Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 07:29 PM EDT

PDB ID	:	1J3M
Title	:	Crystal structure of the conserved hypothetical protein TT1751 from Thermus thermophilus HB8
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Deposited on	:	2003-02-05
Resolution	:	2.00 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
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 (i)) were used in the production of this report:

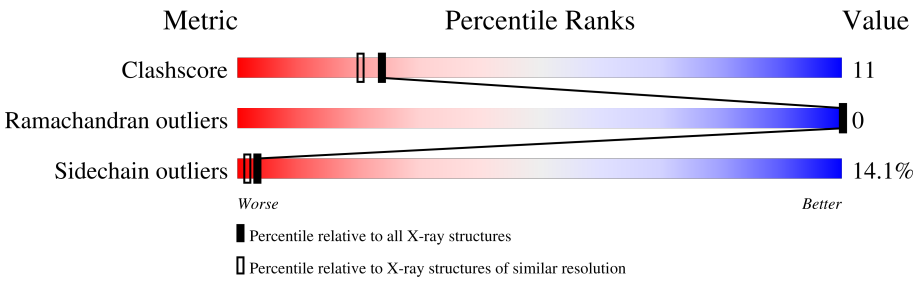
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	129	74% 17% 5% • •
1	B	129	66% 24% 8% • •

2 Entry composition (i)

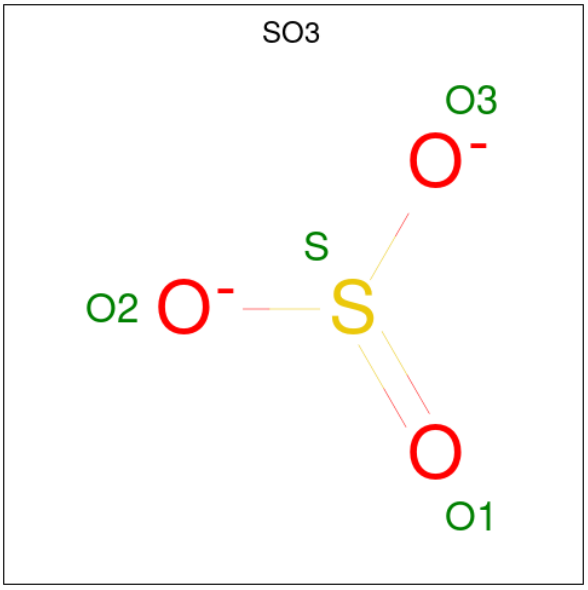
There are 3 unique types of molecules in this entry. The entry contains 2040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 the conserved hypothetical protein TT1751.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	962	609	170	179	4	0	0	0
1	B	127	962	609	170	179	4	0	0	0

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O_3S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	62	62	62	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	50	50	50	0	0

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. 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. 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.

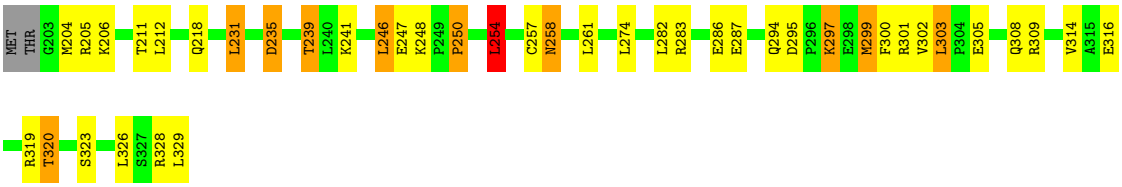
Note EDS was not executed.

• Molecule 1: the conserved hypothetical protein TT1751

Chain A:

• Molecule 1: the conserved hypothetical protein TT1751

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.60Å 78.81Å 44.69Å 90.00° 116.64° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.194 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2040	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO3

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	1.02	0/972	1.21	9/1314 (0.7%)
1	B	0.98	1/972 (0.1%)	1.13	6/1314 (0.5%)
All	All	1.00	1/1944 (0.1%)	1.17	15/2628 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	MET	SD-CE	-6.01	1.44	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	ARG	NE-CZ-NH2	-16.03	112.28	120.30
1	B	235	ASP	CB-CG-OD2	9.98	127.28	118.30
1	A	64	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	64	ARG	CG-CD-NE	-7.45	96.16	111.80
1	A	35	ASP	CB-CG-OD2	7.42	124.98	118.30
1	B	295	ASP	CB-CG-OD2	7.42	124.97	118.30
1	B	283	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	326	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	66	LEU	CA-CB-CG	6.36	129.92	115.30
1	A	126	LEU	CA-CB-CG	6.12	129.38	115.30
1	B	283	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	128	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	254	LEU	CB-CG-CD1	5.20	119.85	111.00
1	A	54	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	107	THR	OG1-CB-CG2	-5.10	98.28	110.00

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	962	0	1024	18	0
1	B	962	0	1024	29	0
2	A	4	0	0	0	0
3	A	62	0	0	0	0
3	B	50	0	0	2	0
All	All	2040	0	2048	44	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 11.

All (44) 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:297:LYS:HD2	1:B:319:ARG:HD2	1.55	0.88
1:A:71:GLU:HG2	1:B:205:ARG:HH22	1.37	0.87
1:A:71:GLU:HG2	1:B:205:ARG:NH2	1.92	0.83
1:A:35:ASP:O	1:A:39:THR:HG23	1.81	0.80
1:B:299:MET:O	1:B:302:VAL:HG22	1.86	0.76
1:B:294:GLN:NE2	1:B:299:MET:SD	2.60	0.75
1:B:309:ARG:HG2	3:B:12:HOH:O	1.86	0.74
1:B:309:ARG:HG2	1:B:309:ARG:HH11	1.56	0.69
1:B:241:LYS:NZ	1:B:247:GLU:OE1	2.23	0.69
1:B:258:ASN:HD22	1:B:261:LEU:H	1.42	0.68
1:B:235:ASP:O	1:B:239:THR:HG23	1.94	0.68
1:B:235:ASP:O	1:B:239:THR:CG2	2.44	0.66
1:A:97:LYS:NZ	1:A:116:GLU:OE2	2.28	0.65
1:A:58:ASN:HD22	1:A:61:LEU:H	1.46	0.64
1:B:246:LEU:HD13	1:B:248:LYS:NZ	2.12	0.63
1:A:83:ARG:NH1	1:A:90:GLU:OE1	2.30	0.58
1:B:294:GLN:HE21	1:B:299:MET:CE	2.18	0.56
1:B:320:THR:HG22	3:B:95:HOH:O	2.08	0.53
1:B:246:LEU:HD12	1:B:248:LYS:HG2	1.90	0.53
1:A:103:LEU:HB3	1:A:107:THR:OG1	2.10	0.52
1:B:254:LEU:HD22	1:B:282:LEU:HD11	1.92	0.51
1:A:105:GLU:CG	1:A:109:ARG:HH22	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:CD1	1:B:248:LYS:HG2	2.40	0.51
1:B:316:GLU:O	1:B:320:THR:HG23	2.11	0.51
1:B:258:ASN:ND2	1:B:261:LEU:H	2.07	0.50
1:B:300:PHE:HA	1:B:303:LEU:HD22	1.94	0.50
1:A:54:LEU:HD22	1:A:82:LEU:CD1	2.42	0.49
1:A:105:GLU:CG	1:A:109:ARG:NH2	2.76	0.49
1:B:302:VAL:HG23	1:B:303:LEU:HD13	1.98	0.46
1:B:309:ARG:HG2	1:B:309:ARG:NH1	2.29	0.46
1:A:94:GLN:NE2	1:B:274:LEU:O	2.41	0.45
1:B:231:LEU:HD22	1:B:257:CYS:HB2	1.97	0.45
1:A:26:GLU:HG2	1:A:128:ARG:HH22	1.81	0.45
1:B:206:LYS:NZ	1:B:329:LEU:O	2.50	0.44
1:B:212:LEU:HD22	1:B:250:PRO:HB3	1.99	0.44
1:B:235:ASP:O	1:B:239:THR:HG22	2.17	0.43
1:A:66:LEU:HD13	1:A:72:ILE:HG22	2.02	0.41
1:A:55:GLY:HA3	1:A:77:PRO:HG2	2.02	0.41
1:A:105:GLU:HG2	1:A:106:ALA:N	2.31	0.41
1:B:218:GLN:HE21	1:B:218:GLN:HB2	1.73	0.41
1:A:16:ARG:NH1	1:A:20:GLU:OE2	2.53	0.41
1:A:94:GLN:CG	1:A:99:MET:HG3	2.51	0.41
1:A:55:GLY:CA	1:A:77:PRO:HG2	2.51	0.41
1:B:231:LEU:HD22	1:B:257:CYS:CB	2.52	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	125/129 (97%)	123 (98%)	2 (2%)	0	100	100
1	B	125/129 (97%)	120 (96%)	5 (4%)	0	100	100
All	All	250/258 (97%)	243 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	99/101 (98%)	90 (91%)	9 (9%)	9 5
1	B	99/101 (98%)	80 (81%)	19 (19%)	1 0
All	All	198/202 (98%)	170 (86%)	28 (14%)	3 1

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	47	GLU
1	A	54	LEU
1	A	66	LEU
1	A	86	GLU
1	A	87	GLU
1	A	97	LYS
1	A	105	GLU
1	A	126	LEU
1	B	211	THR
1	B	231	LEU
1	B	239	THR
1	B	246	LEU
1	B	250	PRO
1	B	254	LEU
1	B	258	ASN
1	B	286	GLU
1	B	287	GLU
1	B	297	LYS
1	B	299	MET
1	B	301	ARG
1	B	303	LEU
1	B	305	GLU
1	B	308	GLN
1	B	314	VAL

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Mol	Chain	Res	Type
1	B	320	THR
1	B	323	SER
1	B	328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	79	ASN
1	B	218	GLN
1	B	258	ASN
1	B	279	ASN
1	B	308	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO3	A	3016	-	1,3,3	1.64	0	0,3,3	-	-

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.

No monomer is involved in short contacts.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.