

wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 12:34 am BST

PDB ID : 2GMQ

Title: Crystal structure of protein EF0006 from Enterococcus faecalis

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tural Genomics (MCSG)

Deposited on : 2006-04-07

Resolution : 1.76 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

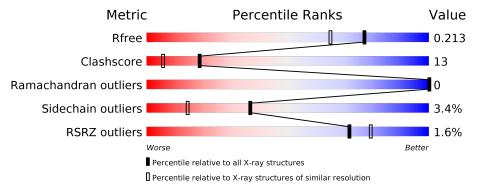
Validation Pipeline (wwPDB-VP) : 2.11

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 1.76 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	$\begin{array}{c} \textbf{Whole archive} \\ (\# \textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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	118	65%	15% •	16%				
1	В	118	50%	33%	• 16%				



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1963 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 Hypothetical protein EF0006.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	99	Total	С	N	О	Se	0	11	0
1	Λ	99	874	575	141	154	4	0	11	U
1	B	99	Total	С	N	О	Se	0	19	0
1	Б	99	912	608	144	157	3		19	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4
A	13	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4
A	45	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4
A	47	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4
В	1	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4
В	13	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4
В	45	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4
В	47	MSE	MET	MODIFIED RESIDUE	UNP Q82YS4

• Molecule 2 is water.

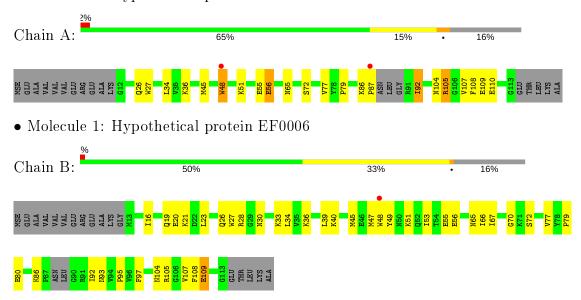
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	92	Total O 92 92	0	0
2	В	85	Total O 85 85	0	0



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: Hypothetical protein EF0006





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants	83.12Å 83.40Å 83.92Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	
Resolution (Å)	50.00 - 1.76	Depositor
resolution (A)	26.52 - 1.75	EDS
% Data completeness	$93.8 \ (50.00 - 1.76)$	Depositor
(in resolution range)	$92.9 \ (26.52 - 1.75)$	EDS
R_{merge}	0.09	Depositor
$\frac{\mathrm{R}_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.83 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.191 , 0.217	Depositor
R, R_{free}	0.188 , 0.213	DCC
R_{free} test set	1390 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 34.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.33$	Xtriage
	0.020 for -h,-l,-k	
	0.018 for l,-k,h	
Estimated twinning fraction	0.479 for -k,-h,-l	Xtriage
	0.017 for k,-l,-h	
	0.017 for -l,h,-k	
F_o, F_c correlation	0.96	EDS
Total number of atoms	1963	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



 $^{^{1}}$ Intensities estimated from amplitudes.

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	Bo	nd lengths	Bond angles		
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z >5	
1	A	1.29	8/919 (0.9%)	1.02	$1/1230 \ (0.1\%)$	
1	В	1.22	7/982 (0.7%)	0.96	1/1317~(0.1%)	
All	All	1.25	15/1901~(0.8%)	0.99	$2/2547 \ (0.1\%)$	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
1	A	56[A]	GLU	CG-CD	6.94	1.62	1.51
1	A	56[B]	GLU	CG-CD	6.94	1.62	1.51
1	В	56[A]	GLU	CG-CD	6.88	1.62	1.51
1	В	56[B]	GLU	CG-CD	6.88	1.62	1.51
1	В	56[A]	GLU	CD-OE2	6.64	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	A	105	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	В	23	LEU	CB-CG-CD2	-6.99	99.11	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	ol Chain R		Type	Group	
1	В	86	LYS	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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	Α	874	0	937	16	0
1	В	912	0	1008	36	2
2	A	92	0	0	3	1
2	В	85	0	0	6	2
All	All	1963	0	1945	49	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 13.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
1:B:26:GLN:NE2	1:B:36[A]:LYS:HE3	1.51	1.23
1:B:39[B]:LEU:HD11	1:B:47:MSE:SE	1.92	1.18
1:B:45[B]:MSE:HE1	1:B:48[B]:TRP:CD1	1.83	1.12
1:B:45[B]:MSE:CE	1:B:48[B]:TRP:CD1	2.40	1.02
1:B:26:GLN:HE22	1:B:36[A]:LYS:HE3	1.14	0.96

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	$egin{array}{l} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	Clash overlap (Å)
1:B:21[B]:LYS:NZ	2:B:163:HOH:O[6_655]	1.93	0.27
2:A:147:HOH:O	2:A:194:HOH:O[6_655]	2.15	0.05
1:B:21[B]:LYS:NZ	2:B:122:HOH:O[6_655]	2.19	0.01

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	Perce	entiles
1	A	106/118 (90%)	104 (98%)	2 (2%)	0	100	100
1	В	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
All	All	$220/236 \ (93\%)$	216 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	S
1	A	100/101 (99%)	97 (97%)	3 (3%)	41 18	
1	В	107/101 (106%)	101 (94%)	6 (6%)	21 5	
All	All	207/202 (102%)	198 (96%)	9 (4%)	37 9	

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	55[B]	GLU
1	В	109[B]	GLU
1	В	80[B]	GLU
1	A	104	ASN
1	В	80[A]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	В	26	GLN
1	В	104	ASN



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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	96/118 (81%)	0.06	2 (2%) 63 71	23, 30, 42, 56	0
1	В	96/118 (81%)	0.06	1 (1%) 82 87	26, 32, 42, 59	0
All	All	192/236 (81%)	0.06	3 (1%) 72 79	23, 31, 42, 59	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	PRO	2.5
1	В	48[A]	TRP	2.2
1	A	48[A]	TRP	2.0

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 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.

