

wwPDB X-ray Structure Validation Summary Report (i)

Oct 18, 2023 – 01:21 PM EDT

PDB ID : 1MC8

Title : Crystal Structure of Flap Endonuclease-1 R42E mutant from Pyrococcus

horikoshii

Authors: Matsui, E.; Musti, K.V.; Abe, J.; Yamazaki, K.; Matsui, I.; Harata, K.

Deposited on : 2002-08-06

Resolution : 3.10 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) : 1.13

henix) : 1.13 EDS : 2.36

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)

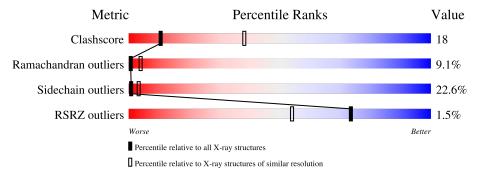
Validation Pipeline (wwPDB-VP) : 2.36

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 3.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	343	40%	37%	13%	6% •	
1	В	343	41%	40%	11%	5% •	



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5274 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 Flap Endonuclease-1.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	331	Total	С	N	О	S	0	0	0
1	71	331	2637	1683	453	494	7	U	U	0
1	D	331	Total	С	N	Ο	S	0	0	0
1	Б	331	2637	1683	453	494	7	0	U	U

There are 2 discrepancies between the modelled and reference sequences:

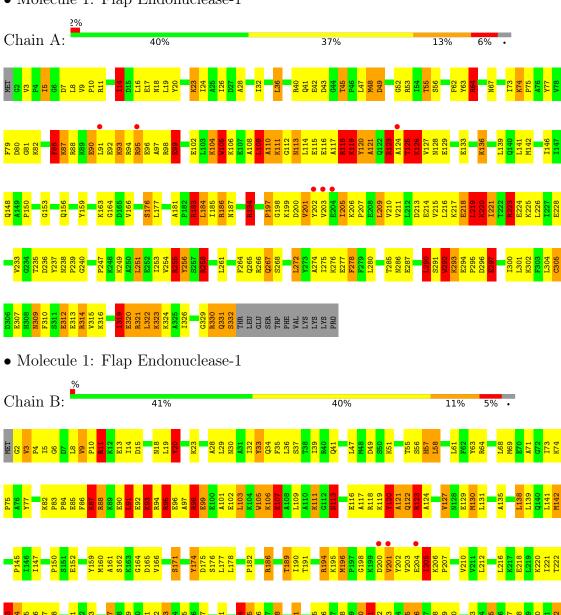
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLU	ARG	engineered mutation	UNP O50123
В	42	GLU	ARG	engineered mutation	UNP O50123



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: Flap Endonuclease-1









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants	62.67Å 62.67Å 180.69Å	D: t
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 - 3.10	Depositor
Resolution (A)	34.72 - 3.00	EDS
% Data completeness	(Not available) (8.00-3.10)	Depositor
(in resolution range)	100.0 (34.72-3.00)	EDS
R_{merge}	0.10	Depositor
R_{sum}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.55 (at 3.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , 0.279	Depositor
it, it free	0.194 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.28, 47.9	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
	0.021 for -h,-k,l	
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage
	0.025 for -k,-h,-l	
F_o, F_c correlation	0.94	EDS
Total number of atoms	5274	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% 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.



¹Intensities 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	Boı	nd lengths	Bond angles		
IVIOI	Cham	Chair RMSZ $\# Z >$		RMSZ	# Z >5	
1	A	0.96	0/2682	1.98	83/3606 (2.3%)	
1	В	0.93	$1/2682 \ (0.0\%)$	1.91	66/3606 (1.8%)	
All	All	0.95	1/5364~(0.0%)	1.94	149/7212 (2.1%)	

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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	В	105	TRP	CG-CD2	-5.06	1.35	1.43

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	321	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	В	98	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	В	120	TYR	CB-CG-CD2	9.98	126.99	121.00
1	A	314	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	В	255	ARG	NE-CZ-NH1	9.40	125.00	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Group
1	В	196	MET	Peptide
1	В	20	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	В	82	LYS	Peptide
1	В	83	PRO	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	2637	0	2719	102	0
1	В	2637	0	2719	99	0
All	All	5274	0	5438	198	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 18.

The worst 5 of 198 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:14:ILE:HD12	1:A:209:LEU:HB2	1.59	0.85
1:A:294:GLU:HG3	1:A:326:ILE:HD13	1.58	0.84
1:A:104:LYS:HD3	1:A:126:LYS:HD2	1.69	0.75
1:A:221:ILE:HD11	1:A:255:ARG:HA	1.67	0.74
1:B:11:ARG:HB3	1:B:210:VAL:HG22	1.70	0.72

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	329/343~(96%)	228 (69%)	68 (21%)	33 (10%)	0 3
1	В	329/343~(96%)	243 (74%)	59 (18%)	27 (8%)	1 5
All	All	658/686 (96%)	471 (72%)	127 (19%)	60 (9%)	1 4

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	90	GLU
1	A	98	ARG
1	A	126	LYS
1	A	194	ARG

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	Pe	erce	enti	les
1	A	281/293 (96%)	210 (75%)	71 (25%)		0	1	
1	В	281/293 (96%)	225 (80%)	56 (20%)		1	5	
All	All	562/586 (96%)	435 (77%)	127 (23%)		1	3	

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	LEU
1	В	224	GLU
1	В	11	ARG
1	В	223	ARG
1	В	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	57	HIS

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Mol	Chain	Res	Type
1	В	122	GLN
1	В	187	ASN
1	A	67	ASN
1	A	113	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 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, 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	331/343 (96%)	-0.54	6 (1%) 68 47	13, 37, 74, 83	0
1	В	331/343 (96%)	-0.54	4 (1%) 79 61	10, 37, 70, 84	0
All	All	662/686 (96%)	-0.54	10 (1%) 73 54	10, 37, 71, 84	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	ALA	3.3
1	A	202	TYR	2.8
1	В	326	ILE	2.8
1	В	204	GLU	2.8
1	В	200	ASP	2.5

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.

