



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:26 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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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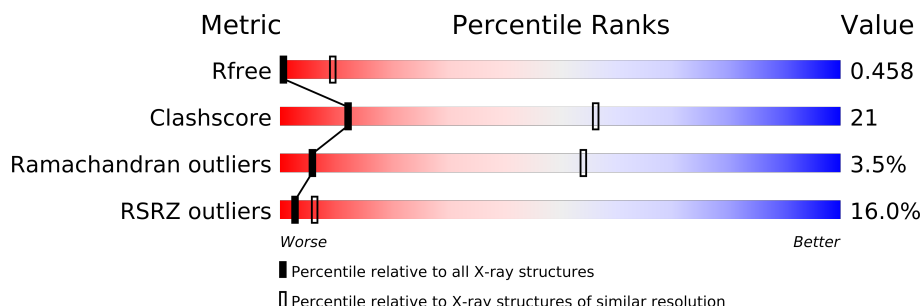
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1046 (6.00-3.50)
Clashscore	79885	1320 (6.00-3.50)
Ramachandran outliers	78287	1236 (6.00-3.50)
RSRZ outliers	66119	1045 (6.00-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	578	
1	B	578	
1	C	578	
1	I	578	
1	J	578	
1	K	578	
2	D	478	
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 hydrogen and 0 are deuterium.

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

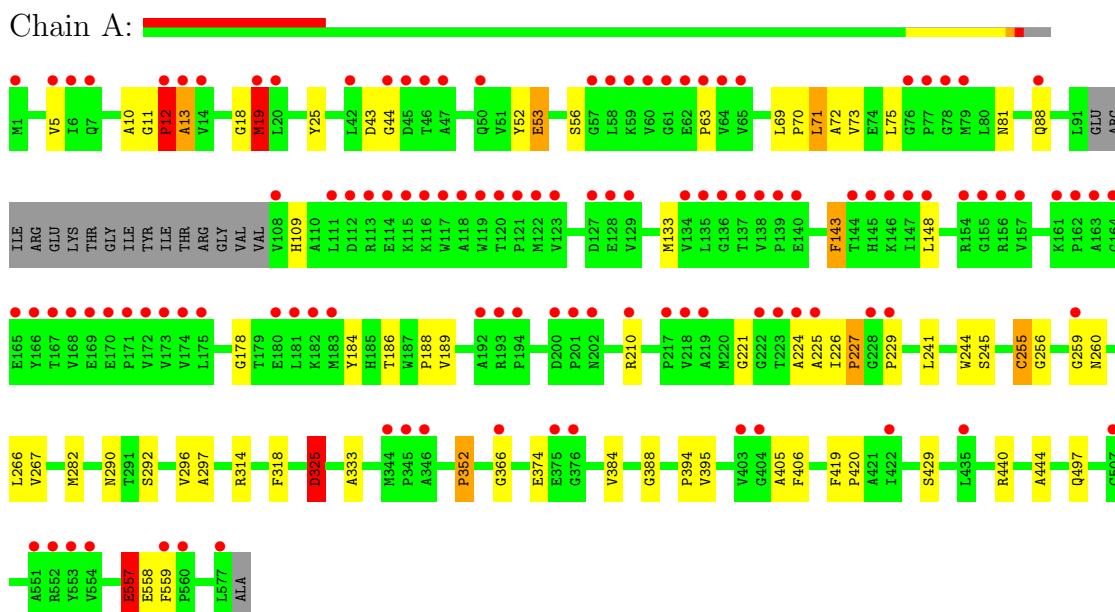
- Molecule 4 is a protein called V-type ATP synthase subunit F.

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

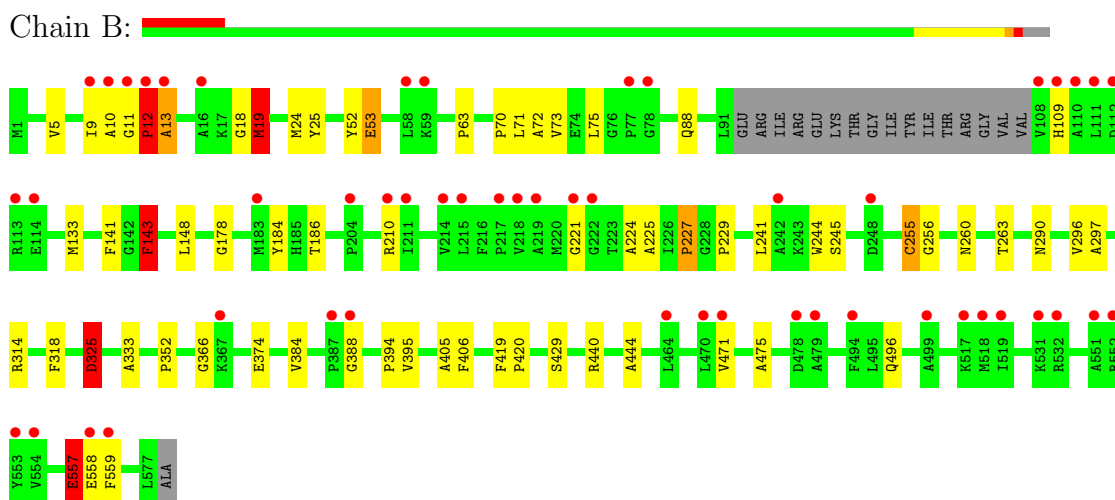
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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

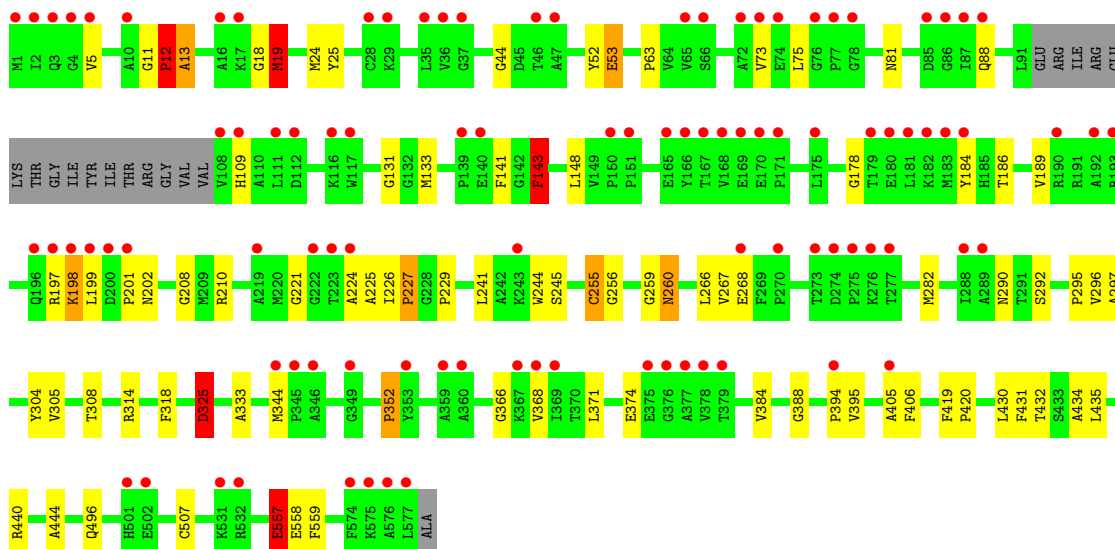


#### • Molecule 1: V-type ATP synthase alpha chain



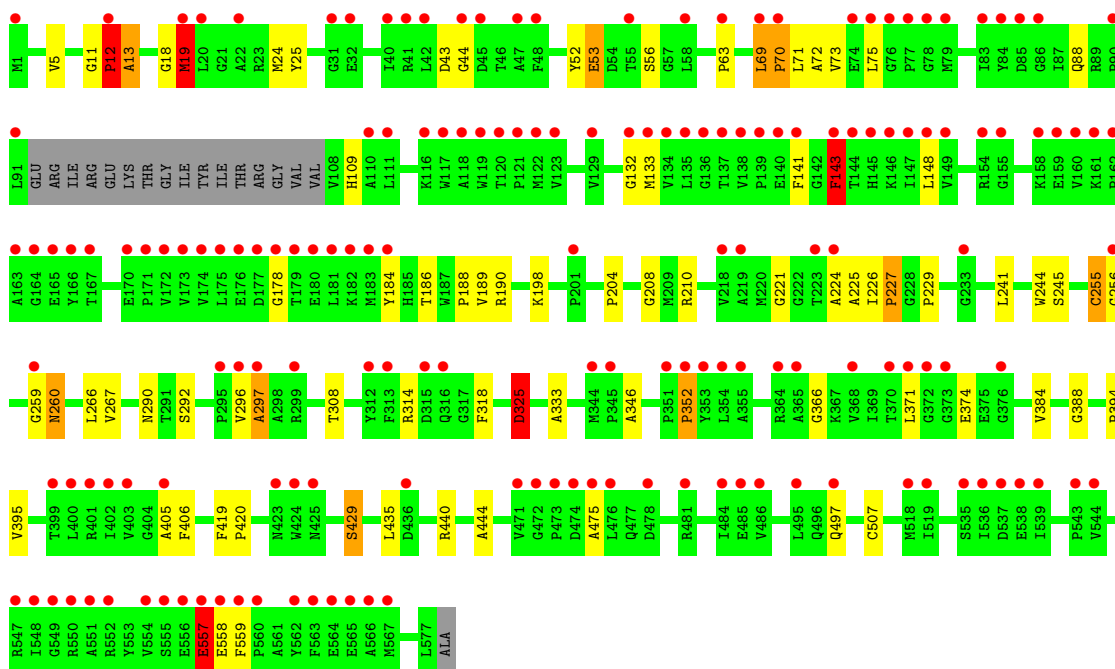
#### • Molecule 1: V-type ATP synthase alpha chain





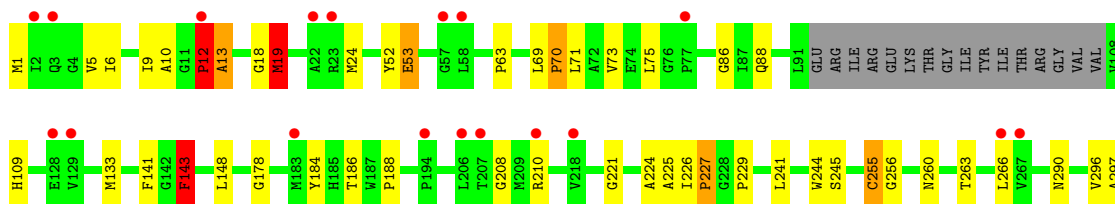
- Molecule 1: V-type ATP synthase alpha chain

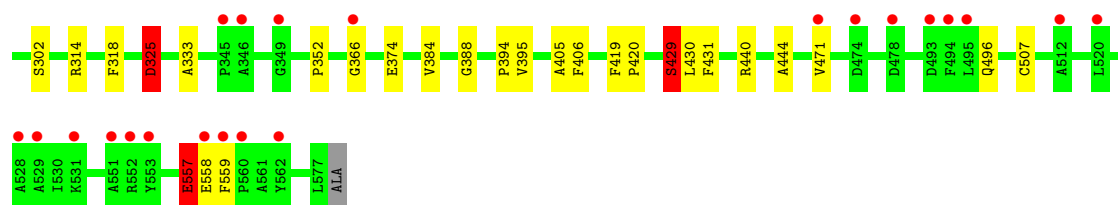
Chain I:



- Molecule 1: V-type ATP synthase alpha chain

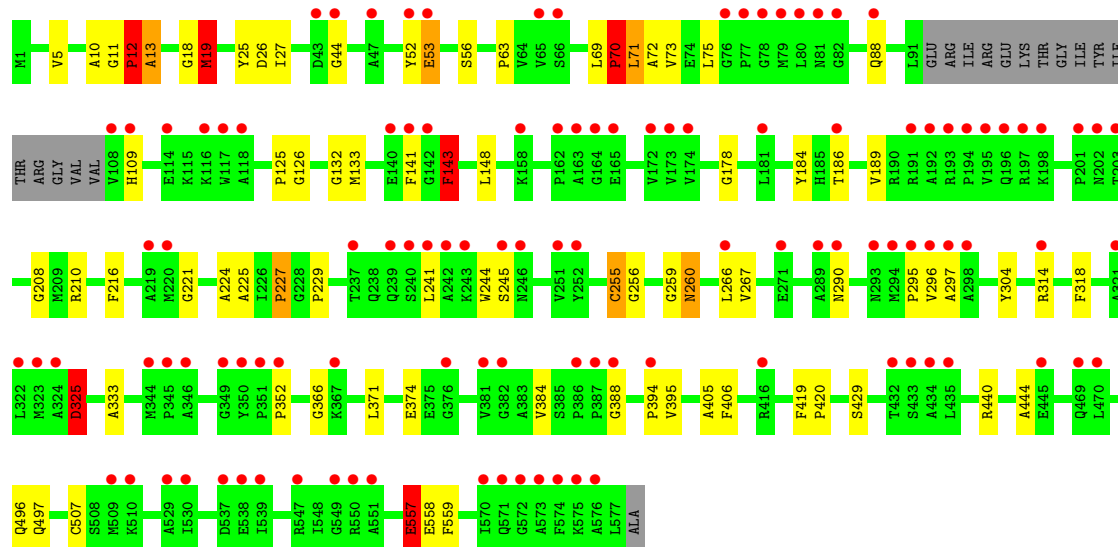
Chain J:





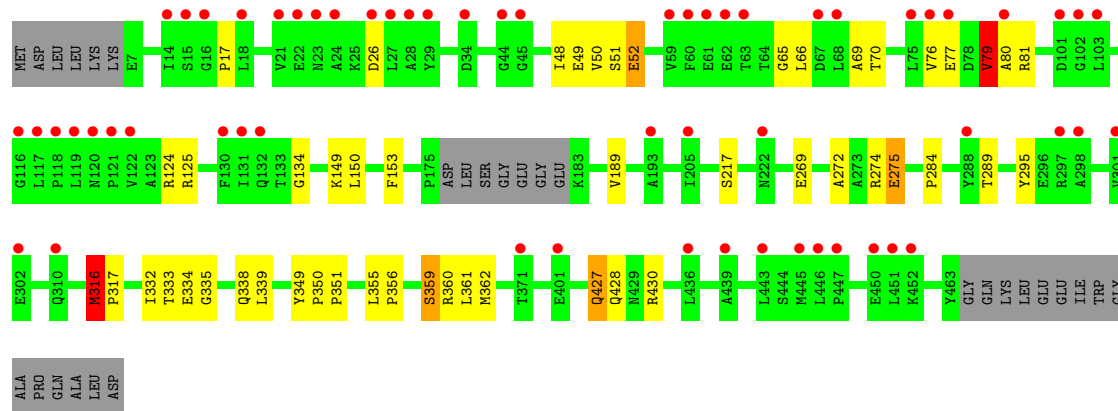
• Molecule 1: V-type ATP synthase alpha chain

Chain K:



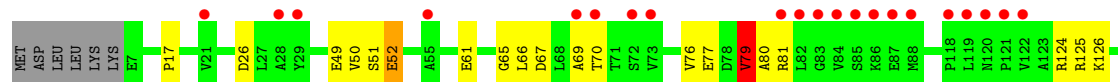
• Molecule 2: V-type ATP synthase beta chain

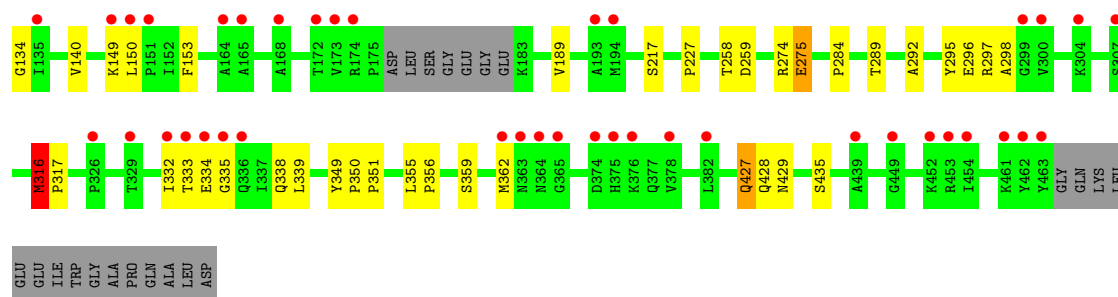
Chain D:



• Molecule 2: V-type ATP synthase beta chain

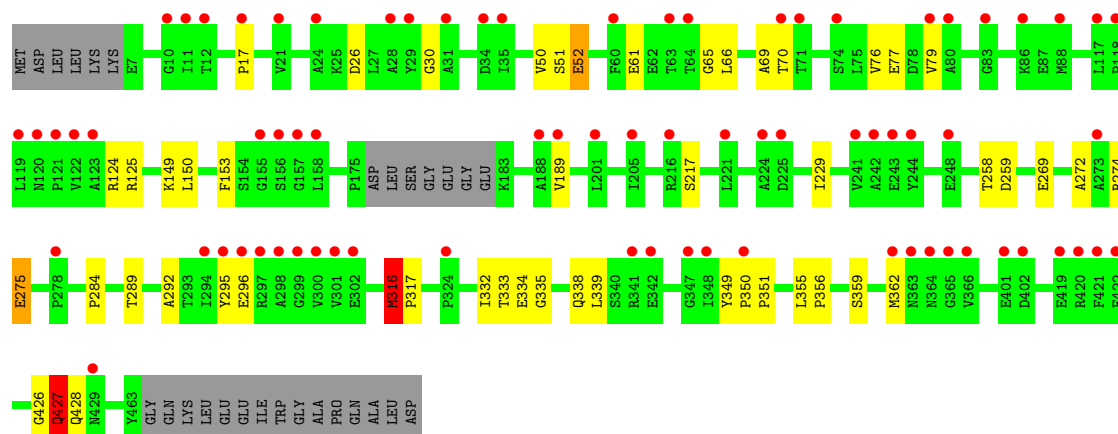
Chain E:





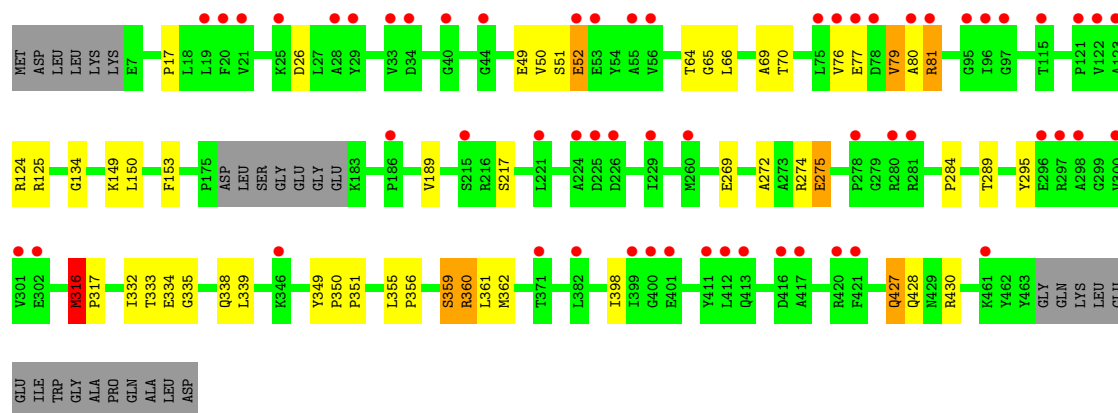
• Molecule 2: V-type ATP synthase beta chain

Chain F:



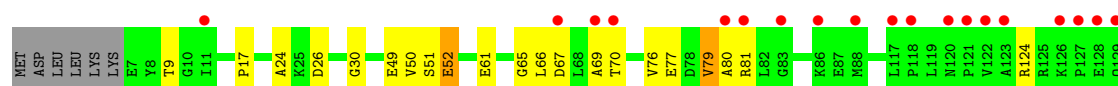
• Molecule 2: V-type ATP synthase beta chain

Chain L:

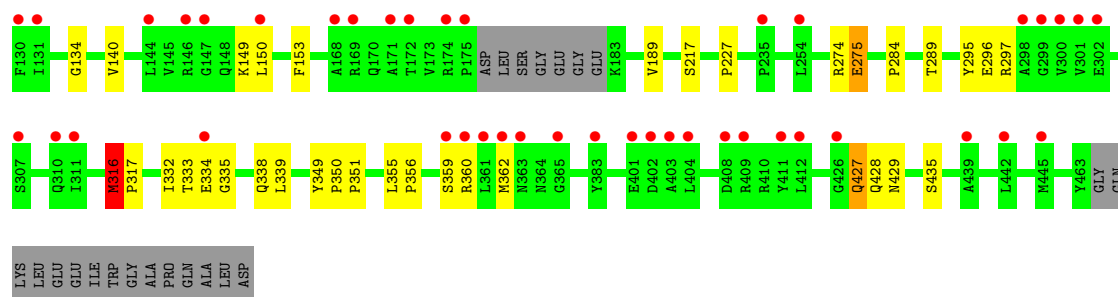


• Molecule 2: V-type ATP synthase beta chain

Chain M:

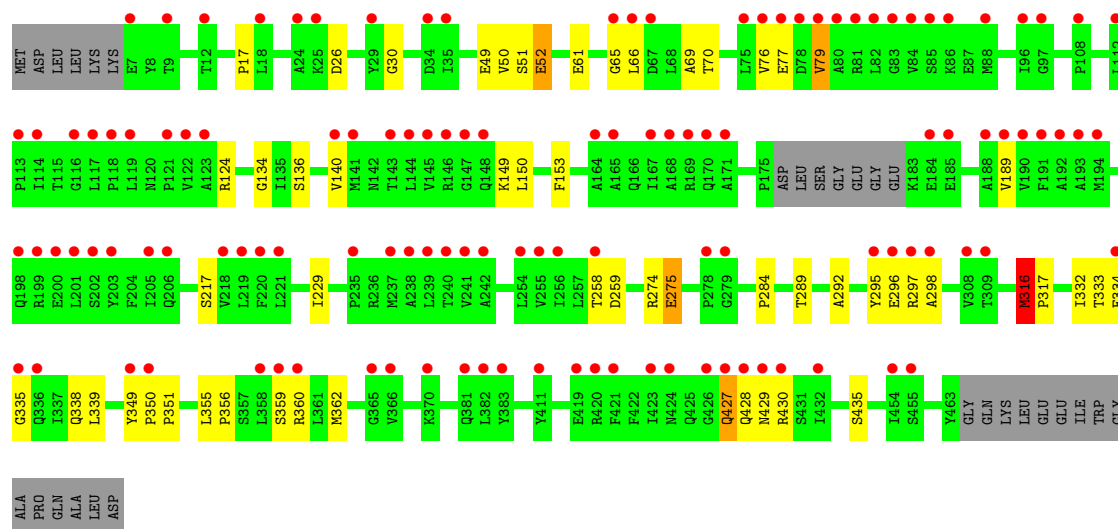






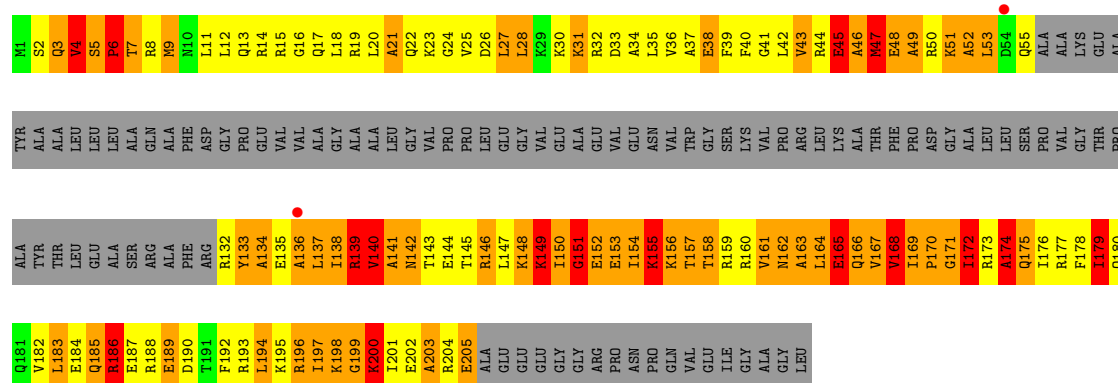
• Molecule 2: V-type ATP synthase beta chain

Chain N:



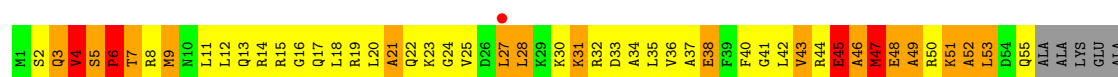
• Molecule 3: V-type ATP synthase subunit D

Chain G:



• Molecule 3: V-type ATP synthase subunit D

Chain O:



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

ALA  
TYR  
THR  
GLU  
GLU  
ALA  
SER  
ARG  
ALA  
PHE  
D190  
ARG  
R132  
Y133  
A134  
E135  
A136  
I137  
I138  
I139  
Y140  
A141  
N142  
T143  
E144  
T145  
R146  
L147  
K148  
K149  
I150  
G151  
E152  
E153  
I154  
K155  
K156  
T157  
T158  
R159  
R160  
V161  
N162  
A163  
L164  
E165  
Q166  
V167  
V168  
I169  
P170  
G171  
I172  
R173  
A174  
Q175  
I176  
R177  
F178  
I179  
Q180

Q181  
V182  
L183  
E184  
Q185  
R186  
S24  
E187  
R188  
E189  
D190  
T191  
F192  
R193  
L194  
K195  
R196  
I197  
K198  
G199  
K200  
I201  
E202  
A203  
R204  
E205  
ALA  
GLU  
GLU  
GLU  
GLY  
GLY  
ARG  
PRO  
ASN  
PRO  
GLN  
VAL  
GLU  
ILE  
GLY  
ALA  
GLY  
LEU

● Molecule 4: V-type ATP synthase subunit F

Chain H: 

W1  
A16  
A23  
S25  
A29  
E34  
E38  
G40  
L62  
M63  
R64  
G65  
R66  
I74  
A75  
G76  
L77  
K78  
E79  
A80  
F81  
Q82  
G83  
H84  
D85  
V86  
I98  
G99  
F100  
D101  
I102  
K103  
L104

● Molecule 4: V-type ATP synthase subunit F

Chain P: 

W1  
A16  
S25  
A29  
E34  
T35  
R39  
G40  
L62  
M63  
R64  
G65  
R66  
I74  
A75  
G76  
L77  
K78  
Q82  
G83  
H84  
D85  
V86  
E87  
G88  
Y89  
V94  
R95  
I98  
G99  
F100  
L104

## 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 0.446 , 0.458	Depositor DCC
$R_{free}$ test set	2935 reflections (5.42%)	DCC
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> )	-0.00 , -10.0	EDS
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.28$ , $\langle L^2 \rangle = 0.12$	Xtriage
Outliers	1 of 57297 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.69	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 1006 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	7	57
1	B	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	7	58
1	C	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	6	56
1	I	557/578 (96%)	491 (88%)	50 (9%)	16 (3%)	7	58
1	J	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	7	57
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	7	57
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	11	67
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	11	67
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	11	67
2	L	446/478 (93%)	419 (94%)	17 (4%)	10 (2%)	10	64
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	11	67
2	N	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	11	67
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	3
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	3
4	H	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	2	38
4	P	102/104 (98%)	86 (84%)	11 (11%)	5 (5%)	3	43
All	All	6472/6990 (93%)	5798 (90%)	449 (7%)	225 (4%)	6	54

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 ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

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	561/578 (97%)	1.37	116 (20%) 1 4	168, 196, 399, 399	0
1	B	561/578 (97%)	0.49	51 (9%) 9 15	97, 98, 159, 159	0
1	C	561/578 (97%)	1.01	99 (17%) 2 5	208, 224, 414, 414	0
1	I	561/578 (97%)	1.73	168 (29%) 1 3	198, 211, 393, 393	0
1	J	561/578 (97%)	0.41	40 (7%) 16 19	90, 94, 161, 161	0
1	K	561/578 (97%)	1.18	113 (20%) 2 4	207, 219, 403, 403	0
2	D	450/478 (94%)	0.72	59 (13%) 4 8	138, 159, 262, 262	0
2	E	450/478 (94%)	0.82	61 (13%) 4 8	157, 157, 176, 176	0
2	F	450/478 (94%)	0.87	75 (16%) 2 5	155, 241, 275, 275	0
2	L	450/478 (94%)	0.78	58 (12%) 4 9	145, 154, 244, 244	0
2	M	450/478 (94%)	0.81	61 (13%) 4 8	151, 151, 191, 191	0
2	N	450/478 (94%)	1.52	121 (26%) 1 4	181, 256, 256, 256	0
3	G	129/223 (57%)	-0.09	2 (1%) 68 56	71, 85, 85, 85	0
3	O	129/223 (57%)	0.04	1 (0%) 83 71	89, 89, 105, 105	0
4	H	104/104 (100%)	0.51	13 (12%) 5 9	159, 185, 185, 185	0
4	P	104/104 (100%)	0.44	9 (8%) 10 16	159, 167, 167, 167	0
All	All	6532/6990 (93%)	0.93	1047 (16%) 3 6	71, 176, 399, 414	0

The worst 5 of 1047 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	147	ILE	27.4
1	A	165	GLU	18.8
1	A	163	ALA	18.4
1	A	166	TYR	18.2
1	A	162	PRO	17.1

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.