



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:58 AM GMT

PDB ID : 3GQB
Title : Crystal Structure of the A3B3 complex from V-ATPase
Authors : Meher, M.; Akimoto, S.; Iwata, M.; Nagata, K.; Hori, Y.; Yoshida, M.;
Yokoyama, S.; Iwata, S.; Yokoyama, K.
Deposited on : 2009-03-24
Resolution : 2.80 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
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

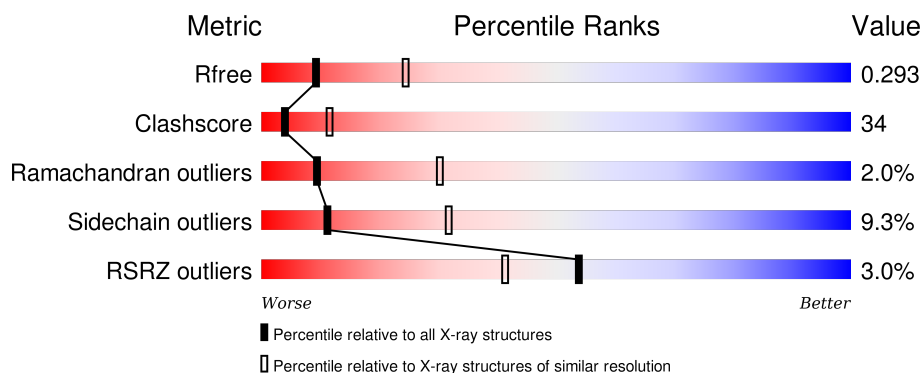
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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>3%</div> <div>52% 41% 7%</div> </div>
1	C	578	<div> <div>3%</div> <div>49% 44% 7%</div> </div>
2	B	464	<div> <div>2%</div> <div>56% 37% 6%</div> </div>
2	D	464	<div> <div>4%</div> <div>59% 35% 5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16863 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	578	Total	C	N	O	S	0	0	0
			4477	2856	763	839	19			
1	C	578	Total	C	N	O	S	0	0	0
			4477	2856	763	839	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SER	CYS	ENGINEERED	UNP Q56403
A	235	SER	THR	ENGINEERED	UNP Q56403
A	255	SER	CYS	ENGINEERED	UNP Q56403
A	507	SER	CYS	ENGINEERED	UNP Q56403
C	28	SER	CYS	ENGINEERED	UNP Q56403
C	235	SER	THR	ENGINEERED	UNP Q56403
C	255	SER	CYS	ENGINEERED	UNP Q56403
C	507	SER	CYS	ENGINEERED	UNP Q56403

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	460	Total	C	N	O	S	0	0	0
			3601	2280	623	689	9			
2	D	460	Total	C	N	O	S	0	0	0
			3601	2280	623	689	9			

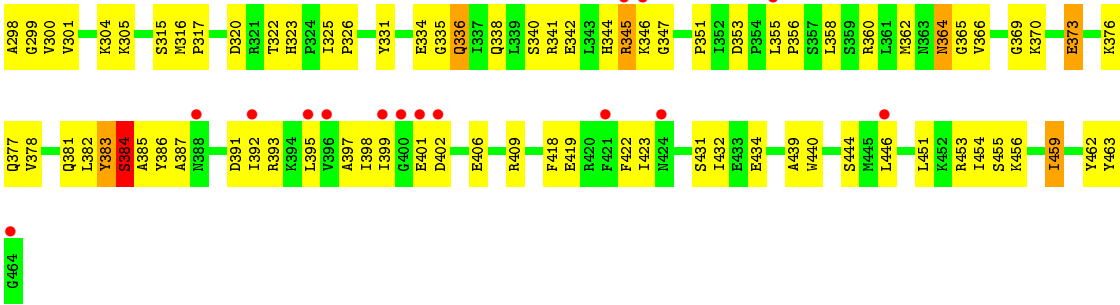
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	SER	CYS	ENGINEERED	UNP Q56404
D	264	SER	CYS	ENGINEERED	UNP Q56404

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total 199	O 199	0	0
3	B	135	Total 135	O 135	0	0
3	C	239	Total 239	O 239	0	0
3	D	134	Total 134	O 134	0	0





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.37Å 199.37Å 179.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.95-2.80) 97.7 (19.94-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.250 , 0.281 0.263 , 0.293	Depositor DCC
R_{free} test set	4941 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 8.9	EDS
Estimated twinning fraction	0.845 for 1.000H, 1.000K, L 0.155 for -1.000H, -1.000K, L 0.077 for -h,-k,l	Xtriage
Reported twinning fraction	0.845 for 1.000H, 1.000K, L 0.155 for -1.000H, -1.000K, L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 98400 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16863	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.56	0/4573	0.71	1/6203 (0.0%)
1	C	0.58	0/4573	0.72	2/6203 (0.0%)
2	B	0.54	0/3668	0.67	0/4965
2	D	0.50	0/3668	0.65	0/4965
All	All	0.55	0/16482	0.69	3/22336 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	241	LEU	CA-CB-CG	5.42	127.76	115.30
1	C	215	LEU	CA-CB-CG	-5.13	103.49	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4477	0	4494	367	0
1	C	4477	0	4494	374	1
2	B	3601	0	3627	193	1
2	D	3601	0	3627	197	0
3	A	199	0	0	120	1
3	B	135	0	0	60	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	239	0	0	135	0
3	D	134	0	0	70	0
All	All	16863	0	16242	1107	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 34.

The worst 5 of 1107 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:256:GLY:O	1:A:329:ARG:HD2	1.24	1.32
1:A:574:PHE:HB3	3:A:697:HOH:O	1.33	1.29
1:A:447:TYR:HA	3:A:651:HOH:O	1.17	1.27
1:C:124:LYS:HD3	3:C:714:HOH:O	1.25	1.26
1:C:256:GLY:O	1:C:329:ARG:HD2	1.22	1.25

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)
2:B:410:ARG:NH2	1:C:478:ASP:OD2[6_555]	2.13	0.07
3:A:653:HOH:O	3:B:704:HOH:O[2_665]	2.14	0.06

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	576/578 (100%)	512 (89%)	51 (9%)	13 (2%)	8	26
1	C	576/578 (100%)	504 (88%)	61 (11%)	11 (2%)	10	32
2	B	458/464 (99%)	407 (89%)	43 (9%)	8 (2%)	11	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	458/464 (99%)	408 (89%)	41 (9%)	9 (2%)	9	30
All	All	2068/2084 (99%)	1831 (88%)	196 (10%)	41 (2%)	9	30

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	GLY
1	A	235	SER
1	A	555	SER
2	B	281	ARG
2	B	346	LYS

5.3.2 Protein sidechains ⓘ

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	468/468 (100%)	425 (91%)	43 (9%)	11	32
1	C	468/468 (100%)	419 (90%)	49 (10%)	8	24
2	B	386/390 (99%)	352 (91%)	34 (9%)	12	35
2	D	386/390 (99%)	354 (92%)	32 (8%)	14	38
All	All	1708/1716 (100%)	1550 (91%)	158 (9%)	11	32

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	MET
1	C	111	LEU
2	D	268	ARG
2	B	370	LYS
1	C	27	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	407	ASN
1	C	202	ASN
2	D	344	HIS
1	C	3	GLN
1	C	196	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 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 [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	578/578 (100%)	0.28	16 (2%) 56 44	9, 29, 57, 63	0
1	C	578/578 (100%)	0.33	16 (2%) 56 44	9, 29, 57, 63	0
2	B	460/464 (99%)	0.21	10 (2%) 65 54	5, 28, 54, 67	0
2	D	460/464 (99%)	0.28	20 (4%) 39 27	5, 28, 54, 67	0
All	All	2076/2084 (99%)	0.28	62 (2%) 54 41	5, 29, 56, 67	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	464	GLY	5.6
2	B	401	GLU	5.3
2	D	395	LEU	5.2
2	D	400	GLY	5.0
1	C	388	GLY	4.8

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.