



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 08:22 am GMT

PDB ID : 2DEO
Title : 1510-N membrane protease specific for a stomatin homolog from *Pyrococcus horikoshii*
Authors : Yokoyama, H.; Matsui, I.
Deposited on : 2006-02-16
Resolution : 3.00 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
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)	:	recalc28949

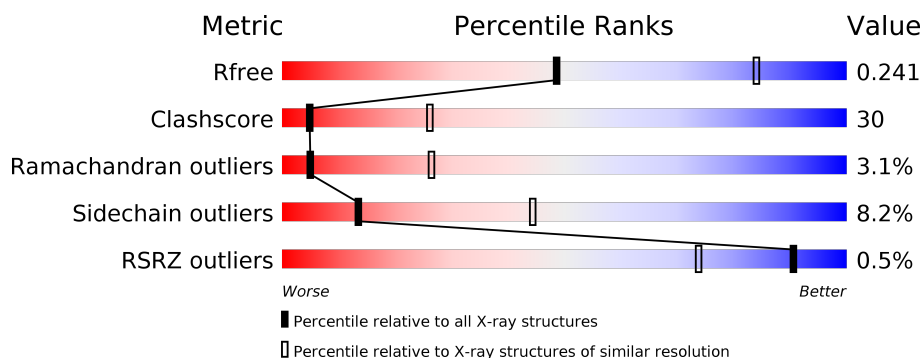
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	230	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 48%, green 35%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 48% 35% 13% </div> </div>
1	B	230	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 43%, yellow 37%, orange 7%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 43% 37% 7% 13% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3124 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 441aa long hypothetical nfeD protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	Se	88	0	0
			1542	986	255	296	1	4			
1	B	200	Total	C	N	O	S	Se	88	0	0
			1550	994	256	295	1	4			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MSE	-	INITIATING METHIONINE	UNP O59179
A	70	MSE	MET	MODIFIED RESIDUE	UNP O59179
A	71	MSE	MET	MODIFIED RESIDUE	UNP O59179
A	111	MSE	MET	MODIFIED RESIDUE	UNP O59179
A	199	MSE	MET	MODIFIED RESIDUE	UNP O59179
A	237	LEU	-	CLONING ARTIFACT	UNP O59179
A	238	GLU	-	CLONING ARTIFACT	UNP O59179
A	239	HIS	-	EXPRESSION TAG	UNP O59179
A	240	HIS	-	EXPRESSION TAG	UNP O59179
A	241	HIS	-	EXPRESSION TAG	UNP O59179
A	242	HIS	-	EXPRESSION TAG	UNP O59179
A	243	HIS	-	EXPRESSION TAG	UNP O59179
A	244	HIS	-	EXPRESSION TAG	UNP O59179
B	15	MSE	-	INITIATING METHIONINE	UNP O59179
B	70	MSE	MET	MODIFIED RESIDUE	UNP O59179
B	71	MSE	MET	MODIFIED RESIDUE	UNP O59179
B	111	MSE	MET	MODIFIED RESIDUE	UNP O59179
B	199	MSE	MET	MODIFIED RESIDUE	UNP O59179
B	237	LEU	-	CLONING ARTIFACT	UNP O59179
B	238	GLU	-	CLONING ARTIFACT	UNP O59179
B	239	HIS	-	EXPRESSION TAG	UNP O59179
B	240	HIS	-	EXPRESSION TAG	UNP O59179
B	241	HIS	-	EXPRESSION TAG	UNP O59179
B	242	HIS	-	EXPRESSION TAG	UNP O59179
B	243	HIS	-	EXPRESSION TAG	UNP O59179

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Chain	Residue	Modelled	Actual	Comment	Reference
B	244	HIS	-	EXPRESSION TAG	UNP O59179

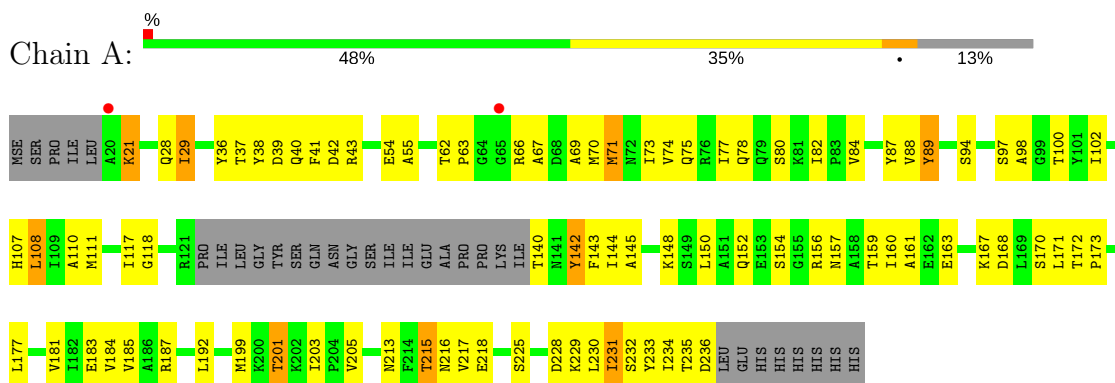
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	12	Total O 12 12	0	0

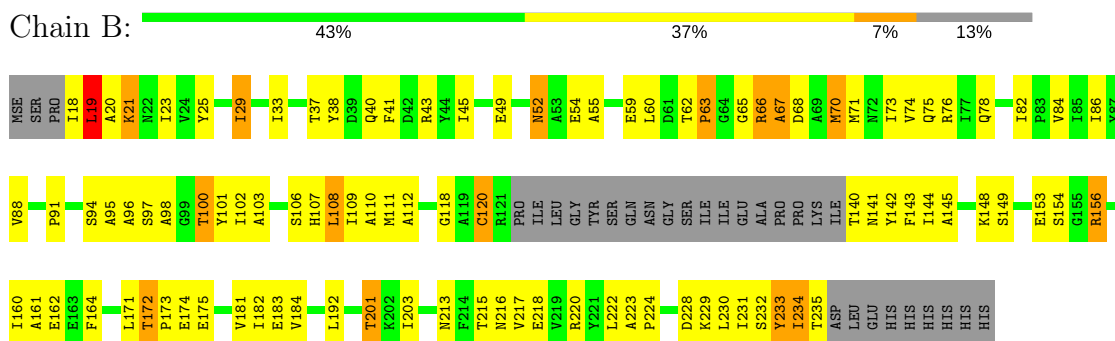
3 Residue-property plots [i](#)

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: 441aa long hypothetical nfeD protein



- Molecule 1: 441aa long hypothetical nfeD protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.21Å 108.40Å 59.34Å 90.00° 110.06° 90.00°	Depositor
Resolution (Å)	19.76 – 3.00 19.76 – 2.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.76-3.00) 99.9 (19.76-2.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.242 0.197 , 0.241	Depositor DCC
R_{free} test set	1263 reflections (10.26%)	DCC
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3124	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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 [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	1.05	0/1563	1.09	2/2113 (0.1%)
1	B	1.07	2/1571 (0.1%)	1.11	3/2124 (0.1%)
All	All	1.06	2/3134 (0.1%)	1.10	5/4237 (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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	CYS	CB-SG	5.55	1.91	1.82
1	B	112	ALA	CA-CB	-5.32	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	N-CA-C	-5.75	95.49	111.00
1	B	63	PRO	N-CA-C	5.56	126.55	112.10
1	A	89	TYR	C-N-CD	-5.46	108.59	120.60
1	B	156	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	59	GLU	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	89	TYR	Sidechain

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	1542	0	1569	81	0
1	B	1550	0	1587	97	0
2	A	20	0	0	0	0
2	B	12	0	0	0	0
All	All	3124	0	3156	176	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 30.

The worst 5 of 176 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:111:MSE:HE2	1:A:173:PRO:HG3	1.47	0.94
1:B:192:LEU:HD12	1:B:192:LEU:O	1.72	0.89
1:A:62:THR:O	1:A:62:THR:HG22	1.72	0.87
1:B:84:VAL:H	1:B:107:HIS:CD2	1.96	0.84
1:A:213:ASN:OD1	1:A:215:THR:HB	1.78	0.84

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	195/230 (85%)	176 (90%)	15 (8%)	4 (2%)	8	38
1	B	196/230 (85%)	171 (87%)	17 (9%)	8 (4%)	3	19
All	All	391/460 (85%)	347 (89%)	32 (8%)	12 (3%)	5	26

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	B	66	ARG
1	B	67	ALA
1	A	231	ILE
1	B	63	PRO

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	165/188 (88%)	153 (93%)	12 (7%)	16	50
1	B	166/188 (88%)	151 (91%)	15 (9%)	11	40
All	All	331/376 (88%)	304 (92%)	27 (8%)	13	44

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	19	LEU
1	B	60	LEU
1	B	172	THR
1	B	21	LYS
1	A	108	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	HIS

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Mol	Chain	Res	Type
1	B	107	HIS
1	B	52	ASN
1	A	75	GLN
1	B	79	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	195/230 (84%)	-0.78	2 (1%) 82 58	26, 47, 117, 141	22 (11%)
1	B	196/230 (85%)	-0.76	0 100 100	21, 45, 116, 138	22 (11%)
All	All	391/460 (85%)	-0.77	2 (0%) 90 74	21, 46, 117, 141	44 (11%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	3.9
1	A	65	GLY	2.1

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.