wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2016 – 03:00 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	:	2015-06-06
Resolution	:	7.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

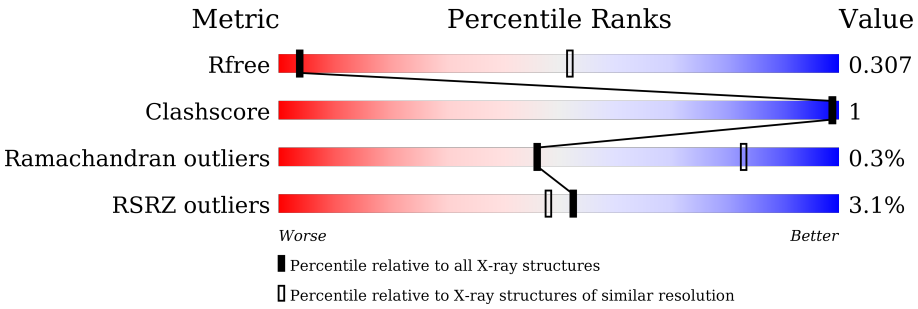
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (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_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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

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Mol	Chain	Length	Quality of chain
2	E	517	85% 12%
2	F	517	84% 13%
2	d	517	89% 11%
2	e	517	88% 12%
2	f	517	87% 13%
3	H	478	92% 7%
3	h	478	93% 7%
4	G	256	54% 46%
4	g	256	55% 45%
5	J	122	85% 15%
5	L	122	56% 44%
5	N	122	66% 34%
5	j	122	83% 17%
5	l	122	5% 54% 46%
5	n	122	48% 52%
6	I	233	93% 7%
6	K	233	76% 24%
6	M	233	5% 86% 13%
6	i	233	3% 93% 7%
6	k	233	9% 72% 28%
6	m	233	4% 78% 22%

2 Entry composition (i)

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 2212	C 1322	N 445	O 445	0	0	0
3	h	444	Total 2208	C 1320	N 444	O 444	0	0	0

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

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

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

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

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.

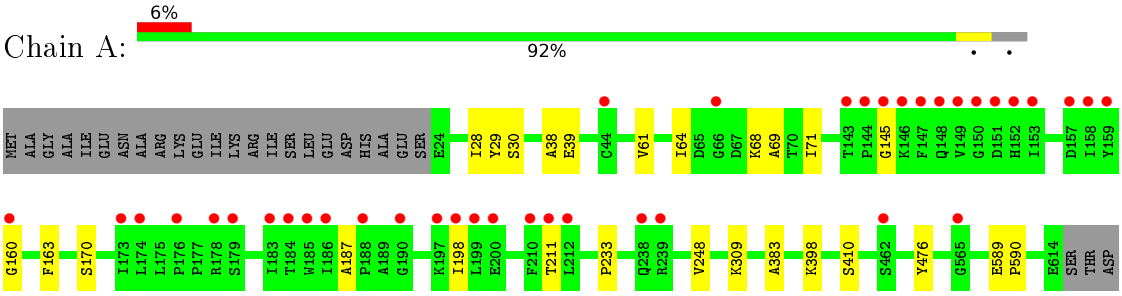
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	216	Total	C	N	O	0	0	0
			1073	641	216	216			
6	K	178	Total	C	N	O	0	0	0
			883	527	178	178			
6	M	203	Total	C	N	O	0	0	0
			1008	602	203	203			
6	i	217	Total	C	N	O	0	0	0
			1078	644	217	217			
6	k	168	Total	C	N	O	0	0	0
			833	497	168	168			
6	m	181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

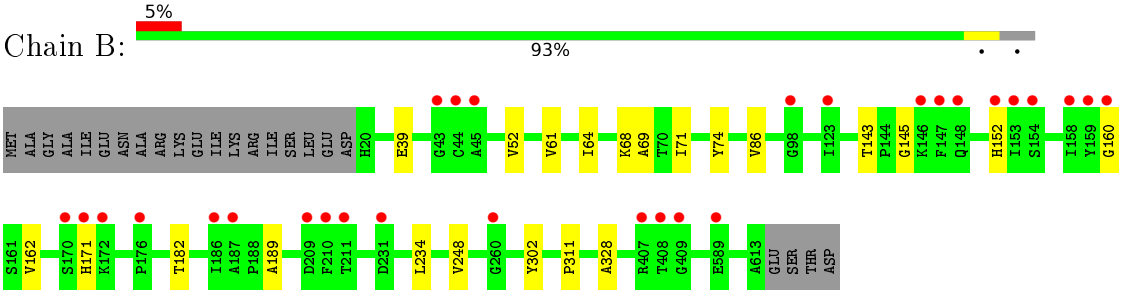
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain A:



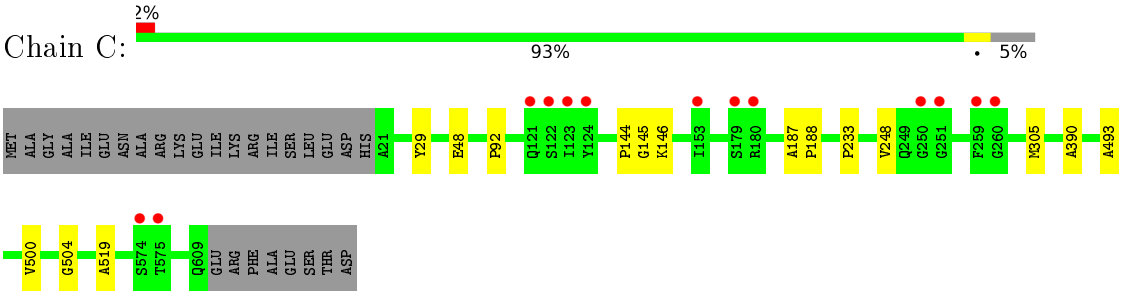
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain B:



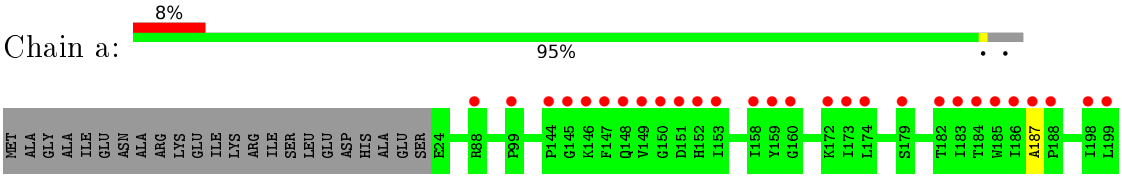
- Molecule 1: V-type proton ATPase catalytic subunit A

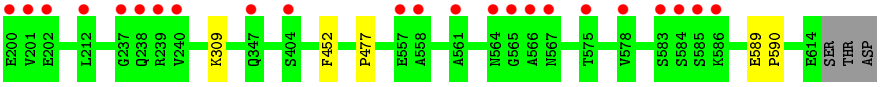
Chain C:



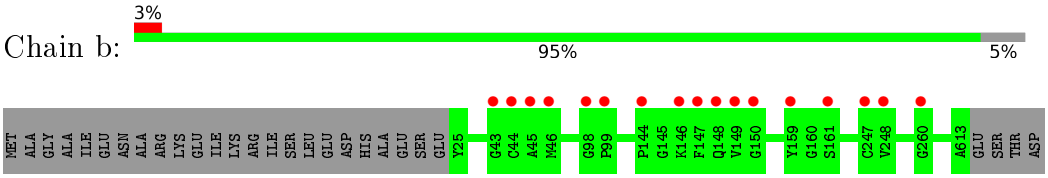
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain a:

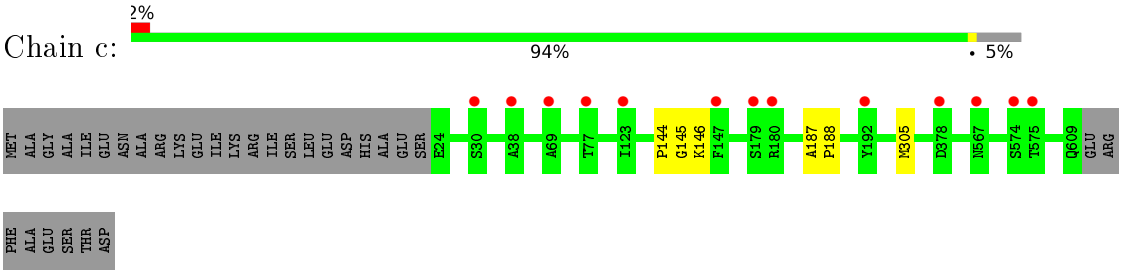




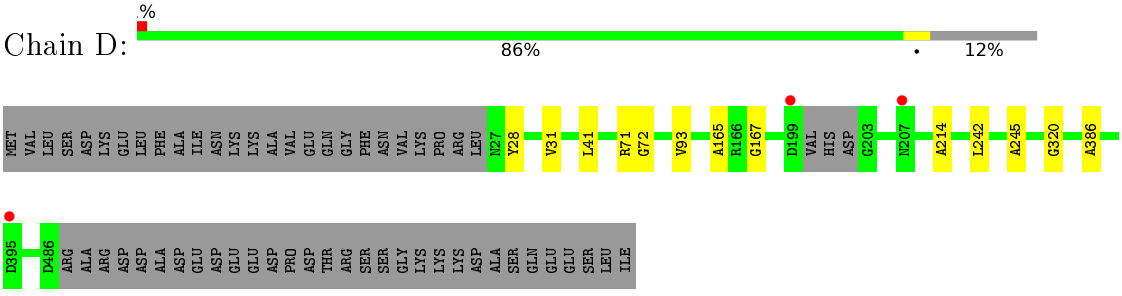
• Molecule 1: V-type proton ATPase catalytic subunit A



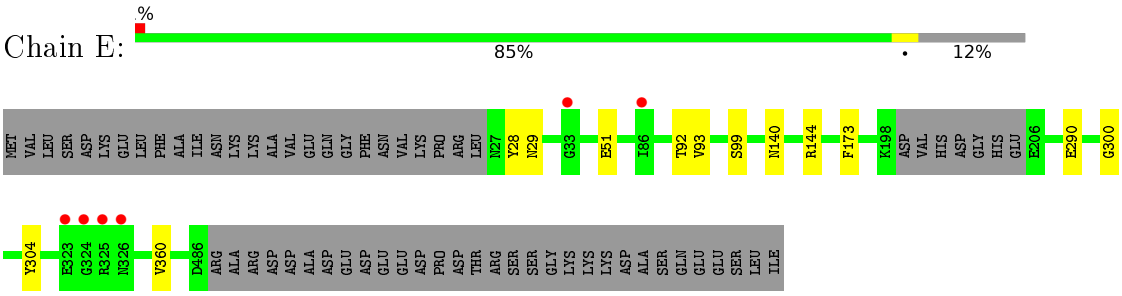
• Molecule 1: V-type proton ATPase catalytic subunit A



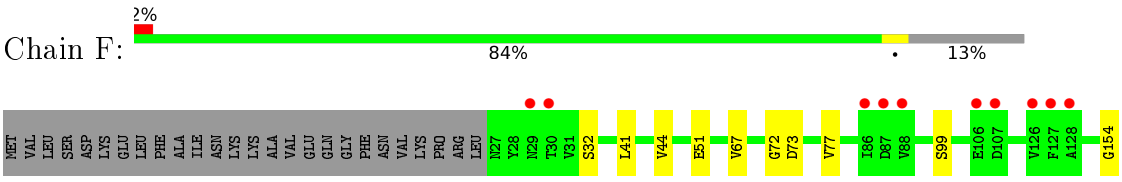
• Molecule 2: V-type proton ATPase subunit B

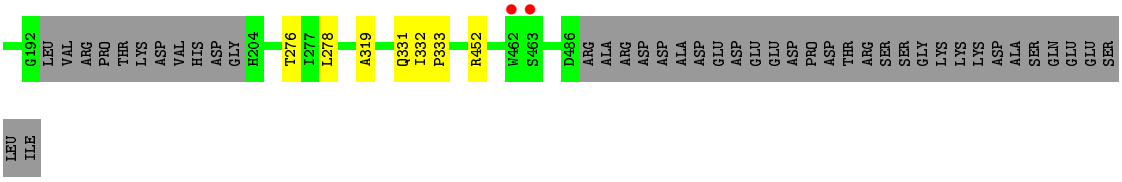


• Molecule 2: V-type proton ATPase subunit B

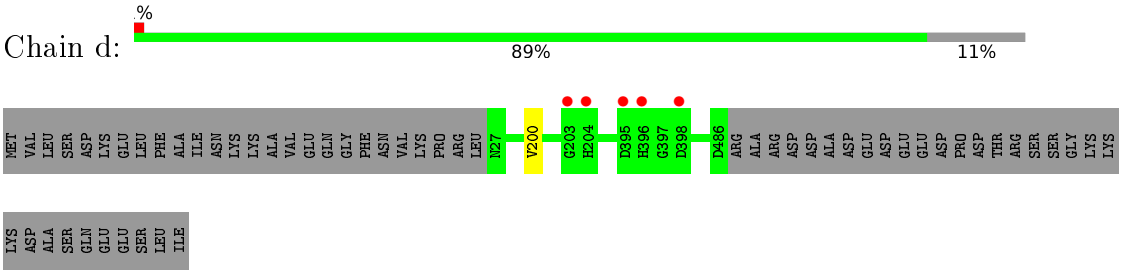


• Molecule 2: V-type proton ATPase subunit B

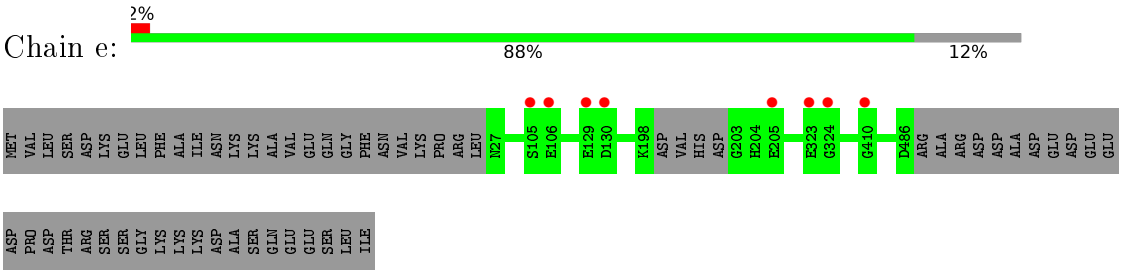




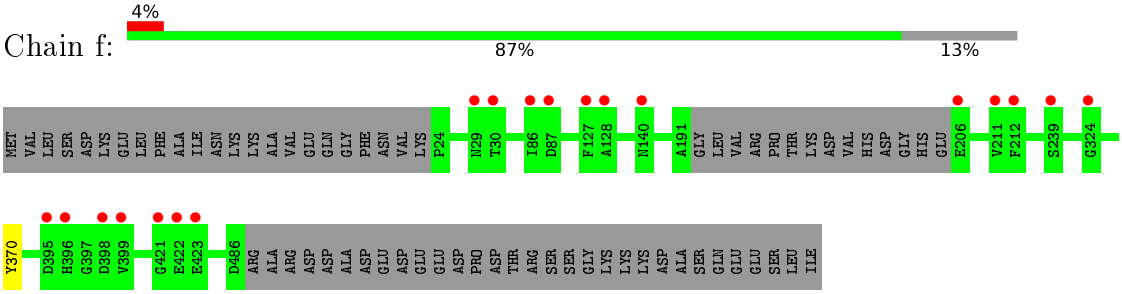
• Molecule 2: V-type proton ATPase subunit B



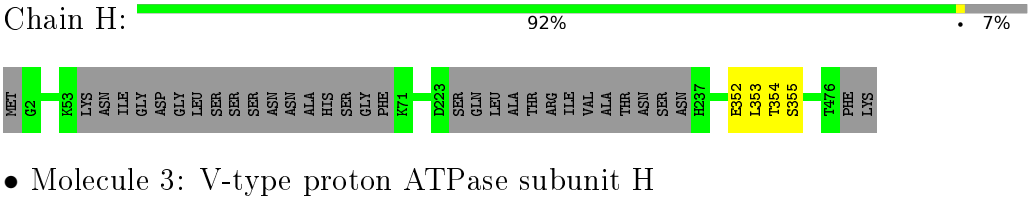
• Molecule 2: V-type proton ATPase subunit B



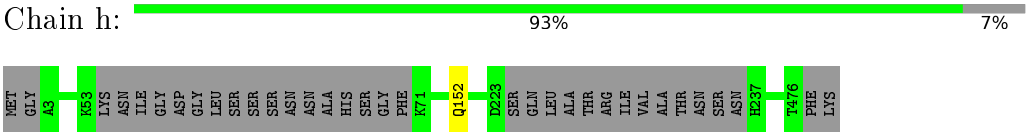
• Molecule 2: V-type proton ATPase subunit B



• Molecule 3: V-type proton ATPase subunit H

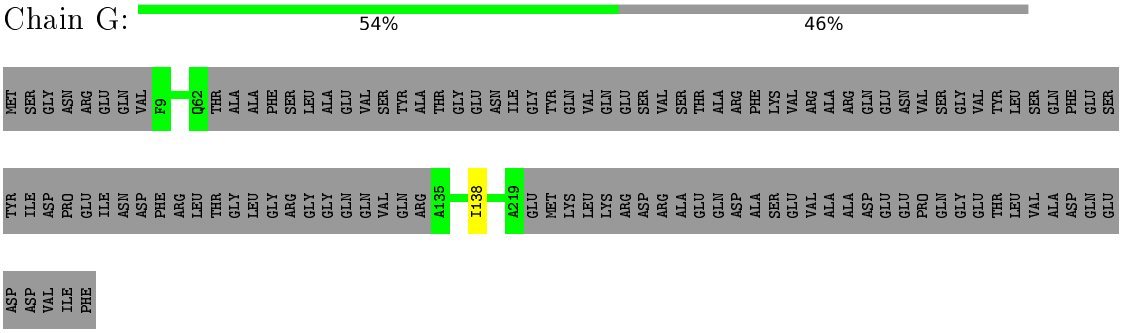


• Molecule 3: V-type proton ATPase subunit H



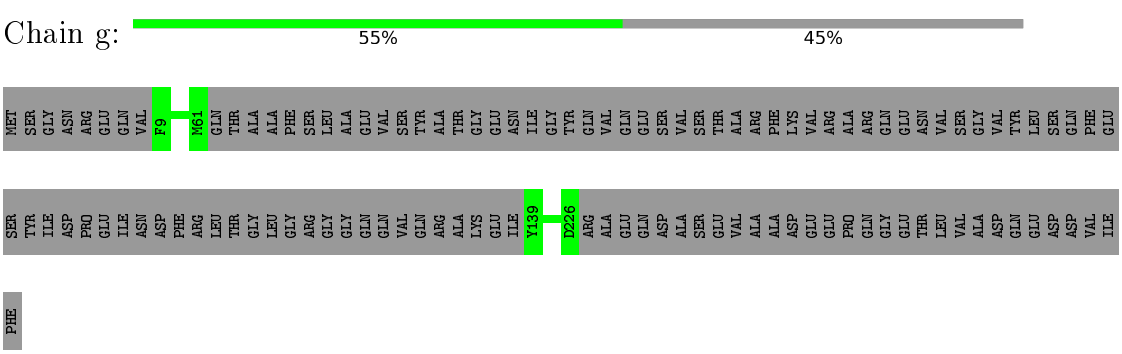
• Molecule 4: V-type proton ATPase subunit D

Chain G:



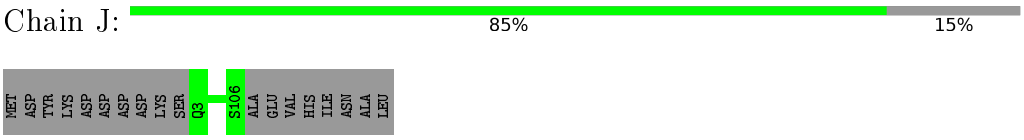
• Molecule 4: V-type proton ATPase subunit D

Chain g:



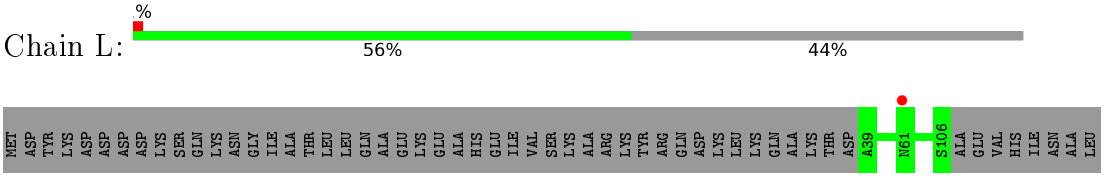
• Molecule 5: V-type proton ATPase subunit G

Chain J:



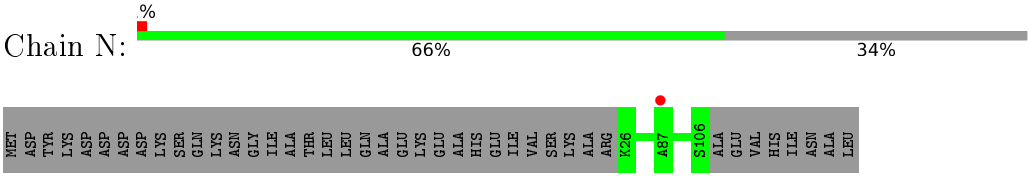
• Molecule 5: V-type proton ATPase subunit G

Chain L:



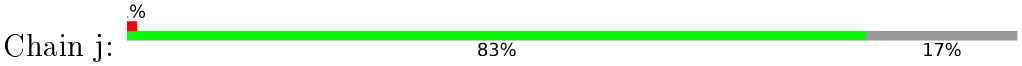
• Molecule 5: V-type proton ATPase subunit G

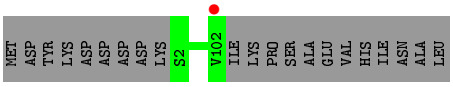
Chain N:



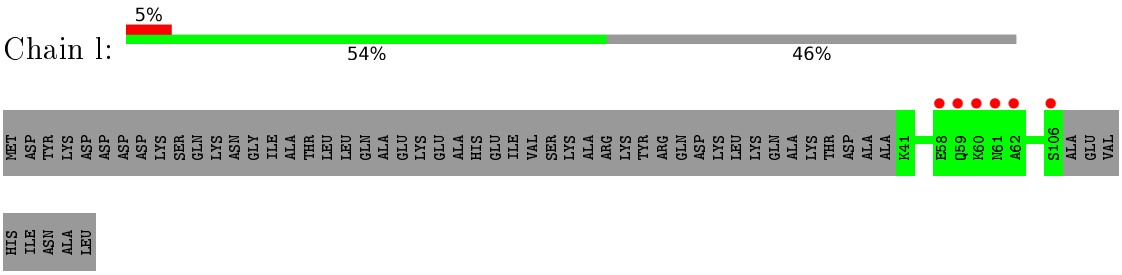
• Molecule 5: V-type proton ATPase subunit G

Chain j:

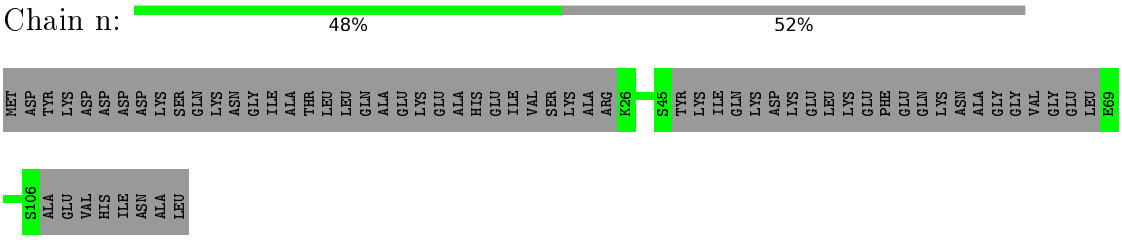




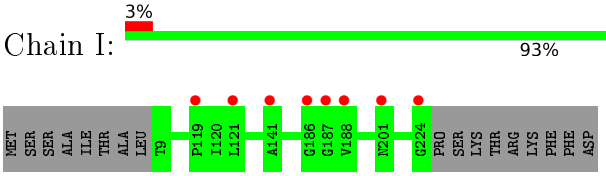
• Molecule 5: V-type proton ATPase subunit G



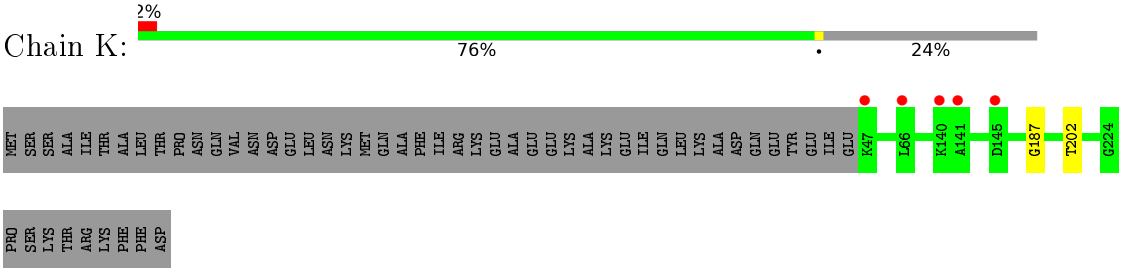
• Molecule 5: V-type proton ATPase subunit G



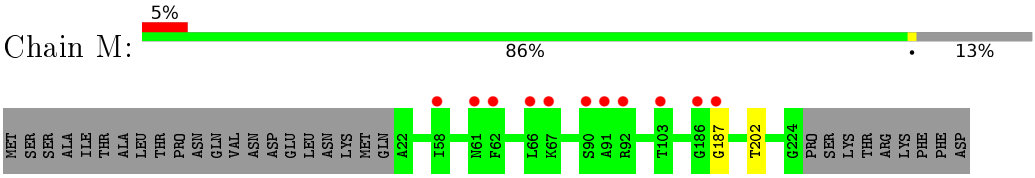
• Molecule 6: V-type proton ATPase subunit E



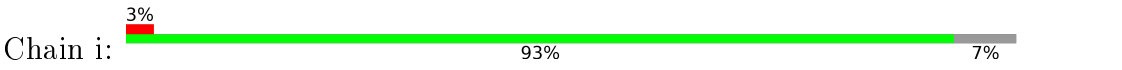
• Molecule 6: V-type proton ATPase subunit E

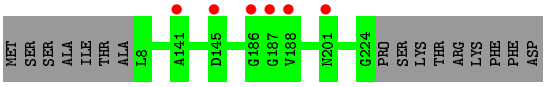


• Molecule 6: V-type proton ATPase subunit E

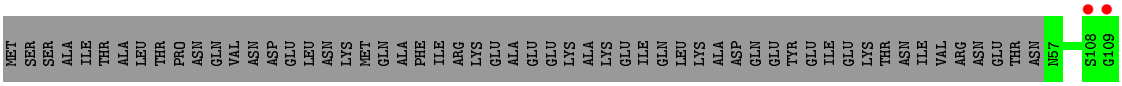


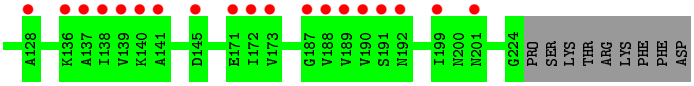
• Molecule 6: V-type proton ATPase subunit E



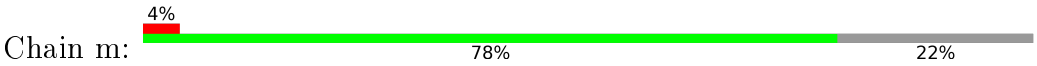


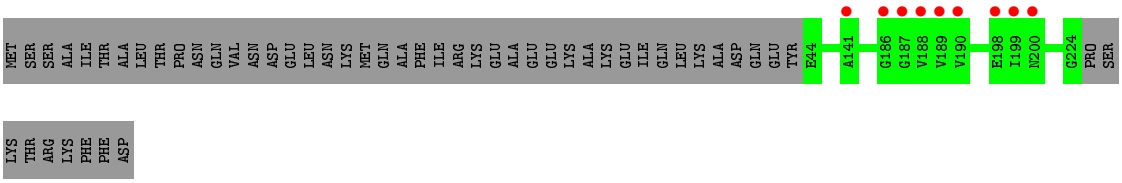
• Molecule 6: V-type proton ATPase subunit E





• Molecule 6: V-type proton ATPase subunit E





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.42 (at 7.33Å)	Xtriage
Refinement program	PHENIX	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^2)	328.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.27 , 6425.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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.

The worst 5 of 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

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%)	550 (93%)	34 (6%)	5 (1%)	24 69
1	B	592/617 (96%)	557 (94%)	35 (6%)	0	100 100
1	C	587/617 (95%)	548 (93%)	33 (6%)	6 (1%)	19 65
1	a	589/617 (96%)	550 (93%)	33 (6%)	6 (1%)	19 65
1	b	587/617 (95%)	552 (94%)	35 (6%)	0	100 100
1	c	584/617 (95%)	545 (93%)	33 (6%)	6 (1%)	19 65
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%)	52 86
2	e	452/517 (87%)	431 (95%)	21 (5%)	0	100 100
2	f	445/517 (86%)	421 (95%)	23 (5%)	1 (0%)	52 86
3	H	439/478 (92%)	412 (94%)	27 (6%)	0	100 100
3	h	438/478 (92%)	412 (94%)	25 (6%)	1 (0%)	52 86
4	G	135/256 (53%)	130 (96%)	4 (3%)	1 (1%)	26 71
4	g	137/256 (54%)	134 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	46	83

5 of 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

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^{th} 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^2)	Q<0.9
1	A	591/617 (95%)	-0.02	39 (6%)	22	23	126, 311, 475, 652	0
1	B	594/617 (96%)	-0.14	29 (4%)	33	33	107, 290, 447, 594	0
1	C	589/617 (95%)	-0.15	13 (2%)	65	61	111, 281, 475, 610	0
1	a	591/617 (95%)	0.24	51 (8%)	13	17	126, 314, 475, 658	0
1	b	589/617 (95%)	-0.15	17 (2%)	55	50	107, 292, 450, 597	0
1	c	586/617 (94%)	-0.15	13 (2%)	65	61	111, 282, 473, 614	0
2	D	457/517 (88%)	-0.47	3 (0%)	89	85	92, 239, 384, 587	0
2	E	453/517 (87%)	-0.31	6 (1%)	79	73	124, 258, 413, 663	0
2	F	449/517 (86%)	-0.28	12 (2%)	58	54	146, 287, 414, 584	0
2	d	460/517 (88%)	-0.33	5 (1%)	82	78	94, 241, 390, 586	0
2	e	456/517 (88%)	-0.30	8 (1%)	71	66	125, 258, 415, 667	0
2	f	449/517 (86%)	-0.18	19 (4%)	40	38	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%)	76	70	283, 418, 525, 566	0
5	N	81/122 (66%)	0.02	1 (1%)	81	75	200, 450, 574, 740	0
5	j	101/122 (82%)	-0.42	1 (0%)	84	79	151, 282, 419, 497	0
5	l	66/122 (54%)	0.26	6 (9%)	11	16	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%)	45	42	112, 345, 497, 643	0
6	K	178/233 (76%)	-0.02	5 (2%)	56	52	186, 344, 491, 599	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
6	M	203/233 (87%)	0.45	11 (5%) 29 30	200, 410, 571, 626	0
6	i	217/233 (93%)	0.01	6 (2%) 56 52	91, 345, 511, 638	0
6	k	168/233 (72%)	0.56	21 (12%) 5 11	187, 331, 466, 514	0
6	m	181/233 (77%)	0.08	9 (4%) 32 32	200, 402, 542, 587	0
All	All	9074/10402 (87%)	-0.21	284 (3%) 52 48	61, 281, 479, 740	0

The worst 5 of 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

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.