



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:33 pm GMT

PDB ID : 3A5C
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 : 4.51 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : trunk28620

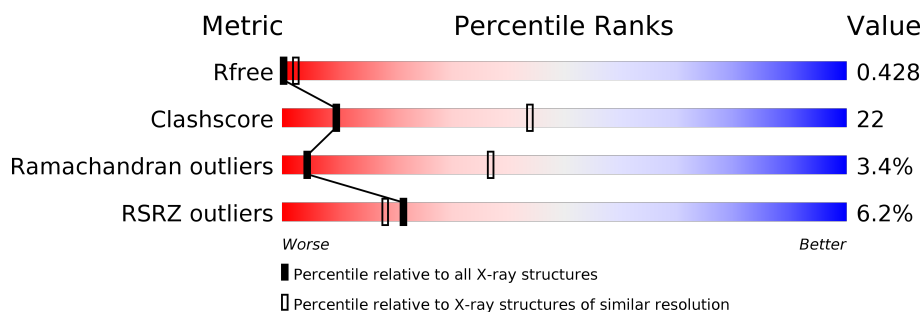
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 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}	100719	1008 (5.40-3.64)
Clashscore	112137	1029 (5.30-3.70)
Ramachandran outliers	110173	1025 (5.30-3.66)
RSRZ outliers	101464	1016 (5.40-3.64)

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 $\leq 5\%$. 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>8%</div> <div>83%</div> <div>12%</div> <div>...</div> </div>
1	B	578	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>...</div> </div>
1	C	578	<div> <div>8%</div> <div>84%</div> <div>11%</div> <div>...</div> </div>
1	I	578	<div> <div>11%</div> <div>81%</div> <div>13%</div> <div>...</div> </div>
1	J	578	<div> <div>%</div> <div>84%</div> <div>11%</div> <div>...</div> </div>
1	K	578	<div> <div>8%</div> <div>83%</div> <div>12%</div> <div>...</div> </div>
2	D	478	<div> <div>5%</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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	K	600	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32188 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			

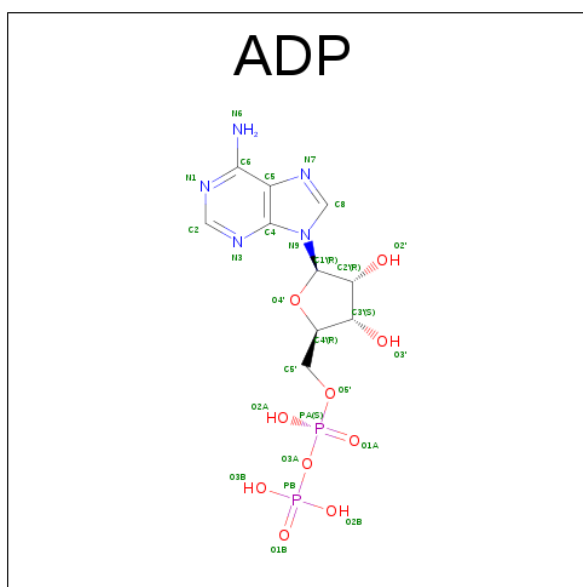
- Molecule 3 is a protein called V-type ATP synthase subunit D.

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

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

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

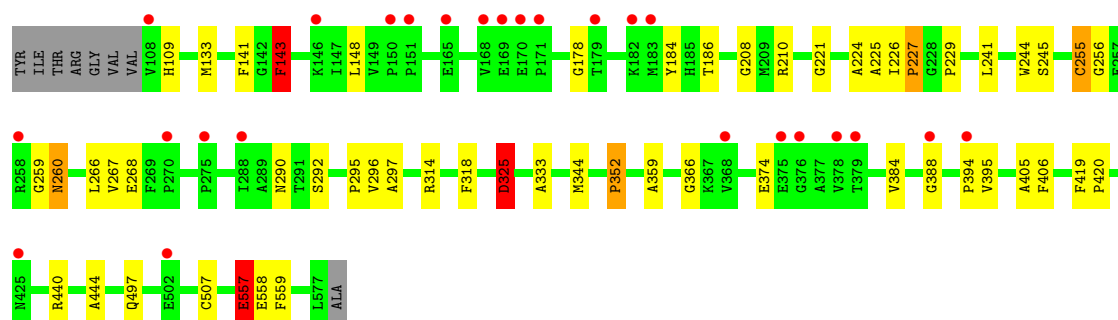
- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



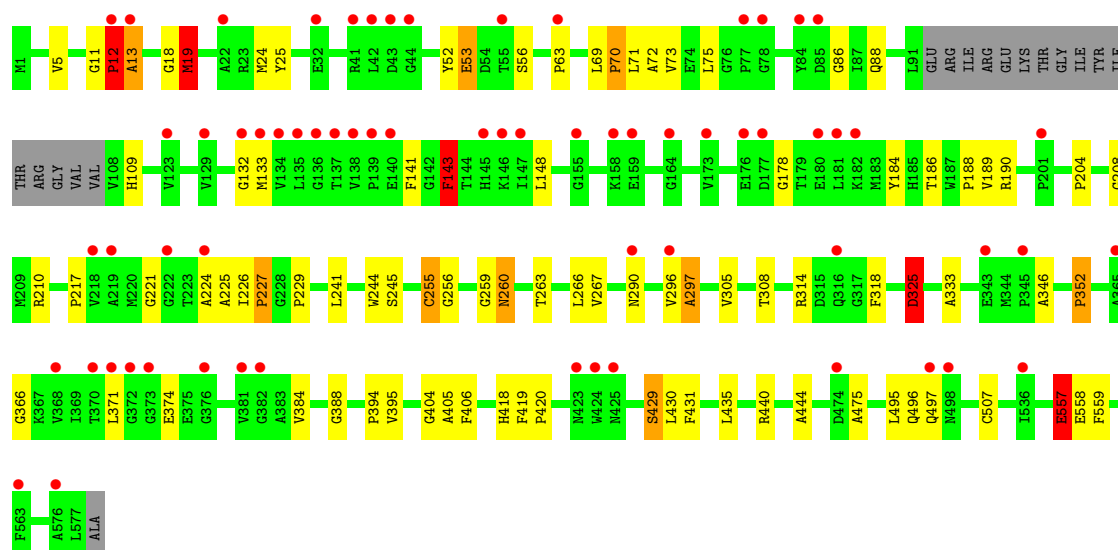
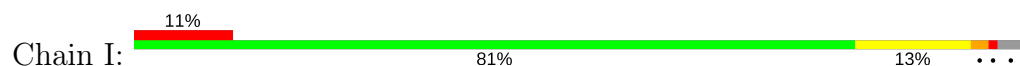
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 1: V-type ATP synthase alpha chain

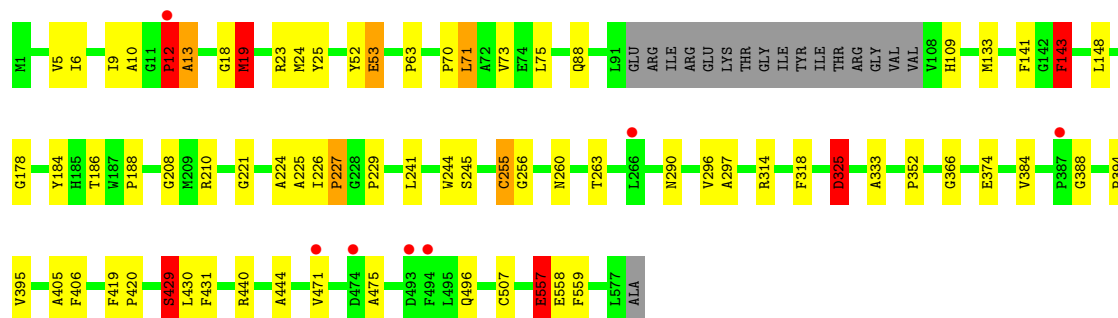
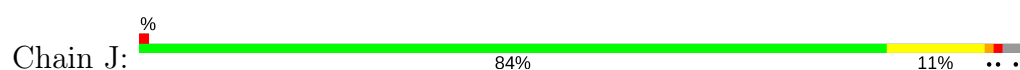




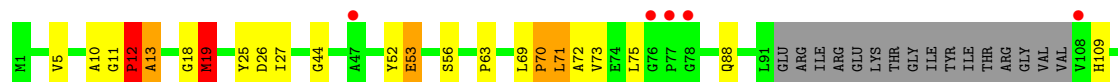
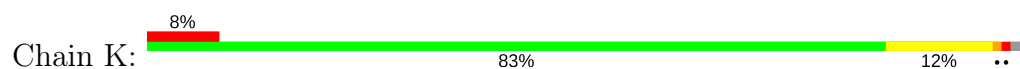
• Molecule 1: V-type ATP synthase alpha chain

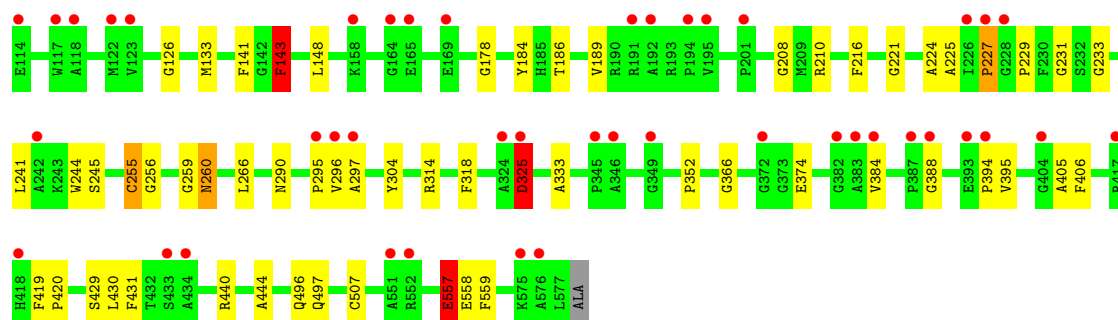


• Molecule 1: V-type ATP synthase alpha chain

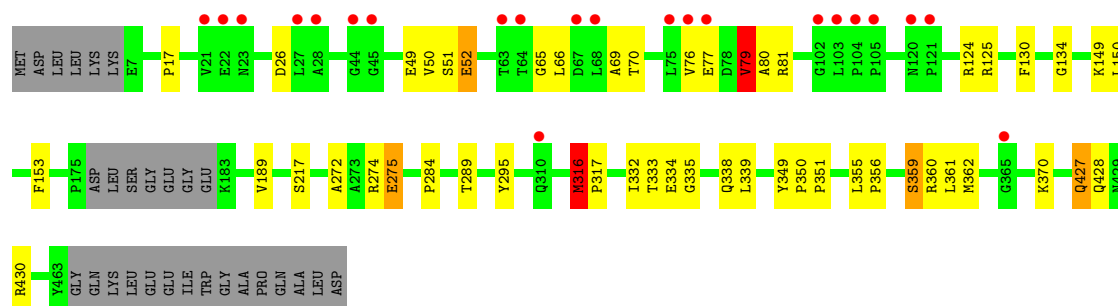
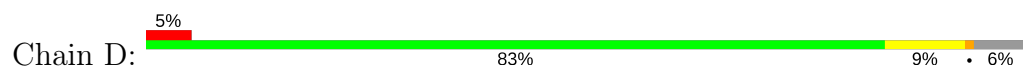


• Molecule 1: V-type ATP synthase alpha chain

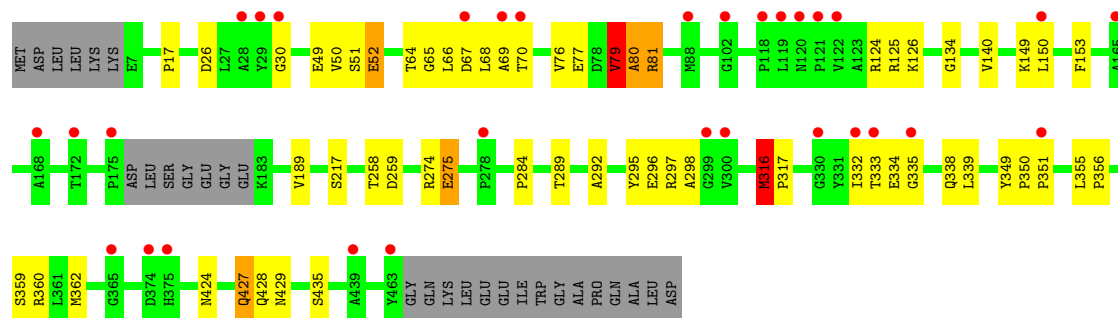
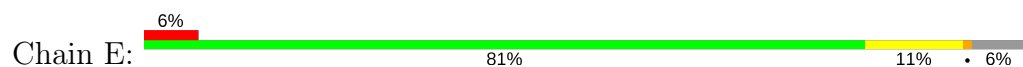




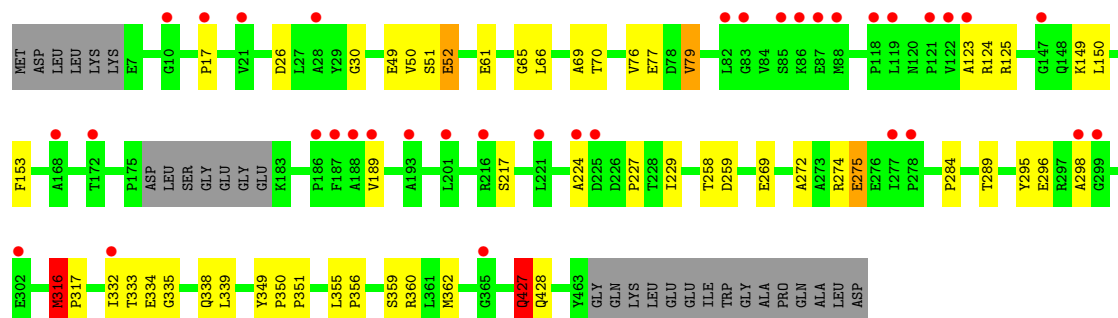
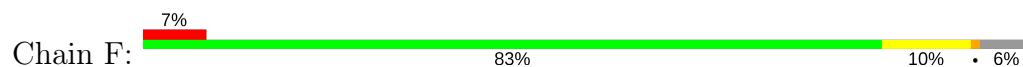
• Molecule 2: V-type ATP synthase beta chain



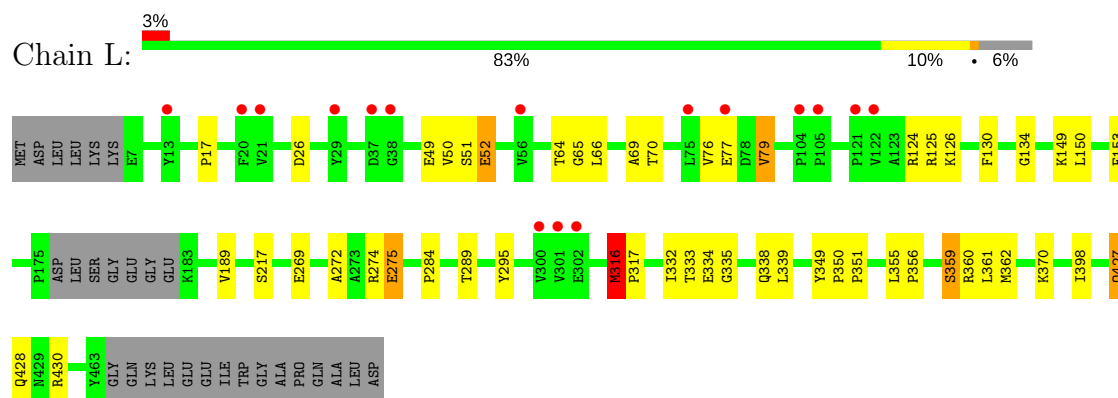
• Molecule 2: V-type ATP synthase beta chain



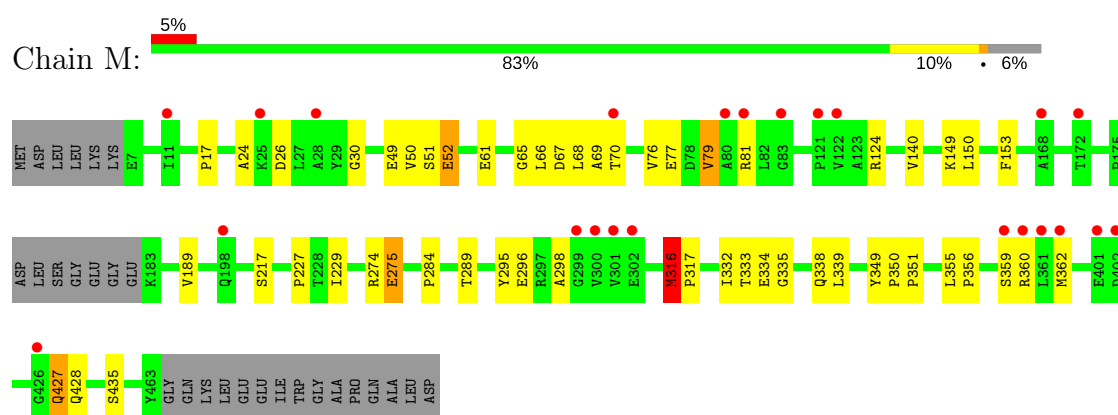
• Molecule 2: V-type ATP synthase beta chain



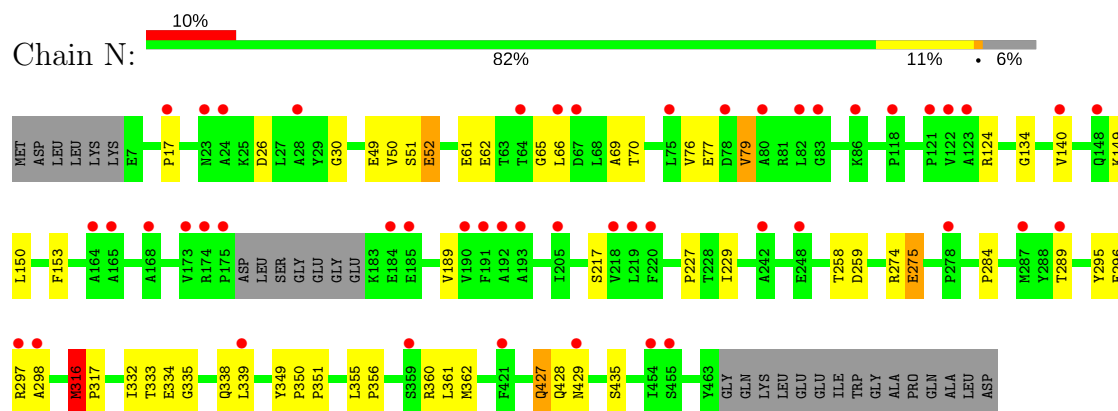
- Molecule 2: V-type ATP synthase beta chain



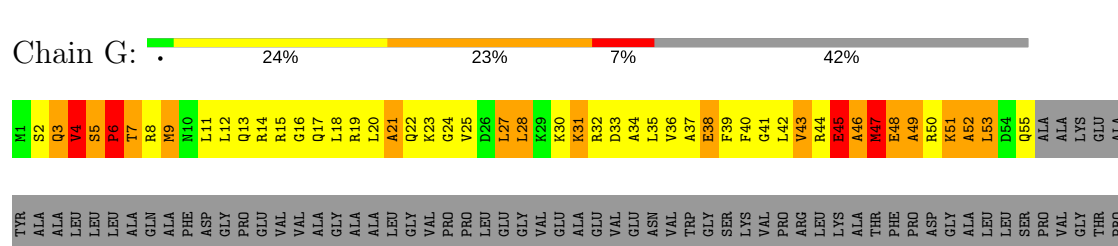
- Molecule 2: V-type ATP synthase beta chain



- Molecule 2: V-type ATP synthase beta chain



- Molecule 3: V-type ATP synthase subunit D



ALA Q181
TYR
THR L183
LEU E184
GLU Q185
ALA R186
SER E187
ARG R188
ALA E189
PHE D190
ARG T191
Y132
Y133
A134
E135
K196
L137
L138
I139
V140
A141
N142
T143
E144
T145
R146
L147
K148
GLU K149
GLY I150
GLY G151
E152
PRO E153
ASN I154
PRO K155
K156
GLN T157
VAL T158
R159
ILE R160
V161
N162
ALA A163
GLY L164
E165
Q166
V167
V168
I169
P170
G171
I172
R173
A174
Q175
I176
R177
F178
I179
Q180

Q181
V182
L183
E184
Q185
R186
E187
R188
E189
D190
T191
F192
R193
L194
K195
A196
I197
K198
G199
K200
I201
E202
A203
R204
E205
ALA
GLU
GLU
GLU
GLY
GLY
ARG
ARG
PRO
ASN
PRO
GLN
VAL
GLU
ILE
GLY
ALA
GLY
LEU

• Molecule 3: V-type ATP synthase subunit D

Chain O: 23% 24% 8% 42%

K1
S2
Q3
V4
S5
P6
T7
R8
M9
N10
L11
L12
L13
R14
R15
G16
Q17
L18
R19
L20
A21
Q22
K23
Q24
V25
D26
L27
L28
K29
K30
K31
R32
D33
GLU A34
L35
V36
A37
E38
F39
F40
G41
L42
V43
R44
E45
A46
M47
E48
A49
R50
K51
A52
L53
D54
Q55
ALA
ALA
LYS
GLY
PRO
ALA

TYR
ALA
ALA
LEU
LEU
LEU
ALA
SER
ALA
GLN
ALA
PHE
ASP
GLY
PRO
GLU
VAL
VAL
ALA
GLY
ALA
ALA
A21
GLY
VAL
PRO
PRO
LEU
GLU
GLY
VAL
GLU
I150
ALA
GLU
VAL
GLU
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

ALA
TYR
THR
LEU
GLU
SER
ALA
ARG
ALA
PHE
ARG
Y132
Y133
A134
E135
A136
I137
I138
R139
V140
A141
N142
T143
E144
T145
R146
L147
K148
K149
I150
G151
E152
E153
I154
K155
K156
T157
T158
R159
I160
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
E187
R188
E189
D190
T191
F192
R193
L194
K195
A196
I197
K198
G199
K200
I201
E202
A203
R204
E205
ALA
GLU
GLU
GLU
GLY
GLY
ARG
ARG
PRO
ASN
PRO
GLN
VAL
GLU
ILE
GLY
ALA
GLY
LEU

• Molecule 4: V-type ATP synthase subunit F

Chain H: 4% 79% 18%

M1
S24
S25
A29
E34
T35
R39
G40
M63
R64
G65
R66
I74
A75
G76
L77
K78
E79
A80
F81
Q82
G83
H84
D85
V86
T98
G99
F100
L104

• Molecule 4: V-type ATP synthase subunit F

Chain P: 7% 77% 16% 7%

M1
A16
S25
A29
E34
T35
R39
G40
L62
M63
R64
G65
R66
I74
A75
G76
L77
K78
Q82
G83
H84
D85
V86
V94
R95
I98
G99
F100
K103
L104

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	381.58Å 381.58Å 147.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 4.51 49.81 – 4.51	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.92-4.51) 96.8 (49.81-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 4.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.429 , 0.437 0.421 , 0.428	Depositor DCC
R_{free} test set	3582 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	145.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	32188	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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%)	1.20	9/3815 (0.2%)
1	B	0.59	3/2750 (0.1%)	1.21	12/3815 (0.3%)
1	C	0.59	3/2750 (0.1%)	1.20	10/3815 (0.3%)
1	I	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	J	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	K	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.80	7/2210 (0.3%)	1.03	13/3068 (0.4%)
2	E	0.85	7/2210 (0.3%)	1.04	10/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
2	L	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	M	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	N	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	122/637 (19.2%)	2.62	48/885 (5.4%)
3	O	4.09	126/637 (19.8%)	2.63	50/885 (5.6%)
4	H	1.48	6/508 (1.2%)	1.43	9/703 (1.3%)
4	P	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
All	All	1.08	308/32050 (1.0%)	1.27	244/44474 (0.5%)

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	6
1	B	0	5
1	C	0	5
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
2	F	0	3
2	L	0	4
2	M	0	3
2	N	0	3
4	H	0	3
4	P	0	2
All	All	0	60

The worst 5 of 308 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-25.00	0.98	1.53
3	G	47	MET	CA-CB	-24.93	0.99	1.53
3	O	27	LEU	CA-CB	14.81	1.87	1.53
3	G	27	LEU	CA-CB	14.78	1.87	1.53
4	P	75	ALA	N-CA	13.48	1.73	1.46

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	325	ASP	O-C-N	-39.90	58.86	122.70
1	J	325	ASP	O-C-N	-39.89	58.87	122.70
1	C	325	ASP	O-C-N	-39.89	58.87	122.70
1	A	325	ASP	O-C-N	-39.88	58.89	122.70
1	K	325	ASP	O-C-N	-39.85	58.94	122.70

There are no chirality outliers.

5 of 60 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	69	LEU	Peptide

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	2752	0	1302	92	0
1	B	2752	0	1303	65	0
1	C	2752	0	1303	100	0
1	I	2752	0	1300	122	0
1	J	2752	0	1303	61	2
1	K	2752	0	1302	94	0
2	D	2212	0	1009	66	0
2	E	2212	0	1008	80	0
2	F	2212	0	1009	94	0
2	L	2212	0	1009	80	0
2	M	2212	0	1009	59	2
2	N	2212	0	1009	76	0
3	G	639	0	299	131	0
3	O	639	0	299	136	0
4	H	509	0	255	12	0
4	P	509	0	255	23	0
5	A	27	0	12	2	0
5	C	27	0	12	1	0
5	I	27	0	12	0	0
5	K	27	0	12	5	0
All	All	32188	0	15022	1021	2

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 22.

The worst 5 of 1021 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	1.65
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
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
3:G:189:GLU:CB	3:G:189:GLU:CA	1.76	1.58

All (2) 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]	2.04	0.16
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	2.10	0.10

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	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	5	38
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	5	38
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	5	39
1	I	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	5	40
1	J	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	5	38
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	5	39
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	9	48
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	9	48
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	9	48
2	L	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	9	48
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	9	48
2	N	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	8	46
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%)	89 (87%)	11 (11%)	2 (2%)	9	48
4	P	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	9	48
All	All	6472/6990 (93%)	5808 (90%)	443 (7%)	221 (3%)	4	37

5 of 221 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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ADP	A	600	-	25,29,29	1.12	3 (12%)	24,45,45	0.76	0
5	ADP	C	600	-	25,29,29	0.94	2 (8%)	24,45,45	1.00	2 (8%)
5	ADP	I	600	-	25,29,29	1.11	3 (12%)	24,45,45	0.76	0
5	ADP	K	600	-	25,29,29	0.93	2 (8%)	24,45,45	1.00	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	600	-	-	0/12/32/32	0/3/3/3
5	ADP	C	600	-	-	0/12/32/32	0/3/3/3
5	ADP	I	600	-	-	0/12/32/32	0/3/3/3
5	ADP	K	600	-	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	600	ADP	PB-O2B	-2.28	1.45	1.54
5	C	600	ADP	PB-O2B	-2.28	1.45	1.54
5	C	600	ADP	PA-O1A	-2.20	1.42	1.50
5	A	600	ADP	PB-O2B	-2.20	1.45	1.54
5	K	600	ADP	PA-O1A	-2.20	1.42	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ADP	O4'-C4'-C3'	-2.05	101.08	105.17
5	C	600	ADP	O4'-C4'-C3'	-2.05	101.09	105.17
5	C	600	ADP	O3B-PB-O2B	2.26	116.71	107.61
5	K	600	ADP	O3B-PB-O2B	2.26	116.72	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ADP	2	0
5	C	600	ADP	1	0
5	K	600	ADP	5	0

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, 95th 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	561/578 (97%)	0.19	44 (7%) 14 13	103, 162, 214, 214	0
1	B	561/578 (97%)	-0.18	10 (1%) 69 62	79, 130, 144, 144	0
1	C	561/578 (97%)	0.22	44 (7%) 14 13	137, 189, 210, 210	0
1	I	561/578 (97%)	0.41	66 (11%) 5 7	172, 172, 232, 232	0
1	J	561/578 (97%)	-0.36	7 (1%) 79 72	50, 58, 104, 104	0
1	K	561/578 (97%)	0.33	48 (8%) 11 11	146, 177, 189, 189	0
2	D	450/478 (94%)	0.00	22 (4%) 30 26	118, 118, 188, 188	0
2	E	450/478 (94%)	0.13	31 (6%) 18 15	122, 130, 162, 162	0
2	F	450/478 (94%)	0.22	35 (7%) 14 13	109, 217, 217, 217	0
2	L	450/478 (94%)	-0.04	16 (3%) 43 36	98, 98, 158, 158	0
2	M	450/478 (94%)	0.02	23 (5%) 29 25	99, 99, 148, 148	0
2	N	450/478 (94%)	0.47	48 (10%) 7 8	158, 250, 250, 250	0
3	G	129/223 (57%)	-0.70	0 100 100	34, 34, 49, 49	0
3	O	129/223 (57%)	-0.62	1 (0%) 86 80	84, 85, 85, 85	0
4	H	104/104 (100%)	0.08	4 (3%) 41 34	110, 110, 134, 134	0
4	P	104/104 (100%)	-0.02	7 (6%) 19 16	94, 94, 141, 141	0
All	All	6532/6990 (93%)	0.08	406 (6%) 21 18	34, 137, 232, 250	0

The worst 5 of 406 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	77	PRO	10.7
2	N	191	PHE	9.3
1	I	372	GLY	9.3
2	N	192	ALA	8.4
2	D	67	ASP	8.3

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	ADP	K	600	27/27	0.63	0.47	0.17	112,112,112,112	0
5	ADP	C	600	27/27	0.79	0.28	-0.26	116,116,116,116	0
5	ADP	A	600	27/27	0.82	0.26	-0.35	109,109,109,109	0
5	ADP	I	600	27/27	0.80	0.28	-0.96	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.