



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:35 AM GMT

PDB ID : 2GOP
Title : The beta-propeller domain of the Trilobed protease from *Pyrococcus furiosus* reveals an open velcro topology
Authors : Bosch, J.; Tamura, T.; Tamura, N.; Baumeister, W.; Essen, L.-O.
Deposited on : 2006-04-13
Resolution : 2.00 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>

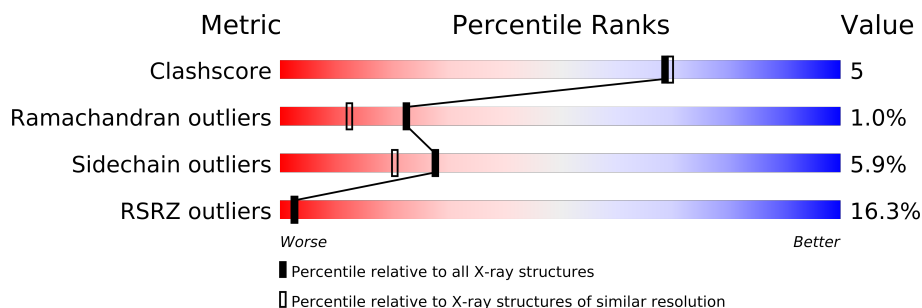
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. 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	347	
1	B	347	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5479 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 Trilobed Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	6	0
			2708	1757	444	500	7			
1	B	304	Total	C	N	O	S	8	1	0
			2529	1635	414	474	6			

- Molecule 2 is water.

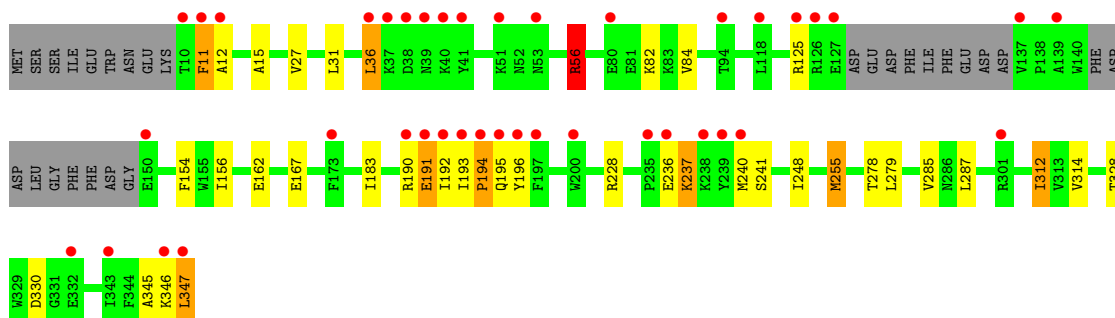
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	156	Total	O	0	0
			156	156		
2	B	86	Total	O	0	0
			86	86		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

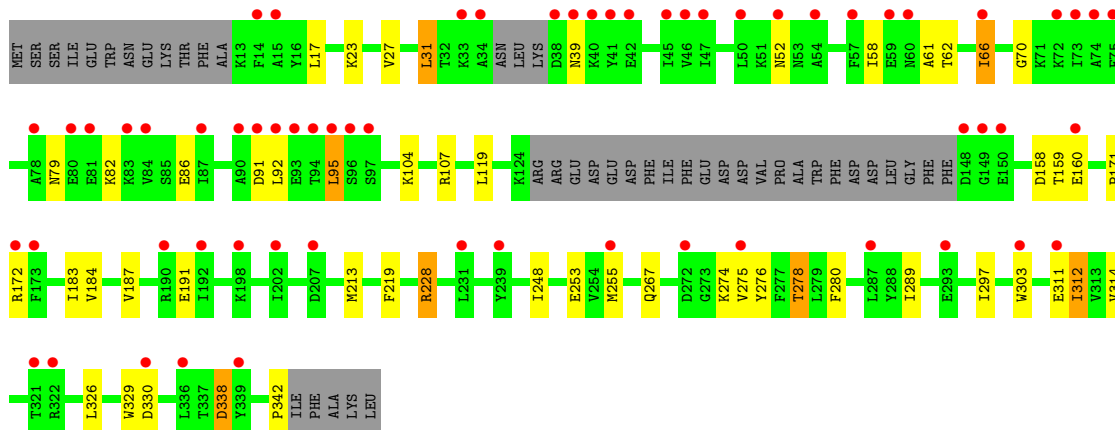
• Molecule 1: Trilobed Protease

Chain A: 



• Molecule 1: Trilobed Protease

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.75Å 88.50Å 153.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.72 – 2.00 18.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (18.72-2.00) 80.2 (18.72-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.258 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 87.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41171 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5479	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.44	0/2789	0.65	2/3755 (0.1%)
1	B	0.57	4/2589 (0.2%)	0.58	3/3484 (0.1%)
All	All	0.51	4/5378 (0.1%)	0.61	5/7239 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	PRO	C-N	-14.56	1.00	1.34
1	B	326	LEU	CA-CB	-11.76	1.26	1.53
1	B	338	ASP	CA-CB	-11.71	1.28	1.53
1	B	172	ARG	C-N	7.27	1.50	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	338	ASP	N-CA-CB	7.14	123.45	110.60
1	B	342	PRO	N-CA-CB	6.28	110.84	103.30
1	B	338	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	56	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TYR	Peptide
1	A	240	MET	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	2708	0	2704	28	0
1	B	2529	0	2489	24	0
2	A	156	0	0	1	0
2	B	86	0	0	0	0
All	All	5479	0	5193	50	0

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 5.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:156:ILE:HD11	1:A:183:ILE:HD11	1.53	0.89
1:A:314[B]:VAL:HG22	1:A:328:THR:HG22	1.57	0.87
1:B:267:GLN:H	1:B:278:THR:HG22	1.51	0.76
1:A:193:ILE:HG22	1:A:193:ILE:O	1.85	0.75
1:A:15:ALA:HB1	1:A:31:LEU:HD11	1.74	0.69
1:B:276:TYR:CE2	1:B:289:ILE:HD13	2.30	0.67
1:A:156:ILE:HD11	1:A:183:ILE:CD1	2.24	0.65
1:B:23:LYS:HB2	1:B:66:ILE:HD11	1.81	0.64
1:A:56:ARG:HH11	1:A:56:ARG:HG3	1.62	0.63
1:A:312:ILE:HD11	1:A:330:ASP:HB3	1.81	0.61
1:B:17:LEU:HD21	1:B:31:LEU:HD22	1.84	0.60
1:B:27:VAL:HG21	1:B:314:VAL:HG21	1.85	0.58
1:B:274:LYS:HB3	1:B:289:ILE:HD11	1.85	0.57
1:A:236:GLU:O	1:A:237:LYS:HG2	2.05	0.56
1:B:184:VAL:HG13	1:B:213:MET:HE3	1.87	0.56
1:B:119:LEU:HD22	1:B:183:ILE:HD12	1.88	0.55
1:A:241:SER:HB3	1:B:280:PHE:CE1	2.40	0.55
1:A:15:ALA:HB1	1:A:31:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278[B]:THR:HG23	1:A:285:VAL:HG13	1.91	0.53
1:B:17:LEU:CD2	1:B:31:LEU:HD22	2.39	0.53
1:B:70:GLY:O	1:B:92:LEU:HD12	2.10	0.52
1:A:36:LEU:H	1:A:36:LEU:HD23	1.76	0.51
1:A:278[B]:THR:HG23	1:A:285:VAL:CG1	2.40	0.51
1:A:278[B]:THR:CG2	1:A:285:VAL:CG1	2.89	0.51
1:A:345:ALA:O	1:A:347:LEU:HD22	2.11	0.50
1:A:278[B]:THR:CG2	1:A:285:VAL:HG13	2.43	0.48
1:B:91:ASP:O	1:B:95:LEU:HA	2.13	0.48
1:A:193:ILE:O	1:A:194:PRO:O	2.32	0.48
1:A:241:SER:HB3	1:B:280:PHE:CD1	2.48	0.48
1:B:27:VAL:CG2	1:B:314:VAL:HG21	2.45	0.47
1:A:156:ILE:CD1	1:A:183:ILE:HD11	2.36	0.46
1:B:276:TYR:CD2	1:B:289:ILE:HD13	2.50	0.46
1:B:158:ASP:OD1	1:B:160:GLU:N	2.48	0.45
1:A:193:ILE:O	1:A:193:ILE:CG2	2.57	0.45
1:A:255[B]:MET:HE3	2:A:459:HOH:O	2.16	0.45
1:B:23:LYS:HB2	1:B:66:ILE:CD1	2.47	0.44
1:B:79:ASN:HD22	1:B:86:GLU:CD	2.20	0.44
1:B:184:VAL:HG13	1:B:213:MET:CE	2.48	0.44
1:A:190:ARG:O	1:A:191:GLU:O	2.35	0.44
1:A:56:ARG:CG	1:A:56:ARG:HH11	2.28	0.43
1:B:267:GLN:N	1:B:278:THR:HG22	2.28	0.43
1:B:58:ILE:HG22	1:B:61:ALA:HB2	2.01	0.43
1:B:297:ILE:HG23	1:B:329:TRP:CD2	2.54	0.43
1:B:228:ARG:HB3	1:B:248:ILE:HG23	2.00	0.43
1:A:27:VAL:HG12	1:A:314[B]:VAL:HG21	2.01	0.42
1:A:154:PHE:O	1:A:167:GLU:HA	2.18	0.42
1:B:312:ILE:HD11	1:B:330:ASP:HB3	2.03	0.41
1:A:82:LYS:HB3	1:A:84:VAL:HG22	2.03	0.40
1:A:228[A]:ARG:HD3	1:A:248:ILE:HG21	2.03	0.40
1:A:192:ILE:HG22	1:A:192:ILE:O	2.22	0.40

There are no symmetry-related clashes.

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	320/347 (92%)	298 (93%)	18 (6%)	4 (1%)	18	8
1	B	299/347 (86%)	281 (94%)	16 (5%)	2 (1%)	30	20
All	All	619/694 (89%)	579 (94%)	34 (6%)	6 (1%)	22	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLU
1	A	194	PRO
1	A	12	ALA
1	B	52	ASN
1	A	11	PHE
1	B	39	ASN

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	293/312 (94%)	279 (95%)	14 (5%)	35	28
1	B	270/312 (86%)	249 (92%)	21 (8%)	18	11
All	All	563/624 (90%)	528 (94%)	35 (6%)	28	18

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	36	LEU
1	A	56	ARG
1	A	125	ARG
1	A	162	GLU
1	A	195	GLN
1	A	237	LYS
1	A	255[A]	MET
1	A	255[B]	MET

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Mol	Chain	Res	Type
1	A	279	LEU
1	A	287	LEU
1	A	312	ILE
1	A	346	LYS
1	A	347	LEU
1	B	31	LEU
1	B	62	THR
1	B	66	ILE
1	B	82	LYS
1	B	95	LEU
1	B	104	LYS
1	B	107	ARG
1	B	159	THR
1	B	187	VAL
1	B	191	GLU
1	B	219	PHE
1	B	228	ARG
1	B	253	GLU
1	B	255	MET
1	B	275	VAL
1	B	278	THR
1	B	303	TRP
1	B	311[A]	GLU
1	B	311[B]	GLU
1	B	312	ILE
1	B	338	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN

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 ⓘ

There are no ligands in this entry.

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	320/347 (92%)	0.86	40 (12%) 5 4	32, 44, 71, 101	0
1	B	304/347 (87%)	1.09	62 (20%) 1 2	20, 62, 86, 97	2 (0%)
All	All	624/694 (89%)	0.97	102 (16%) 2 2	20, 50, 83, 101	2 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ILE	11.4
1	A	10	THR	10.7
1	A	11	PHE	8.7
1	A	127	GLU	8.7
1	B	149	GLY	8.6
1	A	196	TYR	8.0
1	A	239	TYR	7.7
1	A	197	PHE	6.9
1	A	193	ILE	6.6
1	B	14	PHE	6.0
1	A	194	PRO	5.8
1	A	190	ARG	5.8
1	A	126	ARG	5.8
1	A	137	VAL	5.7
1	B	81	GLU	5.6
1	B	192	ILE	5.2
1	B	92	LEU	4.9
1	A	236	GLU	4.9
1	A	191	GLU	4.7
1	A	347	LEU	4.7
1	B	34	ALA	4.1
1	B	52	ASN	4.1
1	A	37	LYS	4.0
1	B	83	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	148	ASP	3.9
1	B	321	THR	3.9
1	A	240	MET	3.8
1	A	36	LEU	3.8
1	B	33	LYS	3.7
1	B	41	TYR	3.6
1	B	172	ARG	3.6
1	B	173	PHE	3.6
1	B	59	GLU	3.6
1	B	303	TRP	3.6
1	B	150	GLU	3.5
1	B	54	ALA	3.3
1	A	150	GLU	3.3
1	B	15	ALA	3.3
1	B	293	GLU	3.2
1	B	93	GLU	3.2
1	A	39	ASN	3.2
1	A	195	GLN	3.0
1	B	287	LEU	3.0
1	A	125	ARG	2.9
1	B	74	ALA	2.9
1	B	94	THR	2.9
1	B	311[A]	GLU	2.9
1	A	332	GLU	2.8
1	A	40	LYS	2.8
1	B	57	PHE	2.8
1	B	50	LEU	2.8
1	B	91	ASP	2.8
1	B	60	ASN	2.7
1	B	339	TYR	2.7
1	B	255	MET	2.7
1	B	66	ILE	2.7
1	B	38	ASP	2.7
1	B	190	ARG	2.7
1	A	235	PRO	2.6
1	A	173	PHE	2.6
1	B	202	ILE	2.6
1	B	42	GLU	2.6
1	B	80	GLU	2.5
1	B	160	GLU	2.5
1	B	231	LEU	2.5
1	B	90	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	275	VAL	2.5
1	A	53	ASN	2.4
1	B	78	ALA	2.4
1	A	346	LYS	2.4
1	A	301	ARG	2.4
1	B	336	LEU	2.4
1	A	238	LYS	2.4
1	A	200	TRP	2.4
1	A	139	ALA	2.4
1	A	343	ILE	2.4
1	A	51	LYS	2.3
1	B	72	LYS	2.3
1	B	39	ASN	2.3
1	A	94	THR	2.3
1	B	46	VAL	2.3
1	B	40	LYS	2.3
1	B	47	ILE	2.3
1	B	73	ILE	2.3
1	A	12	ALA	2.2
1	B	322	ARG	2.2
1	B	198	LYS	2.2
1	B	239	TYR	2.2
1	A	118	LEU	2.2
1	B	96	SER	2.2
1	B	207	ASP	2.2
1	B	87	ILE	2.1
1	B	97	SER	2.1
1	B	75	PHE	2.1
1	B	272	ASP	2.1
1	B	45	ILE	2.1
1	A	80	GLU	2.1
1	A	41	TYR	2.1
1	A	38	ASP	2.0
1	B	84	VAL	2.0
1	B	95	LEU	2.0
1	B	330	ASP	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.