wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1R5Z
Title	:	Crystal Structure of Subunit C of V-ATPase
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Deposited on	:	2003-10-14
Resolution	:	1.95 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

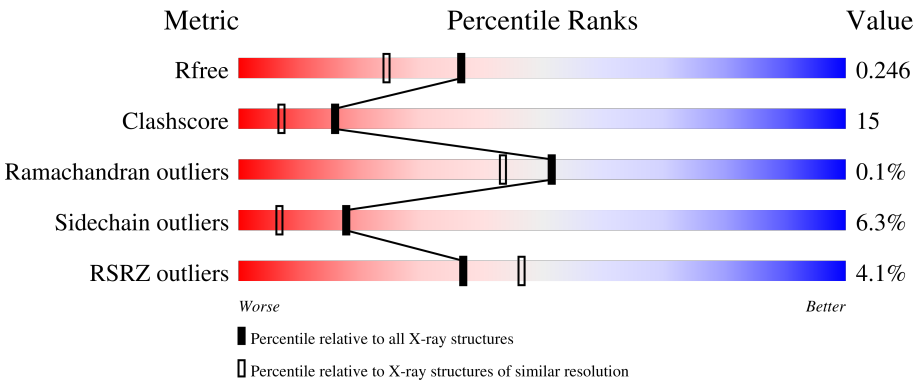
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	323	3% 78% 20% ••
1	B	323	3% 75% 19% • ••
1	C	323	6% 73% 22% • ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8179 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 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2514	1599	460	451	4	0	0	0
1	B	320	2514	1599	460	451	4	0	0	0
1	C	320	2514	1599	460	451	4	0	0	0

- Molecule 2 is water.

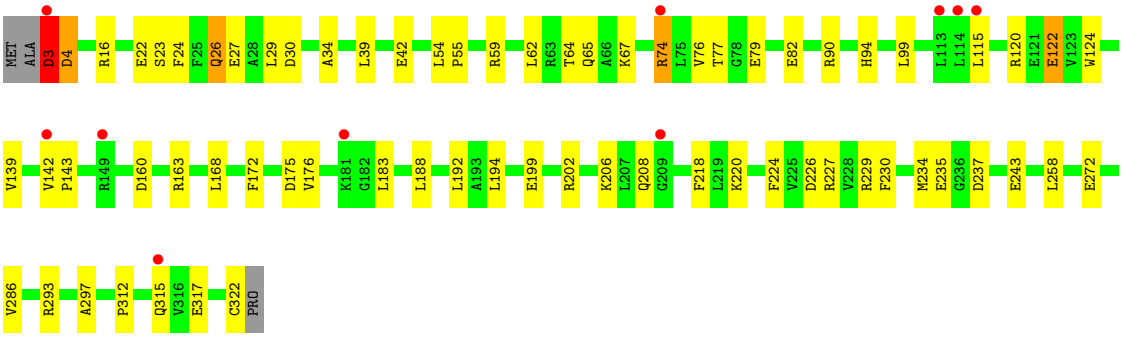
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	237	237	237	0	0
2	B	217	217	217	0	0
2	C	183	183	183	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

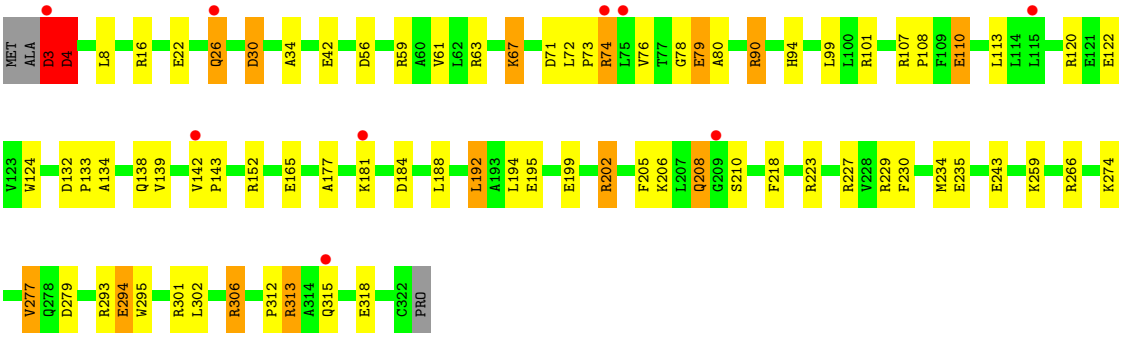
• Molecule 1: V-type ATP synthase subunit C

Chain A:



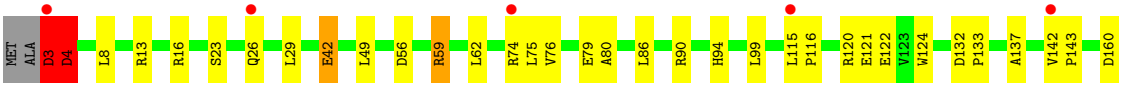
• Molecule 1: V-type ATP synthase subunit C

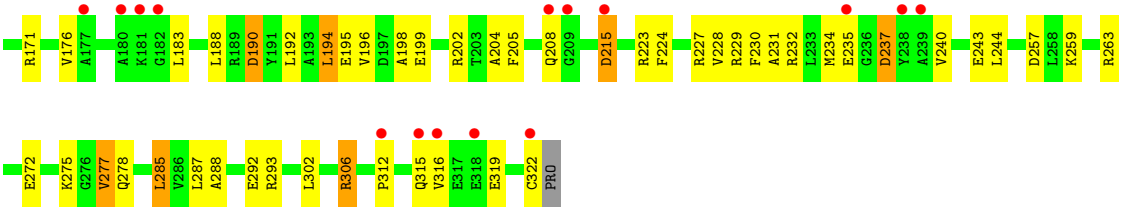
Chain B:



• Molecule 1: V-type ATP synthase subunit C

Chain C:




R171
V176
A177
A180
K181
G182
L183
L188
R189
D190
Y191
L192
A193
L194
E195
V196
D197
A198
E199
R202
T203
A204
F205
Q208
G209
D215
R223
F224
R227
V228
R229
F230
A231
R232
L233
M234
E235
G236
D237
Y238
A239
V240
E243
L244
D257
L258
K259
R263
E272
K275
G276
V277
Q278
L285
V286
L287
A288
E292
R293
L302
R306
P312
Q315
V316
E317
E318
E319
C322
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	118.43Å 118.43Å 152.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.95 37.56 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.95) 99.4 (37.56-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.191 , 0.249 0.192 , 0.246	Depositor DCC
R_{free} test set	4353 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8179	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2787e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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	1.22	6/2553 (0.2%)	1.11	12/3447 (0.3%)
1	B	1.14	3/2553 (0.1%)	1.08	10/3447 (0.3%)
1	C	1.11	4/2553 (0.2%)	1.07	11/3447 (0.3%)
All	All	1.16	13/7659 (0.2%)	1.09	33/10341 (0.3%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	ALA	CA-CB	6.39	1.65	1.52
1	A	224	PHE	CE2-CZ	5.75	1.48	1.37
1	C	137	ALA	CA-CB	5.68	1.64	1.52
1	A	293	ARG	CG-CD	5.67	1.66	1.51
1	A	297	ALA	CA-CB	5.65	1.64	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3	ASP	CB-CG-OD2	9.28	126.65	118.30
1	B	3	ASP	CB-CG-OD2	8.67	126.10	118.30
1	A	3	ASP	CB-CG-OD2	8.53	125.98	118.30
1	A	160	ASP	CB-CG-OD2	7.68	125.21	118.30
1	C	237	ASP	CB-CG-OD2	6.48	124.13	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	ASP	Peptide
1	B	3	ASP	Peptide
1	C	3	ASP	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	2514	0	2587	67	0
1	B	2514	0	2587	71	0
1	C	2514	0	2587	85	0
2	A	237	0	0	23	0
2	B	217	0	0	21	0
2	C	183	0	0	21	0
All	All	8179	0	7761	223	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 15.

The worst 5 of 223 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)
1:A:229:ARG:NH1	1:A:243:GLU:OE1	1.77	1.17
1:B:142:VAL:HG23	1:B:143:PRO:CD	1.75	1.14
1:B:142:VAL:HG23	1:B:143:PRO:HD3	1.11	1.09
1:A:94:HIS:HB2	2:A:529:HOH:O	1.51	1.08
1:B:165:GLU:HG2	2:B:523:HOH:O	1.51	1.08

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	318/323 (98%)	314 (99%)	4 (1%)	0	100	100
1	B	318/323 (98%)	312 (98%)	5 (2%)	1 (0%)	41	30
1	C	318/323 (98%)	311 (98%)	7 (2%)	0	100	100
All	All	954/969 (98%)	937 (98%)	16 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	210	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/256 (99%)	246 (97%)	8 (3%)	40	28
1	B	254/256 (99%)	230 (91%)	24 (9%)	8	2
1	C	254/256 (99%)	238 (94%)	16 (6%)	18	7
All	All	762/768 (99%)	714 (94%)	48 (6%)	18	7

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	302	LEU
1	C	59	ARG

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Mol	Chain	Res	Type
1	B	306	ARG
1	C	3	ASP
1	C	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	GLN
1	B	94	HIS
1	C	208	GLN
1	C	65	GLN
1	B	26	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	320/323 (99%)	0.06	10 (3%)	49	58	18, 28, 47, 57	0
1	B	320/323 (99%)	0.07	9 (2%)	53	62	22, 32, 51, 65	0
1	C	320/323 (99%)	0.31	20 (6%)	20	28	22, 34, 61, 70	0
All	All	960/969 (99%)	0.15	39 (4%)	37	46	18, 31, 56, 70	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	GLY	5.5
1	A	209	GLY	4.7
1	C	209	GLY	4.7
1	C	181	LYS	4.3
1	C	315	GLN	4.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.