0.260 , 0.309 0.255 , 0.307	Depositor DCC
$R_{free}$ test set	1808 reflections (7.63%)	DCC
Wilson B-factor (Å <sup>2</sup> )	328.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	1.27 , 6425.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	44760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	290.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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	0.18	0/2904	0.31	0/4034
1	B	0.18	0/2919	0.31	0/4055
1	C	0.19	0/2894	0.32	0/4020
1	a	0.18	0/2904	0.31	0/4034
1	b	0.18	0/2894	0.30	0/4020
1	c	0.18	0/2879	0.32	0/3999
2	D	0.18	0/2248	0.30	0/3123
2	E	0.18	0/2229	0.30	0/3097
2	F	0.18	0/2209	0.30	0/3069
2	d	0.18	0/2264	0.30	0/3147
2	e	0.18	0/2243	0.30	0/3116
2	f	0.18	0/2210	0.30	0/3071
3	H	0.19	0/2209	0.32	0/3080
3	h	0.19	0/2205	0.32	0/3075
4	G	0.18	0/689	0.31	0/959
4	g	0.18	0/699	0.30	0/973
5	J	0.18	0/513	0.30	0/713
5	L	0.19	0/334	0.30	0/463
5	N	0.18	0/399	0.30	0/554
5	j	0.18	0/498	0.30	0/692
5	l	0.19	0/324	0.30	0/449
5	n	0.18	0/286	0.29	0/396
6	I	0.18	0/1072	0.29	0/1495
6	K	0.18	0/882	0.29	0/1229
6	M	0.18	0/1007	0.28	0/1404
6	i	0.18	0/1077	0.29	0/1502
6	k	0.18	0/832	0.28	0/1159
6	m	0.18	0/897	0.28	0/1250
All	All	0.18	0/44720	0.31	0/62178

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	12	0
1	B	2920	0	1348	11	0
1	C	2895	0	1335	6	0
1	a	2905	0	1339	0	0
1	b	2895	0	1335	0	0
1	c	2880	0	1326	0	0
2	D	2250	0	1015	8	0
2	E	2231	0	1006	7	0
2	F	2211	0	999	9	0
2	d	2265	0	1022	0	0
2	e	2245	0	1013	0	0
2	f	2212	0	998	0	0
3	H	2212	0	951	2	0
3	h	2208	0	948	0	0
4	G	691	0	311	0	0
4	g	701	0	312	0	0
5	J	514	0	248	0	0
5	L	335	0	160	0	0
5	N	400	0	189	0	0
5	j	499	0	243	0	0
5	l	325	0	150	0	0
5	n	288	0	136	0	0
6	I	1073	0	481	0	0
6	K	883	0	394	1	0
6	M	1008	0	456	1	0
6	i	1078	0	483	0	0
6	k	833	0	374	0	0
6	m	898	0	400	0	0
All	All	44760	0	20311	52	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 (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:352:GLU:HA	3:H:355:SER:HA	1.72	0.72
2:D:28:TYR:H	2:D:93:VAL:H	1.39	0.69
3:H:353:LEU:H	3:H:354:THR:C	1.97	0.68
1:A:383:ALA:HB1	2:E:290:GLU:HA	1.95	0.63
2:D:31:VAL:HA	2:D:41:LEU:HA	1.80	0.63
6:M:187:GLY:HA3	6:M:202:THR:HA	1.80	0.63
1:C:390:ALA:HB1	2:D:245:ALA:HB1	1.80	0.62
6:K:187:GLY:HA3	6:K:202:THR:HA	1.85	0.59
1:A:29:TYR:O	2:D:72:GLY:N	2.37	0.57
2:F:51:GLU:HA	2:F:99:SER:HA	1.87	0.56
2:F:319:ALA:HB2	2:F:331:GLN:H	1.71	0.56
1:B:302:TYR:HA	1:B:311:PRO:HA	1.88	0.55
1:A:145:GLY:H	1:A:160:GLY:HA2	1.73	0.54
1:A:28:ILE:HA	1:A:38:ALA:HA	1.90	0.54
1:B:234:LEU:H	1:B:248:VAL:HA	1.73	0.54
1:B:145:GLY:H	1:B:160:GLY:HA2	1.73	0.54
1:A:233:PRO:HA	1:A:248:VAL:HA	1.90	0.54
1:C:48:GLU:HA	1:C:92:PRO:HA	1.89	0.53
1:B:64:ILE:HA	1:B:69:ALA:HA	1.91	0.53
2:E:300:GLY:N	2:E:304:TYR:O	2.34	0.53
1:B:52:VAL:HA	1:B:86:VAL:HA	1.91	0.53
2:F:154:GLY:O	2:F:452:ARG:N	2.40	0.51
2:D:165:ALA:HB2	2:D:386:ALA:HB2	1.93	0.50
2:F:32:SER:H	2:F:41:LEU:HA	1.77	0.49
1:A:39:GLU:HA	1:A:68:LYS:HA	1.94	0.49
1:B:39:GLU:HA	1:B:68:LYS:HA	1.95	0.49
2:E:51:GLU:HA	2:E:99:SER:HA	1.95	0.48
1:B:152:HIS:HA	1:B:182:THR:HA	1.96	0.48
1:B:74:TYR:HA	1:B:328:ALA:HB3	1.96	0.48
1:A:30:SER:HA	2:D:71:ARG:HA	1.96	0.48
2:F:44:VAL:N	2:F:73:ASP:O	2.37	0.47
1:B:61:VAL:HA	1:B:71:ILE:HA	1.97	0.46
2:F:278:LEU:H	2:F:333:PRO:HA	1.81	0.46
1:A:61:VAL:HA	1:A:71:ILE:HA	1.99	0.45
1:C:493:ALA:HB1	1:C:519:ALA:HB2	1.99	0.44
1:C:500:VAL:O	1:C:504:GLY:N	2.48	0.44
1:C:29:TYR:O	2:F:72:GLY:N	2.44	0.44
2:E:28:TYR:N	2:E:93:VAL:O	2.52	0.43
2:E:29:ASN:HA	2:E:92:THR:HA	1.99	0.43
1:A:398:LYS:HA	1:A:410:SER:HA	2.01	0.43
2:E:140:ASN:O	2:E:144:ARG:N	2.52	0.43
1:A:163:PHE:HA	1:A:170:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:PRO:HA	1:C:248:VAL:HA	2.01	0.43
1:A:64:ILE:HA	1:A:69:ALA:HA	2.02	0.42
1:B:143:THR:HA	1:B:189:ALA:HB1	2.01	0.42
1:A:198:ILE:H	1:A:211:THR:HA	1.85	0.42
1:B:162:VAL:O	1:B:171:HIS:N	2.40	0.42
2:D:214:ALA:HB3	2:D:242:LEU:HA	2.02	0.41
2:F:67:VAL:HA	2:F:77:VAL:HA	2.02	0.41
2:E:173:PHE:O	2:E:360:VAL:N	2.49	0.41
2:D:167:GLY:HA2	2:D:320:GLY:HA2	2.03	0.41
2:F:276:THR:O	2:F:332:ILE:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	550 (93%)	34 (6%)	5 (1%)	22	67
1	B	592/617 (96%)	557 (94%)	35 (6%)	0	100	100
1	C	587/617 (95%)	548 (93%)	33 (6%)	6 (1%)	18	61
1	a	589/617 (96%)	550 (93%)	33 (6%)	6 (1%)	18	61
1	b	587/617 (95%)	552 (94%)	35 (6%)	0	100	100
1	c	584/617 (95%)	545 (93%)	33 (6%)	6 (1%)	18	61
2	D	453/517 (88%)	425 (94%)	28 (6%)	0	100	100
2	E	449/517 (87%)	428 (95%)	21 (5%)	0	100	100
2	F	445/517 (86%)	420 (94%)	25 (6%)	0	100	100
2	d	458/517 (89%)	429 (94%)	28 (6%)	1 (0%)	51	84
2	e	452/517 (87%)	431 (95%)	21 (5%)	0	100	100
2	f	445/517 (86%)	421 (95%)	23 (5%)	1 (0%)	51	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	439/478 (92%)	412 (94%)	27 (6%)	0	100	100
3	h	438/478 (92%)	412 (94%)	25 (6%)	1 (0%)	51	84
4	G	135/256 (53%)	130 (96%)	4 (3%)	1 (1%)	25	68
4	g	137/256 (54%)	134 (98%)	3 (2%)	0	100	100
5	J	102/122 (84%)	100 (98%)	2 (2%)	0	100	100
5	L	66/122 (54%)	65 (98%)	1 (2%)	0	100	100
5	N	79/122 (65%)	75 (95%)	4 (5%)	0	100	100
5	j	99/122 (81%)	97 (98%)	2 (2%)	0	100	100
5	l	64/122 (52%)	63 (98%)	1 (2%)	0	100	100
5	n	54/122 (44%)	51 (94%)	3 (6%)	0	100	100
6	I	214/233 (92%)	213 (100%)	1 (0%)	0	100	100
6	K	176/233 (76%)	175 (99%)	1 (1%)	0	100	100
6	M	201/233 (86%)	200 (100%)	1 (0%)	0	100	100
6	i	215/233 (92%)	213 (99%)	2 (1%)	0	100	100
6	k	166/233 (71%)	165 (99%)	1 (1%)	0	100	100
6	m	179/233 (77%)	178 (99%)	1 (1%)	0	100	100
All	All	8994/10402 (86%)	8539 (95%)	428 (5%)	27 (0%)	44	81

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	ALA
1	C	188	PRO
4	G	138	ILE
1	c	187	ALA
1	c	188	PRO
1	A	589	GLU
1	C	144	PRO
1	a	589	GLU
1	c	144	PRO
1	A	590	PRO
1	C	305	MET
3	h	152	GLN
1	a	590	PRO
1	c	305	MET
2	d	200	VAL

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Mol	Chain	Res	Type
1	A	187	ALA
1	A	309	LYS
1	A	476	TYR
1	a	187	ALA
1	a	309	LYS
1	C	145	GLY
1	C	146	LYS
1	c	145	GLY
1	c	146	LYS
1	a	477	PRO
1	a	452	PHE
2	f	370	TYR

### 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

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%)	-0.02	39 (6%)	19	23	126, 311, 475, 652	0
1	B	594/617 (96%)	-0.14	29 (4%)	30	33	107, 290, 447, 594	0
1	C	589/617 (95%)	-0.15	13 (2%)	62	60	111, 281, 475, 610	0
1	a	591/617 (95%)	0.24	51 (8%)	11	18	126, 314, 475, 658	0
1	b	589/617 (95%)	-0.15	17 (2%)	52	50	107, 292, 450, 597	0
1	c	586/617 (94%)	-0.15	13 (2%)	62	60	111, 282, 473, 614	0
2	D	457/517 (88%)	-0.47	3 (0%)	87	84	92, 239, 384, 587	0
2	E	453/517 (87%)	-0.31	6 (1%)	77	72	124, 258, 413, 663	0
2	F	449/517 (86%)	-0.28	12 (2%)	55	52	146, 287, 414, 584	0
2	d	460/517 (88%)	-0.33	5 (1%)	80	76	94, 241, 390, 586	0
2	e	456/517 (88%)	-0.30	8 (1%)	69	65	125, 258, 415, 667	0
2	f	449/517 (86%)	-0.18	19 (4%)	37	37	145, 288, 416, 573	0
3	H	445/478 (93%)	-0.83	0	100	100	65, 163, 317, 625	0
3	h	444/478 (92%)	-0.79	0	100	100	61, 164, 321, 631	0
4	G	139/256 (54%)	-0.48	0	100	100	93, 212, 488, 554	0
4	g	141/256 (55%)	-0.85	0	100	100	97, 213, 493, 560	0
5	J	104/122 (85%)	-0.51	0	100	100	154, 290, 427, 498	0
5	L	68/122 (55%)	-0.03	1 (1%)	74	69	283, 418, 525, 566	0
5	N	81/122 (66%)	0.02	1 (1%)	79	74	200, 450, 574, 740	0
5	j	101/122 (82%)	-0.42	1 (0%)	82	78	151, 282, 419, 497	0
5	l	66/122 (54%)	0.26	6 (9%)	10	17	279, 422, 522, 566	0
5	n	58/122 (47%)	-0.42	0	100	100	200, 441, 509, 541	0
6	I	216/233 (92%)	-0.01	8 (3%)	42	42	112, 345, 497, 643	0
6	K	178/233 (76%)	-0.02	5 (2%)	53	51	186, 344, 491, 599	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
6	M	203/233 (87%)	0.45	11 (5%) 26 30	200, 410, 571, 626	0
6	i	217/233 (93%)	0.01	6 (2%) 53 51	91, 345, 511, 638	0
6	k	168/233 (72%)	0.56	21 (12%) 4 12	187, 331, 466, 514	0
6	m	181/233 (77%)	0.08	9 (4%) 30 32	200, 402, 542, 587	0
All	All	9074/10402 (87%)	-0.21	284 (3%) 49 48	61, 281, 479, 740	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	149	VAL	17.1
1	a	148	GLN	15.9
1	a	184	THR	10.8
1	a	150	GLY	9.9
1	a	185	TRP	9.4
1	a	159	TYR	7.5
1	a	151	ASP	7.5
1	A	148	GLN	7.2
1	a	183	ILE	7.2
1	a	565	GLY	7.1
1	a	186	ILE	6.8
6	I	187	GLY	6.6
6	i	187	GLY	6.3
1	A	151	ASP	6.1
1	C	123	ILE	6.0
1	a	566	ALA	6.0
1	A	147	PHE	5.9
6	I	186	GLY	5.5
1	a	173	ILE	5.5
6	M	187	GLY	5.5
1	A	149	VAL	5.4
1	A	159	TYR	5.4
1	a	147	PHE	5.4
1	a	160	GLY	5.3
6	i	186	GLY	5.3
1	a	158	ILE	5.3
1	A	144	PRO	5.2
6	k	137	ALA	5.0
1	a	564	ASN	5.0
6	k	171	GLU	4.9
1	a	188	PRO	4.9
1	A	211	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	146	LYS	4.7
6	M	186	GLY	4.7
2	F	87	ASP	4.6
5	l	61	ASN	4.6
1	a	187	ALA	4.5
1	a	146	LYS	4.5
1	C	122	SER	4.5
1	B	147	PHE	4.5
1	C	259	PHE	4.5
1	A	152	HIS	4.5
1	a	200	GLU	4.4
6	m	187	GLY	4.2
2	f	395	ASP	4.1
6	k	191	SER	4.0
6	k	173	VAL	4.0
2	f	206	GLU	4.0
1	A	150	GLY	4.0
6	k	187	GLY	4.0
1	A	173	ILE	3.9
1	B	408	THR	3.9
1	C	574	SER	3.9
6	k	190	VAL	3.8
2	F	86	ILE	3.8
1	A	190	GLY	3.8
1	b	99	PRO	3.8
1	A	158	ILE	3.7
1	b	44	CYS	3.7
6	k	138	ILE	3.7
1	a	586	LYS	3.7
1	b	149	VAL	3.6
2	f	211	VAL	3.6
1	a	585	SER	3.6
6	i	188	VAL	3.6
1	A	145	GLY	3.6
1	B	146	LYS	3.5
6	k	172	ILE	3.5
1	C	251	GLY	3.5
1	A	185	TRP	3.5
6	m	198	GLU	3.5
1	B	44	CYS	3.5
2	f	87	ASP	3.5
1	A	210	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	b	45	ALA	3.4
6	m	199	ILE	3.4
2	E	325	ARG	3.4
1	C	180	ARG	3.4
2	F	29	ASN	3.4
2	f	239	SER	3.3
1	a	198	ILE	3.3
2	f	422	GLU	3.3
2	E	324	GLY	3.3
1	A	198	ILE	3.3
1	c	575	THR	3.3
2	e	129	GLU	3.3
1	A	160	GLY	3.3
1	b	148	GLN	3.3
6	m	186	GLY	3.2
1	B	159	TYR	3.2
1	B	148	GLN	3.2
1	a	182	THR	3.1
6	K	141	ALA	3.1
6	m	141	ALA	3.1
1	A	197	LYS	3.1
1	a	239	ARG	3.1
1	A	184	THR	3.1
1	B	153	ILE	3.1
1	B	209	ASP	3.0
1	B	45	ALA	3.0
2	f	127	PHE	3.0
2	e	105	SER	3.0
1	A	212	LEU	3.0
6	i	141	ALA	3.0
2	f	86	ILE	3.0
6	k	188	VAL	3.0
1	a	238	GLN	3.0
1	a	202	GLU	3.0
2	F	127	PHE	3.0
1	b	161	SER	3.0
5	l	106	SER	2.9
6	M	91	ALA	2.9
6	k	141	ALA	2.9
1	A	174	LEU	2.9
1	A	186	ILE	2.9
1	B	231	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	d	395	ASP	2.9
1	a	561	ALA	2.8
2	f	30	THR	2.8
6	k	201	ASN	2.8
1	C	124	TYR	2.8
1	c	192	TYR	2.8
5	j	102	VAL	2.8
2	e	106	GLU	2.8
1	b	147	PHE	2.8
6	k	199	ILE	2.8
1	c	180	ARG	2.8
1	a	212	LEU	2.8
1	c	123	ILE	2.7
2	F	126	VAL	2.7
1	b	43	GLY	2.7
6	m	188	VAL	2.7
1	A	153	ILE	2.7
1	c	567	ASN	2.7
1	a	144	PRO	2.7
2	f	423	GLU	2.7
2	f	29	ASN	2.7
6	k	192	ASN	2.7
1	a	179	SER	2.7
1	c	38	ALA	2.7
1	c	574	SER	2.7
1	a	145	GLY	2.7
2	d	398	ASP	2.7
5	l	58	GLU	2.7
1	b	98	GLY	2.7
5	l	59	GLN	2.7
1	a	557	GLU	2.7
1	b	150	GLY	2.7
1	a	152	HIS	2.6
6	I	141	ALA	2.6
1	B	160	GLY	2.6
1	a	567	ASN	2.6
2	f	128	ALA	2.6
6	M	90	SER	2.6
1	a	347	GLN	2.6
1	A	183	ILE	2.6
2	E	323	GLU	2.6
1	a	558	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	e	323	GLU	2.5
2	F	107	ASP	2.5
1	A	462	SER	2.5
6	I	188	VAL	2.5
6	k	136	LYS	2.5
1	A	188	PRO	2.5
1	A	199	LEU	2.5
1	B	187	ALA	2.5
5	L	61	ASN	2.5
1	c	179	SER	2.5
6	K	140	LYS	2.5
1	b	248	VAL	2.5
2	F	88	VAL	2.5
1	A	157	ASP	2.5
1	C	121	GLN	2.5
1	a	240	VAL	2.4
1	A	239	ARG	2.4
1	c	147	PHE	2.4
2	f	398	ASP	2.4
1	a	237	GLY	2.4
6	k	109	GLY	2.4
1	a	201	VAL	2.4
2	F	462	TRP	2.4
2	e	324	GLY	2.4
6	k	189	VAL	2.4
5	l	60	LYS	2.4
2	D	199	ASP	2.4
1	B	43	GLY	2.4
6	M	61	ASN	2.4
1	B	409	GLY	2.4
6	m	190	VAL	2.4
1	B	176	PRO	2.4
1	b	247	CYS	2.4
1	a	583	SER	2.4
2	d	203	GLY	2.4
1	a	174	LEU	2.4
6	K	145	ASP	2.4
6	i	201	ASN	2.4
6	k	108	SER	2.4
2	F	30	THR	2.3
1	B	123	ILE	2.3
2	F	128	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	e	130	ASP	2.3
1	c	378	ASP	2.3
2	d	204	HIS	2.3
1	C	575	THR	2.3
1	A	176	PRO	2.3
1	C	250	GLY	2.3
1	a	172	LYS	2.3
1	c	77	THR	2.3
6	K	66	LEU	2.3
1	A	66	GLY	2.3
1	B	154	SER	2.3
1	a	88	ARG	2.3
2	E	326	ASN	2.3
6	k	145	ASP	2.3
6	M	58	ILE	2.3
2	D	395	ASP	2.3
1	B	260	GLY	2.3
1	A	179	SER	2.3
6	k	139	VAL	2.3
1	a	153	ILE	2.3
1	c	69	ALA	2.3
1	a	578	VAL	2.3
1	c	30	SER	2.2
1	B	158	ILE	2.2
1	A	565	GLY	2.2
2	E	86	ILE	2.2
2	F	106	GLU	2.2
6	i	145	ASP	2.2
6	m	200	ASN	2.2
5	N	87	ALA	2.2
2	E	33	GLY	2.2
6	M	66	LEU	2.2
6	M	67	LYS	2.2
1	A	200	GLU	2.2
1	B	589	GLU	2.2
2	f	212	PHE	2.2
1	b	260	GLY	2.2
6	I	119	PRO	2.2
1	A	178	ARG	2.2
1	C	179	SER	2.2
6	M	103	THR	2.2
2	D	207	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	a	584	SER	2.1
6	I	201	ASN	2.1
6	M	62	PHE	2.1
1	B	407	ARG	2.1
1	A	143	THR	2.1
6	k	140	LYS	2.1
6	m	189	VAL	2.1
1	A	44	CYS	2.1
2	f	396	HIS	2.1
1	B	172	LYS	2.1
1	a	575	THR	2.1
2	f	324	GLY	2.1
6	k	128	ALA	2.1
1	C	153	ILE	2.1
1	B	98	GLY	2.1
5	l	62	ALA	2.1
1	a	199	LEU	2.1
6	I	121	LEU	2.1
6	M	92	ARG	2.1
1	a	404	SER	2.1
2	e	205	GLU	2.1
2	f	399	VAL	2.1
1	B	211	THR	2.1
1	B	170	SER	2.1
2	F	463	SER	2.1
2	f	421	GLY	2.1
1	b	159	TYR	2.1
1	A	238	GLN	2.1
6	K	47	LYS	2.1
1	C	260	GLY	2.0
1	b	144	PRO	2.0
2	d	396	HIS	2.0
1	B	152	HIS	2.0
1	b	46	MET	2.0
1	a	99	PRO	2.0
1	b	146	LYS	2.0
1	B	171	HIS	2.0
2	f	140	ASN	2.0
6	I	224	GLY	2.0
1	B	186	ILE	2.0
1	B	210	PHE	2.0
2	e	410	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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.