



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:43 PM GMT

PDB ID : 2A6A
Title : Crystal structure of Glycoprotein endopeptidase (tm0874) from THERMOTOGA MARITIMA at 2.50 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-07-02
Resolution : 2.50 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

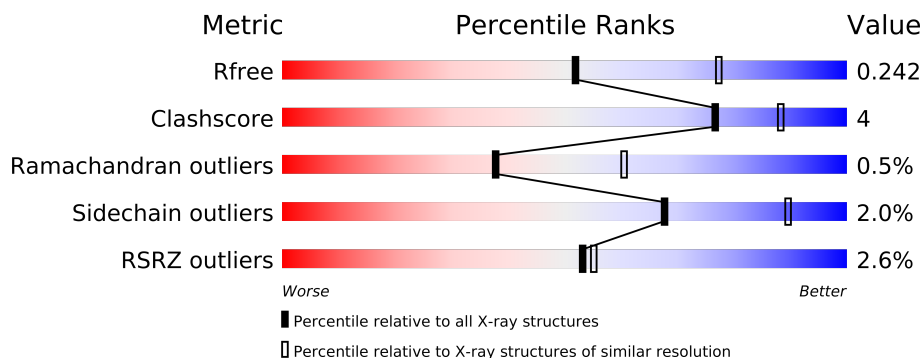
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	218	
1	B	218	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	UNL	A	301	-	X
2	UNL	B	302	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2889 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TM0874.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	Se	0	0	0
			1434	926	235	269	2	2			
1	B	188	Total	C	N	O	S	Se	0	0	0
			1426	922	234	266	2	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	MODIFIED RESIDUE	GB 15643636
A	-10	GLY	-	LEADER SEQUENCE	GB 15643636
A	-9	SER	-	LEADER SEQUENCE	GB 15643636
A	-8	ASP	-	LEADER SEQUENCE	GB 15643636
A	-7	LYS	-	LEADER SEQUENCE	GB 15643636
A	-6	ILE	-	LEADER SEQUENCE	GB 15643636
A	-5	HIS	-	LEADER SEQUENCE	GB 15643636
A	-4	HIS	-	LEADER SEQUENCE	GB 15643636
A	-3	HIS	-	LEADER SEQUENCE	GB 15643636
A	-2	HIS	-	LEADER SEQUENCE	GB 15643636
A	-1	HIS	-	LEADER SEQUENCE	GB 15643636
A	0	HIS	-	LEADER SEQUENCE	GB 15643636
A	1	MSE	MET	MODIFIED RESIDUE	GB 15643636
A	96	MSE	MET	MODIFIED RESIDUE	GB 15643636
B	-11	MSE	-	MODIFIED RESIDUE	GB 15643636
B	-10	GLY	-	LEADER SEQUENCE	GB 15643636
B	-9	SER	-	LEADER SEQUENCE	GB 15643636
B	-8	ASP	-	LEADER SEQUENCE	GB 15643636
B	-7	LYS	-	LEADER SEQUENCE	GB 15643636
B	-6	ILE	-	LEADER SEQUENCE	GB 15643636
B	-5	HIS	-	LEADER SEQUENCE	GB 15643636
B	-4	HIS	-	LEADER SEQUENCE	GB 15643636
B	-3	HIS	-	LEADER SEQUENCE	GB 15643636
B	-2	HIS	-	LEADER SEQUENCE	GB 15643636
B	-1	HIS	-	LEADER SEQUENCE	GB 15643636

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	LEADER SEQUENCE	GB 15643636
B	1	MSE	MET	MODIFIED RESIDUE	GB 15643636
B	96	MSE	MET	MODIFIED RESIDUE	GB 15643636

- Molecule 2 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

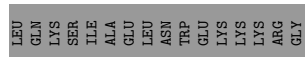
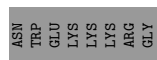
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 3 3	0	0
2	A	1	Total O 4 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	16	Total O 16 16	0	0

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- Molecule 1: hypothetical protein TM0874



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.27Å 217.11Å 51.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.24 – 2.50 29.24 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.24-2.50) 99.5 (29.24-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.191 , 0.235 0.197 , 0.242	Depositor DCC
R_{free} test set	955 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 18685 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2889	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL

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	0.76	1/1458 (0.1%)	0.82	0/1983
1	B	0.90	1/1448 (0.1%)	0.85	0/1963
All	All	0.83	2/2906 (0.1%)	0.84	0/3946

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	GLU	CB-CG	5.31	1.62	1.52
1	A	120	CYS	CB-SG	-5.15	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	LEU	Peptide

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1434	0	1419	10	0
1	B	1426	0	1449	12	1
2	A	4	0	0	0	0
2	B	3	0	0	1	0
3	A	6	0	0	0	0
3	B	16	0	0	1	0
All	All	2889	0	2868	22	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (22) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:LYS:CB	1:A:128:GLY:HA3	2.11	0.80
1:A:101:CYS:O	1:A:125:LYS:NZ	2.15	0.80
1:A:96:MSE:HE1	1:A:170:GLU:HG3	1.74	0.70
1:B:170:GLU:OE1	3:B:314:HOH:O	2.09	0.69
2:B:302:UNL:O1	2:B:302:UNL:O2	2.12	0.66
1:A:1:MSE:HE1	1:A:175:PHE:CD2	2.30	0.66
1:B:118:HIS:ND1	1:B:140:ASP:OD1	2.33	0.58
1:B:125:LYS:HG2	1:B:129:LEU:HD12	1.87	0.56
1:B:32:LYS:O	1:B:35:GLU:HG2	2.09	0.53
1:A:33:HIS:HA	1:B:47:GLU:OE2	2.12	0.50
1:A:150:PHE:O	1:A:151:SER:C	2.52	0.48
1:B:77:VAL:O	1:B:81:VAL:HG22	2.16	0.46
1:A:1:MSE:HE1	1:A:175:PHE:HD2	1.78	0.45
1:B:82:SER:N	1:B:83:PRO:CD	2.80	0.45
1:A:127:LYS:CB	1:A:128:GLY:CA	2.90	0.44
1:A:187:GLU:CB	1:A:188:PRO:HD3	2.49	0.42
1:B:1:MSE:HE1	1:B:176:ARG:HG3	2.01	0.42
1:B:83:PRO:HB2	1:B:84:TYR:CE1	2.55	0.41
1:A:96:MSE:CE	1:A:170:GLU:HG3	2.47	0.41
1:B:157:LYS:O	1:B:159:ASP:N	2.51	0.41
1:B:37:LEU:HB2	1:B:38:PRO:HD3	2.02	0.40
1:B:67:LEU:HG	1:B:71:ARG:HD2	2.03	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:84:TYR:OH	1:B:84:TYR:OH[6_555]	1.92	0.28

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	191/218 (88%)	175 (92%)	14 (7%)	2 (1%)	22	38
1	B	186/218 (85%)	180 (97%)	6 (3%)	0	100	100
All	All	377/436 (86%)	355 (94%)	20 (5%)	2 (0%)	38	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	LYS
1	A	158	ASP

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	145/188 (77%)	142 (98%)	3 (2%)	66	88
1	B	150/188 (80%)	147 (98%)	3 (2%)	68	89
All	All	295/376 (78%)	289 (98%)	6 (2%)	68	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	111	ARG
1	A	122	VAL

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Mol	Chain	Res	Type
1	B	1	MSE
1	B	125	LYS
1	B	163	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	193/218 (88%)	0.03	8 (4%) 35 36	44, 55, 77, 97	0
1	B	188/218 (86%)	0.02	2 (1%) 77 79	47, 56, 71, 79	0
All	All	381/436 (87%)	0.02	10 (2%) 53 55	44, 55, 73, 97	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ASP	3.1
1	A	192	GLN	2.8
1	A	190	TYR	2.8
1	B	113	ALA	2.6
1	A	128	GLY	2.6
1	A	49	ASP	2.3
1	B	79	GLY	2.2
1	A	113	ALA	2.2
1	A	77	VAL	2.1
1	A	191	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	UNL	B	302	3/-	1.20	23.37	57,57,61,70	0
2	UNL	A	301	4/-	0.90	12.84	57,59,80,82	0

6.5 Other polymers

There are no such residues in this entry.