



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 08:45 pm GMT

PDB ID : 3A5D  
Title : Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase  
Authors : Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.  
Deposited on : 2009-08-06  
Resolution : 4.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

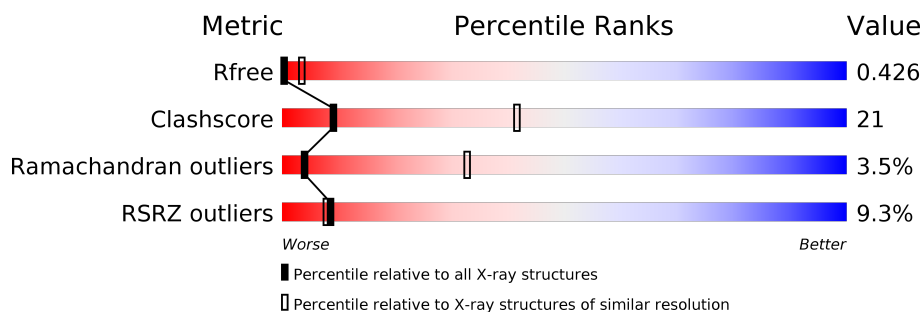
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 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))
$R_{free}$	111664	1105 (5.90-3.70)
Clashscore	122126	1004 (5.82-3.78)
Ramachandran outliers	120053	1119 (5.90-3.70)
RSRZ outliers	108989	1027 (5.98-3.62)

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	578	<div> <div>11%</div> <div>84%</div> <div>11%</div> <div>...</div> </div>
1	B	578	<div> <div>4%</div> <div>85%</div> <div>10%</div> <div>...</div> </div>
1	C	578	<div> <div>11%</div> <div>82%</div> <div>13%</div> <div>...</div> </div>
1	I	578	<div> <div>15%</div> <div>83%</div> <div>12%</div> <div>...</div> </div>
1	J	578	<div> <div>2%</div> <div>84%</div> <div>11%</div> <div>...</div> </div>
1	K	578	<div> <div>15%</div> <div>83%</div> <div>12%</div> <div>...</div> </div>
2	D	478	<div> <div>7%</div> <div>83%</div> <div>9%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	478	
2	F	478	
2	L	478	
2	M	478	
2	N	478	
3	G	223	
3	O	223	
4	H	104	
4	P	104	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32080 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 ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	B	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	C	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	I	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	J	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	K	561	Total	C	N	O	0	0	0
			2752	1630	561	561			

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	E	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	F	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	L	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	M	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	N	450	Total	C	N	O	0	0	0
			2212	1312	450	450			

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total 639	C 381	N 129	O 129	0	0	0
3	O	129	Total 639	C 381	N 129	O 129	0	0	0

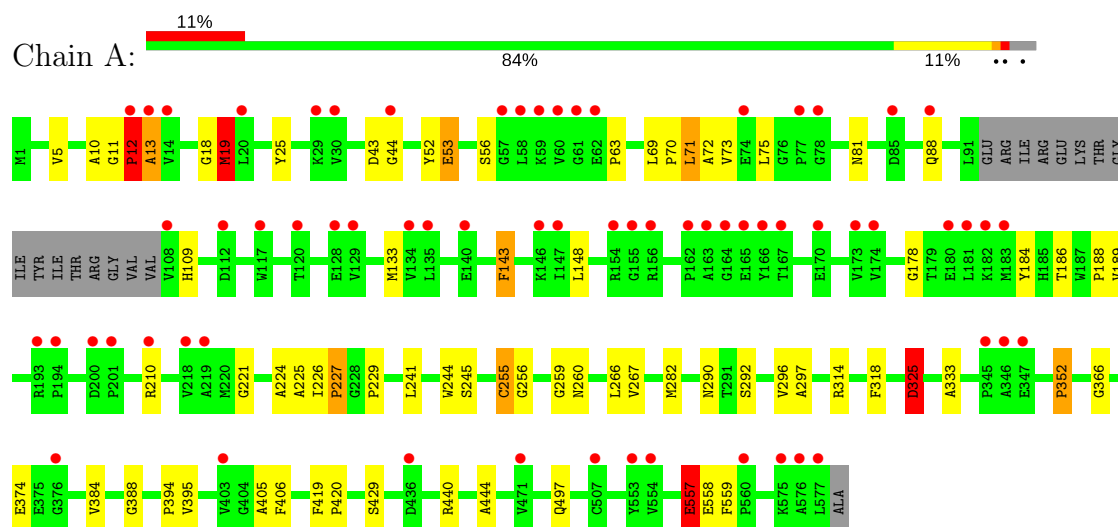
- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total 509	C 301	N 104	O 104	0	0	0
4	P	104	Total 509	C 301	N 104	O 104	0	0	0

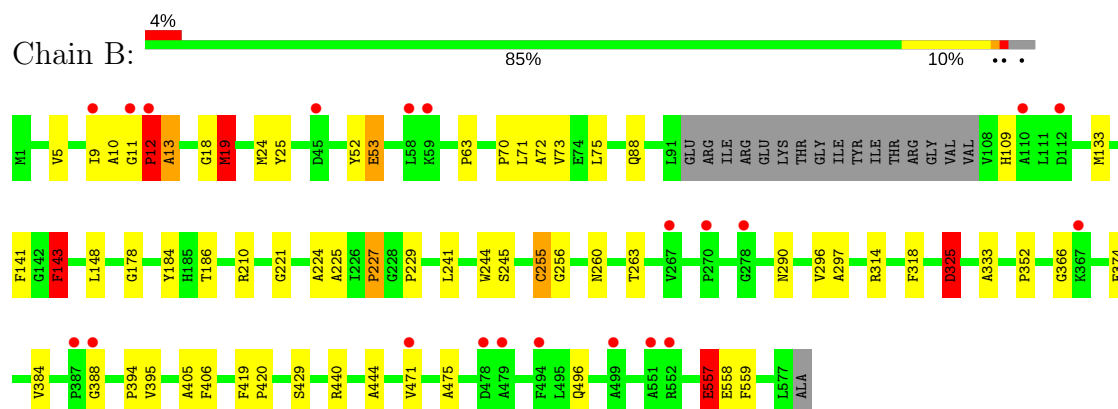
### 3 Residue-property plots [i](#)

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.

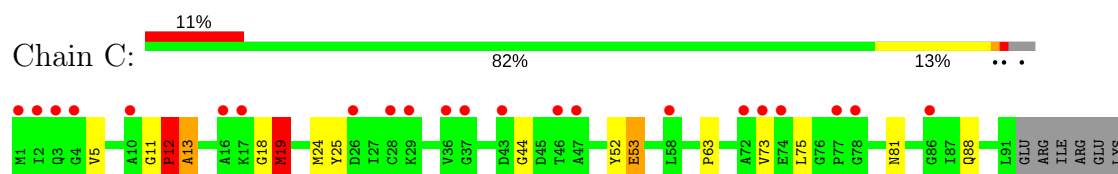
#### • Molecule 1: V-type ATP synthase alpha chain

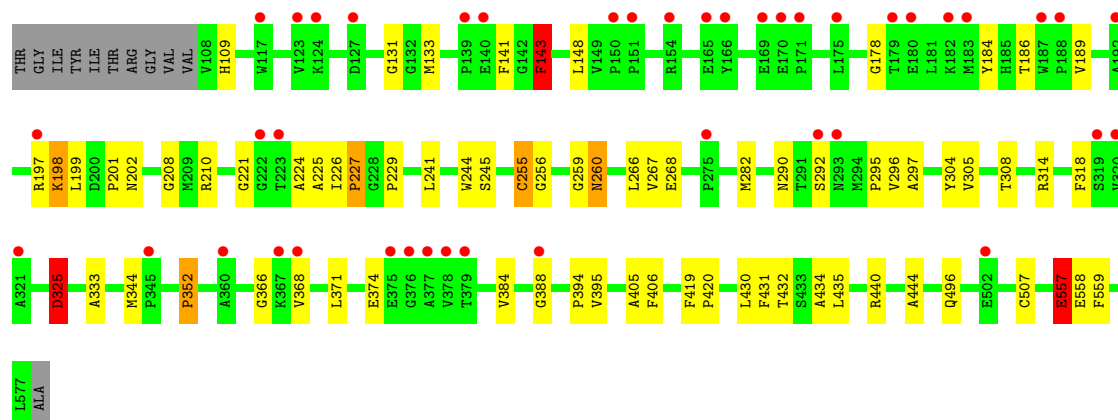


#### • Molecule 1: V-type ATP synthase alpha chain

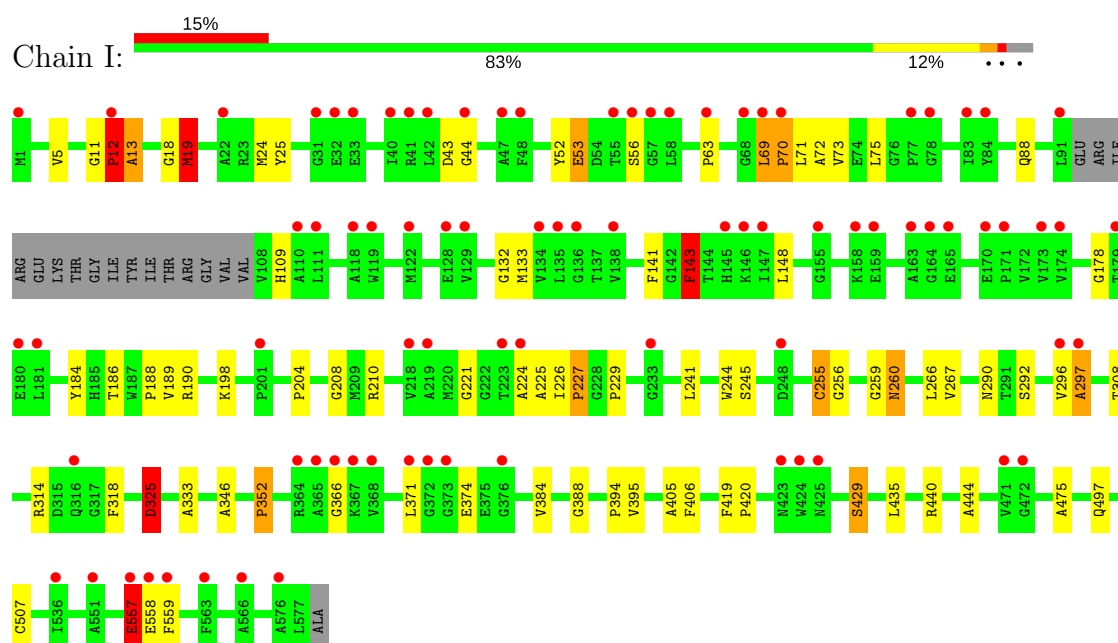


#### • Molecule 1: V-type ATP synthase alpha chain

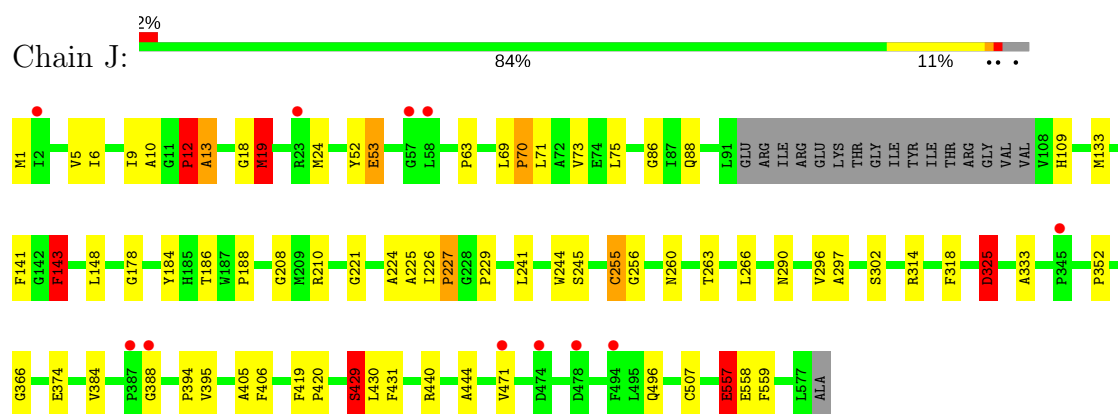




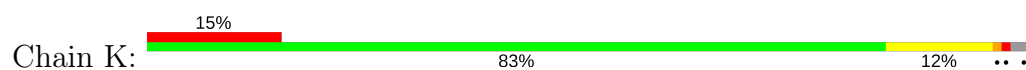
• Molecule 1: V-type ATP synthase alpha chain

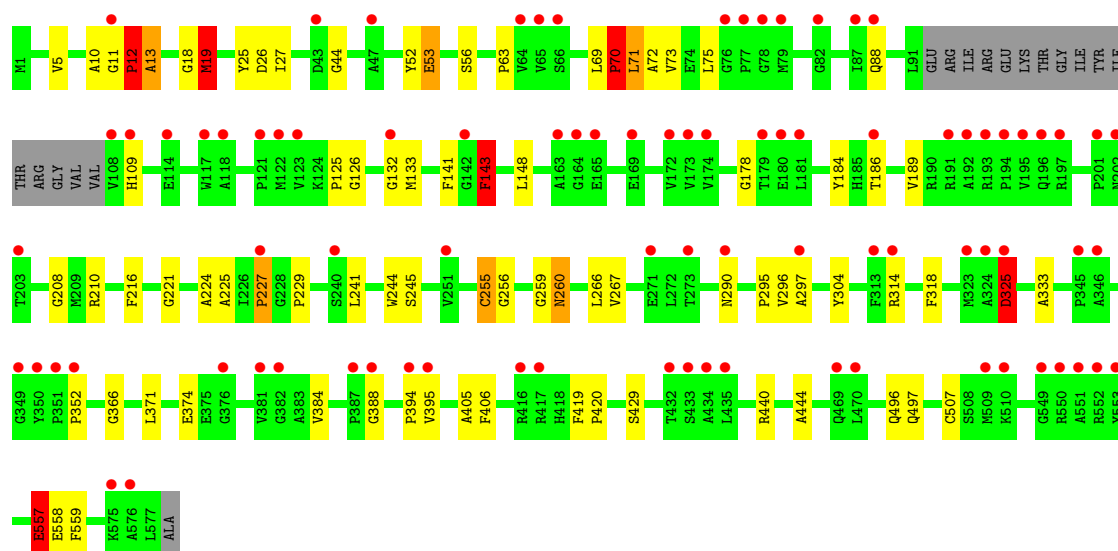


• Molecule 1: V-type ATP synthase alpha chain

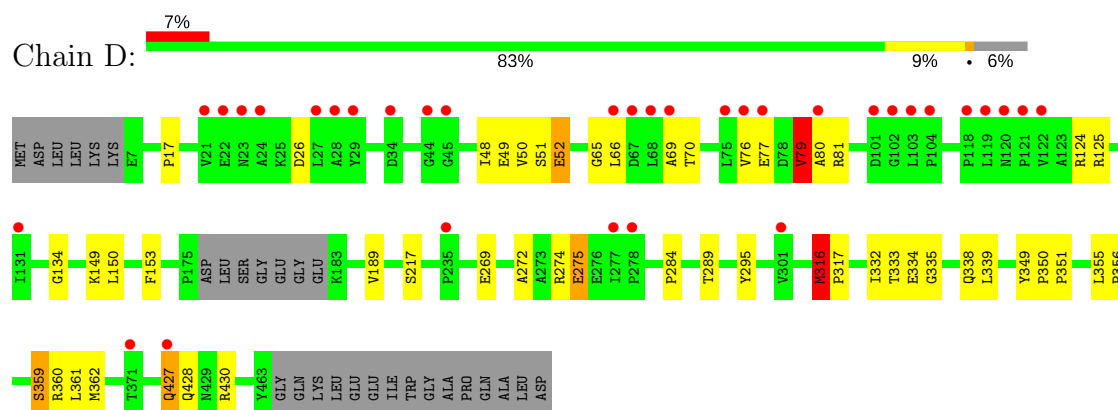


• Molecule 1: V-type ATP synthase alpha chain

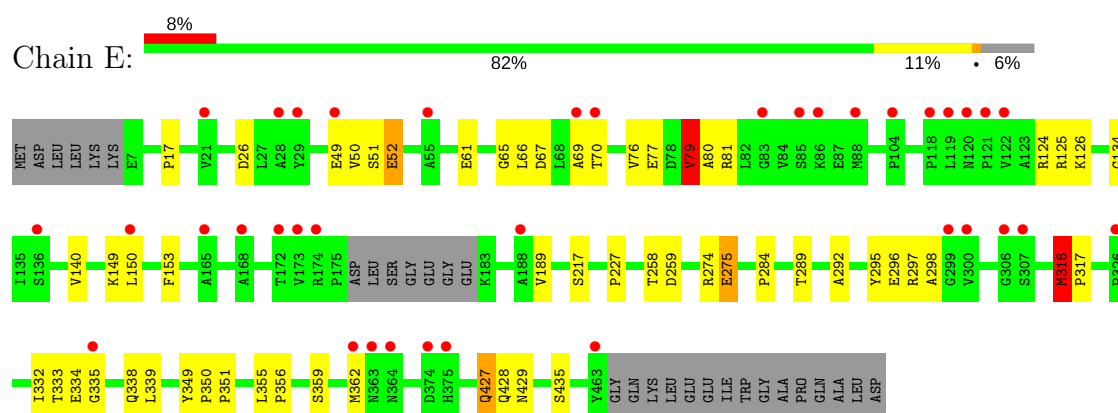




• Molecule 2: V-type ATP synthase beta chain



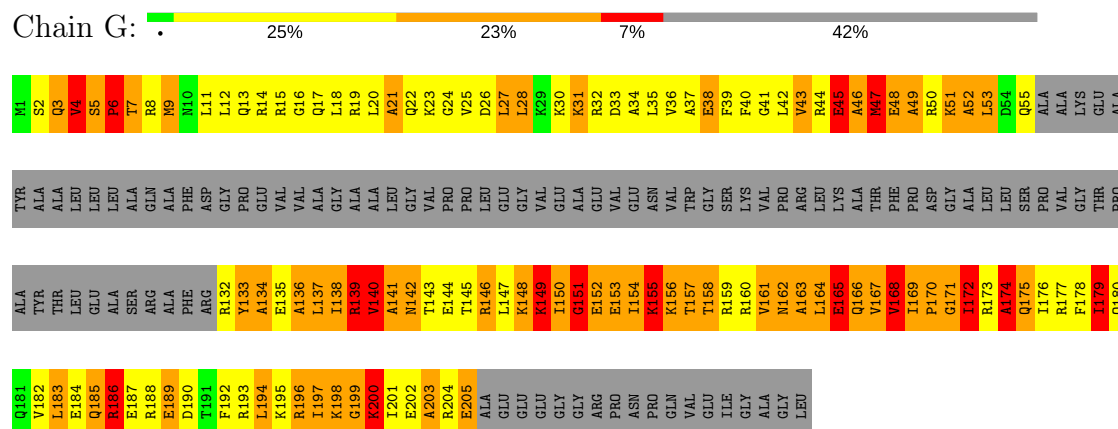
• Molecule 2: V-type ATP synthase beta chain



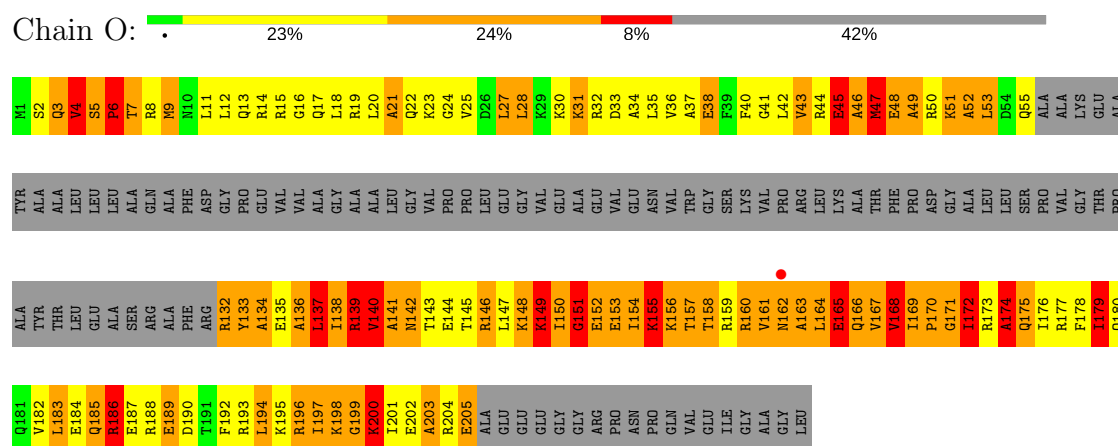




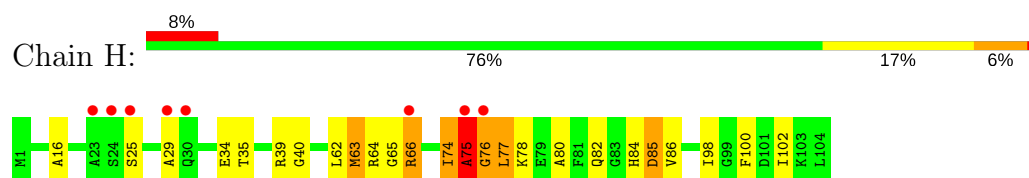
- Molecule 3: V-type ATP synthase subunit D



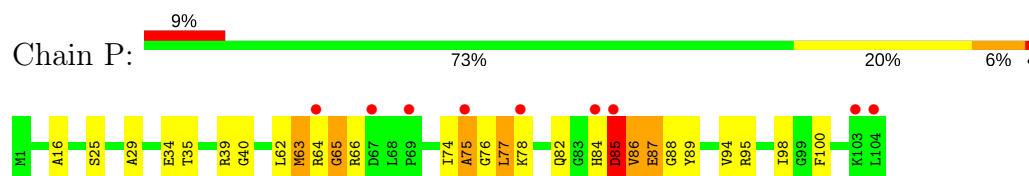
- Molecule 3: V-type ATP synthase subunit D



- Molecule 4: V-type ATP synthase subunit F



- Molecule 4: V-type ATP synthase subunit F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	380.70Å 380.70Å 147.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 4.80 49.72 – 4.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (29.97-4.80) 95.2 (49.72-4.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 4.86Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.441 , 0.454 0.413 , 0.426	Depositor DCC
$R_{free}$ test set	2935 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	173.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.13 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.28$ , $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	32080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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	0.59	3/2750 (0.1%)	1.25	12/3815 (0.3%)
1	B	0.62	4/2750 (0.1%)	1.19	9/3815 (0.2%)
1	C	0.60	4/2750 (0.1%)	1.20	10/3815 (0.3%)
1	I	0.61	4/2750 (0.1%)	1.30	17/3815 (0.4%)
1	J	0.61	4/2750 (0.1%)	1.26	13/3815 (0.3%)
1	K	0.61	4/2750 (0.1%)	1.43	12/3815 (0.3%)
2	D	0.77	6/2210 (0.3%)	1.02	11/3068 (0.4%)
2	E	0.77	6/2210 (0.3%)	1.01	9/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
2	L	0.79	6/2210 (0.3%)	1.07	14/3068 (0.5%)
2	M	0.76	5/2210 (0.2%)	1.00	8/3068 (0.3%)
2	N	0.75	3/2210 (0.1%)	1.00	7/3068 (0.2%)
3	G	4.09	125/637 (19.6%)	2.63	49/885 (5.5%)
3	O	4.09	125/637 (19.6%)	2.63	50/885 (5.6%)
4	H	1.50	9/508 (1.8%)	1.43	10/703 (1.4%)
4	P	1.61	10/508 (2.0%)	2.13	17/703 (2.4%)
All	All	1.08	321/32050 (1.0%)	1.28	255/44474 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	6
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	3
2	E	0	3
2	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	3
2	M	0	3
2	N	0	3
4	H	0	2
4	P	0	2
All	All	0	55

The worst 5 of 321 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-24.95	0.99	1.53
3	G	47	MET	CA-CB	-24.94	0.99	1.53
3	O	27	LEU	CA-CB	14.84	1.87	1.53
3	G	27	LEU	CA-CB	14.76	1.87	1.53
3	O	7	THR	CA-CB	12.80	1.86	1.53

The worst 5 of 255 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	325	ASP	O-C-N	-39.90	58.87	122.70
1	J	325	ASP	O-C-N	-39.90	58.87	122.70
1	A	325	ASP	O-C-N	-39.88	58.90	122.70
1	C	325	ASP	O-C-N	-39.88	58.90	122.70
1	B	325	ASP	O-C-N	-39.85	58.94	122.70

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	557	GLU	Mainchain

## 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	2752	0	1302	87	0
1	B	2752	0	1303	71	0
1	C	2752	0	1303	98	0
1	I	2752	0	1301	134	0
1	J	2752	0	1303	52	3
1	K	2752	0	1303	91	0
2	D	2212	0	1009	73	0
2	E	2212	0	1009	56	0
2	F	2212	0	1009	78	0
2	L	2212	0	1009	94	0
2	M	2212	0	1009	50	3
2	N	2212	0	1009	78	0
3	G	639	0	299	133	0
3	O	639	0	299	135	0
4	H	509	0	255	22	0
4	P	509	0	254	18	0
All	All	32080	0	14976	1006	3

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 21.

The worst 5 of 1006 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:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.64
3:O:189:GLU:CA	3:O:189:GLU:CB	1.76	1.64
3:G:205:GLU:CA	3:G:205:GLU:CB	1.78	1.62
1:K:52:TYR:CA	1:K:295:PRO:CB	1.79	1.59
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:ILE:CB	2:M:24:ALA:O[5_555]	1.43	0.77
1:J:1:MET:N	2:M:9:THR:CA[5_555]	1.83	0.37
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	1.92	0.28

## 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	557/578 (96%)	488 (88%)	52 (9%)	17 (3%)	4	35
1	B	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	5	36
1	C	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	4	34
1	I	557/578 (96%)	491 (88%)	50 (9%)	16 (3%)	5	36
1	J	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	4	35
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	4	35
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	8	44
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	8	44
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	8	44
2	L	446/478 (93%)	419 (94%)	17 (4%)	10 (2%)	7	42
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	8	44
2	N	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	8	44
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	2	22
4	P	102/104 (98%)	86 (84%)	11 (11%)	5 (5%)	2	26
All	All	6472/6990 (93%)	5798 (90%)	449 (7%)	225 (4%)	4	33

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	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<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	561/578 (97%)	0.42	66 (11%) 4 5	168, 196, 399, 399	0
1	B	561/578 (97%)	-0.07	21 (3%) 41 32	97, 98, 159, 159	0
1	C	561/578 (97%)	0.50	64 (11%) 5 5	208, 224, 414, 414	0
1	I	561/578 (97%)	0.64	84 (14%) 2 3	198, 211, 393, 393	0
1	J	561/578 (97%)	-0.22	11 (1%) 65 56	90, 94, 161, 161	0
1	K	561/578 (97%)	0.78	86 (15%) 2 2	207, 219, 403, 403	0
2	D	450/478 (94%)	0.13	34 (7%) 14 11	138, 159, 262, 262	0
2	E	450/478 (94%)	0.25	37 (8%) 11 10	157, 157, 176, 176	0
2	F	450/478 (94%)	0.33	49 (10%) 5 5	155, 241, 275, 275	0
2	L	450/478 (94%)	0.25	37 (8%) 11 10	145, 154, 244, 244	0
2	M	450/478 (94%)	0.22	32 (7%) 16 12	151, 151, 191, 191	0
2	N	450/478 (94%)	0.75	68 (15%) 2 3	181, 256, 256, 256	0
3	G	129/223 (57%)	-0.71	0 100 100	71, 85, 85, 85	0
3	O	129/223 (57%)	-0.43	1 (0%) 86 80	89, 89, 105, 105	0
4	H	104/104 (100%)	0.03	8 (7%) 13 11	159, 185, 185, 185	0
4	P	104/104 (100%)	0.02	9 (8%) 10 9	159, 167, 167, 167	0
All	All	6532/6990 (93%)	0.29	607 (9%) 8 8	71, 176, 399, 414	0

The worst 5 of 607 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	78	GLY	21.1
1	K	77	PRO	20.6
1	A	155	GLY	12.5
1	C	376	GLY	10.5
2	N	191	PHE	10.4

## 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.