



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:17 AM GMT

PDB ID : 2GHB
Title : Thermotoga maritima maltotriose binding protein, ligand free form
Authors : Cuneo, M.J.; Changela, A.; Hocker, B.; Beese, L.S.; Hellinga, H.W.
Deposited on : 2006-03-27
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

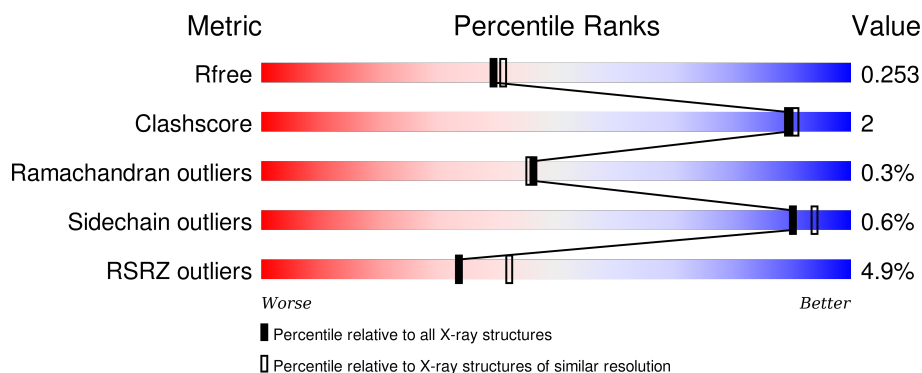
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 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	382	<div> <div>2%</div> <div>91%</div> <div>7% •</div> </div>
1	B	382	<div> <div>5%</div> <div>92%</div> <div>5% •</div> </div>
1	C	382	<div> <div>8%</div> <div>90%</div> <div>7% •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9151 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 maltose ABC transporter, periplasmic maltose-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	4	0
			2919	1894	466	548	11			
1	B	372	Total	C	N	O	S	0	4	0
			2906	1887	463	545	11			
1	C	372	Total	C	N	O	S	0	1	0
			2895	1878	463	543	11			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	INSERTION	GB 4981756
A	377	GLY	-	INSERTION	GB 4981756
A	378	SER	-	INSERTION	GB 4981756
A	379	HIS	-	INSERTION	GB 4981756
A	380	HIS	-	INSERTION	GB 4981756
A	381	HIS	-	INSERTION	GB 4981756
A	382	HIS	-	INSERTION	GB 4981756
A	383	HIS	-	INSERTION	GB 4981756
A	384	HIS	-	INSERTION	GB 4981756
B	3	MET	-	INSERTION	GB 4981756
B	377	GLY	-	INSERTION	GB 4981756
B	378	SER	-	INSERTION	GB 4981756
B	379	HIS	-	INSERTION	GB 4981756
B	380	HIS	-	INSERTION	GB 4981756
B	381	HIS	-	INSERTION	GB 4981756
B	382	HIS	-	INSERTION	GB 4981756
B	383	HIS	-	INSERTION	GB 4981756
B	384	HIS	-	INSERTION	GB 4981756
C	3	MET	-	INSERTION	GB 4981756
C	377	GLY	-	INSERTION	GB 4981756
C	378	SER	-	INSERTION	GB 4981756
C	379	HIS	-	INSERTION	GB 4981756
C	380	HIS	-	INSERTION	GB 4981756

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Chain	Residue	Modelled	Actual	Comment	Reference
C	381	HIS	-	INSERTION	GB 4981756
C	382	HIS	-	INSERTION	GB 4981756
C	383	HIS	-	INSERTION	GB 4981756
C	384	HIS	-	INSERTION	GB 4981756

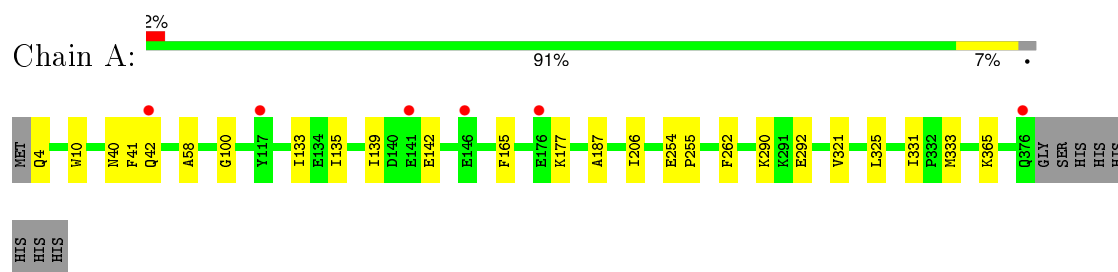
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	147	Total O 147 147	0	0
2	B	118	Total O 118 118	0	0
2	C	166	Total O 166 166	0	0

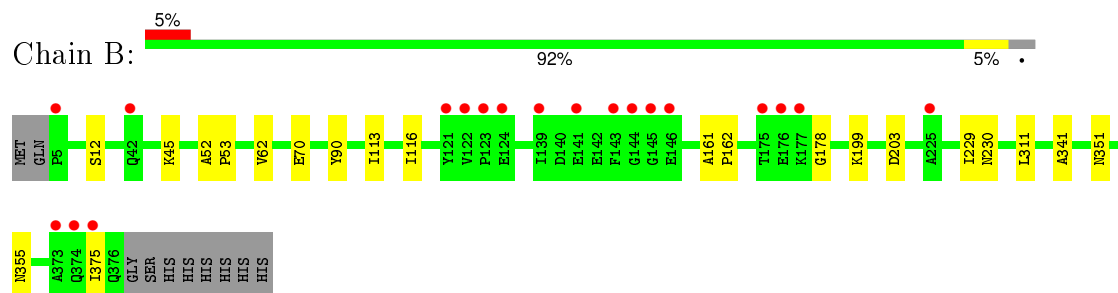
3 Residue-property plots [i](#)

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

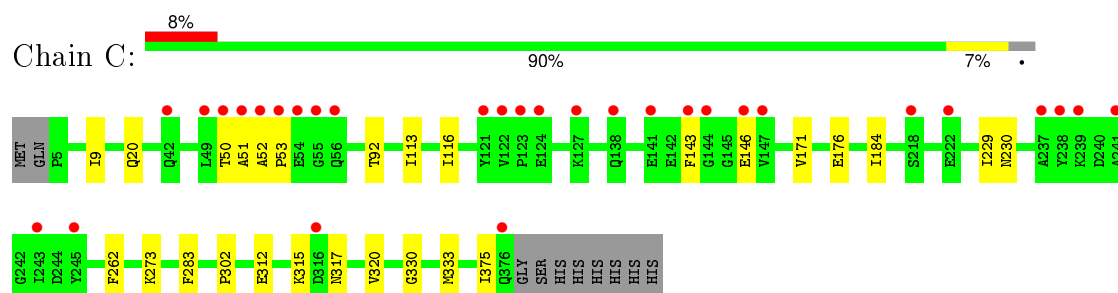
- Molecule 1: maltose ABC transporter, periplasmic maltose-binding protein



- Molecule 1: maltose ABC transporter, periplasmic maltose-binding protein



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.04Å 106.23Å 186.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.19 – 2.10 43.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.19-2.10) 99.3 (43.19-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.212 , 0.249 0.220 , 0.253	Depositor DCC
R_{free} test set	4230 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84589 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9151	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	0/2997	0.63	0/4066
1	B	0.58	0/2984	0.62	0/4048
1	C	0.65	1/2964 (0.0%)	0.67	0/4020
All	All	0.61	1/8945 (0.0%)	0.64	0/12134

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	GLU	CG-CD	6.94	1.62	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2919	0	2928	14	0
1	B	2906	0	2921	13	0
1	C	2895	0	2900	15	0
2	A	147	0	0	0	0
2	B	118	0	0	1	0
2	C	166	0	0	1	0
All	All	9151	0	8749	42	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 2.

All (42) 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:B:375:ILE:O	1:B:375:ILE:HG22	1.84	0.77
1:A:321:VAL:O	1:A:325:LEU:HG	1.98	0.64
1:C:52:ALA:O	1:C:273:LYS:HG3	1.98	0.62
1:C:312:GLU:OE1	1:C:315:LYS:NZ	2.32	0.58
1:C:113:ILE:HD12	1:C:229:ILE:HG22	1.87	0.57
1:A:133:ILE:HG23	1:A:206:ILE:CD1	2.35	0.56
1:A:133:ILE:HG23	1:A:206:ILE:HD11	1.87	0.55
1:A:165:PHE:HB3	1:A:331:ILE:CD1	2.37	0.55
1:B:341:ALA:HB3	1:B:375:ILE:HD11	1.88	0.55
1:A:262:PHE:CD1	1:A:333:MET:HG2	2.44	0.53
1:B:90:TYR:OH	1:B:311:LEU:HD22	2.09	0.52
1:B:199:LYS:NZ	1:B:203:ASP:OD1	2.42	0.52
1:B:375:ILE:O	1:B:375:ILE:CG2	2.55	0.50
1:A:165:PHE:HB3	1:A:331:ILE:HD12	1.95	0.49
1:B:45:LYS:NZ	1:B:70:GLU:OE1	2.35	0.49
1:C:51:ALA:HB1	2:C:440:HOH:O	2.13	0.48
1:B:178:GLY:HA3	2:B:429:HOH:O	2.15	0.47
1:C:171:VAL:O	1:C:184:ILE:HA	2.15	0.47
1:A:187:ALA:HB1	1:A:365:LYS:HE2	1.96	0.46
1:A:40:ASN:OD1	1:A:42:GLN:N	2.46	0.46
1:C:375:ILE:CG2	1:C:375:ILE:O	2.64	0.46
1:B:351:ASN:OD1	1:B:355:ASN:ND2	2.48	0.45
1:C:262:PHE:CD1	1:C:333:MET:HG2	2.52	0.45
1:C:92:THR:HG21	1:C:330:GLY:O	2.17	0.45
1:C:116:ILE:HD12	1:C:230:ASN:HB3	2.00	0.44
1:C:143:PHE:O	1:C:146:GLU:HG2	2.18	0.44
1:A:10:TRP:CE2	1:A:58:ALA:HB2	2.54	0.43
1:A:100:GLY:HA2	1:A:177:LYS:O	2.18	0.43
1:C:9:ILE:HD11	1:C:283:PHE:CE2	2.53	0.43
1:A:135:ILE:O	1:A:139:ILE:HG12	2.18	0.43
1:A:290:LYS:HB3	1:A:292:GLU:OE1	2.19	0.42
1:C:143:PHE:O	1:C:146:GLU:CG	2.66	0.42
1:A:40:ASN:OD1	1:A:40:ASN:C	2.57	0.42
1:B:90:TYR:OH	1:B:311:LEU:CD2	2.67	0.42
1:B:52:ALA:HB3	1:B:53:PRO:HD3	2.01	0.42
1:B:116:ILE:HD12	1:B:230:ASN:HB3	2.01	0.42
1:B:161:ALA:N	1:B:162:PRO:CD	2.83	0.42
1:B:113:ILE:HD12	1:B:229:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HB2	1:A:255:PRO:HD2	2.02	0.41
1:C:9:ILE:CD1	1:C:283:PHE:CE2	3.04	0.41
1:C:52:ALA:N	1:C:53:PRO:CD	2.84	0.41
1:C:317:ASN:O	1:C:320:VAL:HG12	2.22	0.40

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	375/382 (98%)	368 (98%)	6 (2%)	1 (0%)	46	45
1	B	374/382 (98%)	365 (98%)	9 (2%)	0	100	100
1	C	371/382 (97%)	359 (97%)	10 (3%)	2 (0%)	34	30
All	All	1120/1146 (98%)	1092 (98%)	25 (2%)	3 (0%)	46	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLU
1	C	50	THR
1	C	302	PRO

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	
1	A	307/311 (99%)	305 (99%)	2 (1%)	88	92
1	B	306/311 (98%)	302 (99%)	4 (1%)	76	82
1	C	303/311 (97%)	301 (99%)	2 (1%)	88	92
All	All	916/933 (98%)	908 (99%)	8 (1%)	90	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	PHE
1	B	12[A]	SER
1	B	12[B]	SER
1	B	62[A]	VAL
1	B	62[B]	VAL
1	C	20[A]	GLN
1	C	20[B]	GLN

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 molecules 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	373/382 (97%)	0.18	6 (1%) 74 79	24, 37, 56, 70	0
1	B	372/382 (97%)	0.26	19 (5%) 32 40	26, 41, 63, 75	0
1	C	372/382 (97%)	0.43	30 (8%) 15 20	24, 36, 61, 71	0
All	All	1117/1146 (97%)	0.29	55 (4%) 33 42	24, 38, 61, 75	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	PRO	6.4
1	C	51	ALA	5.6
1	C	55	GLY	5.5
1	C	50	THR	5.2
1	C	52	ALA	5.0
1	C	54	GLU	4.9
1	C	121	TYR	4.7
1	C	144	GLY	4.3
1	B	146	GLU	4.3
1	B	143	PHE	3.9
1	B	121	TYR	3.8
1	C	143	PHE	3.5
1	C	241	ALA	3.3
1	B	176	GLU	3.1
1	B	42	GLN	3.0
1	A	141	GLU	3.0
1	B	175	THR	3.0
1	A	42	GLN	2.9
1	A	176	GLU	2.9
1	C	245	TYR	2.9
1	C	49	LEU	2.8
1	B	374	GLN	2.8
1	C	243	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	56	GLN	2.8
1	A	117	TYR	2.8
1	B	375	ILE	2.7
1	B	122	VAL	2.7
1	C	237	ALA	2.7
1	C	122	VAL	2.6
1	C	147	VAL	2.5
1	C	316	ASP	2.5
1	C	124	GLU	2.5
1	C	218	SER	2.4
1	C	141	GLU	2.4
1	C	146	GLU	2.4
1	A	376	GLN	2.4
1	B	139	ILE	2.4
1	B	145	GLY	2.4
1	B	124	GLU	2.3
1	B	141	GLU	2.3
1	C	123	PRO	2.3
1	B	123	PRO	2.3
1	C	42	GLN	2.3
1	B	144	GLY	2.2
1	A	146	GLU	2.2
1	C	376	GLN	2.2
1	C	222	GLU	2.1
1	B	177	LYS	2.1
1	B	225	ALA	2.1
1	C	238	TYR	2.1
1	B	373	ALA	2.1
1	C	127	LYS	2.1
1	C	239	LYS	2.1
1	B	5	PRO	2.0
1	C	138	GLN	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.