



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:08 AM GMT

PDB ID : 3O7O
Title : Use of synthetic symmetrization in the crystallization and structure determination of CelA from *Thermotoga maritima*
Authors : Forse, G.J.; Ram, N.; Yeates, T.O.
Deposited on : 2010-07-30
Resolution : 2.41 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

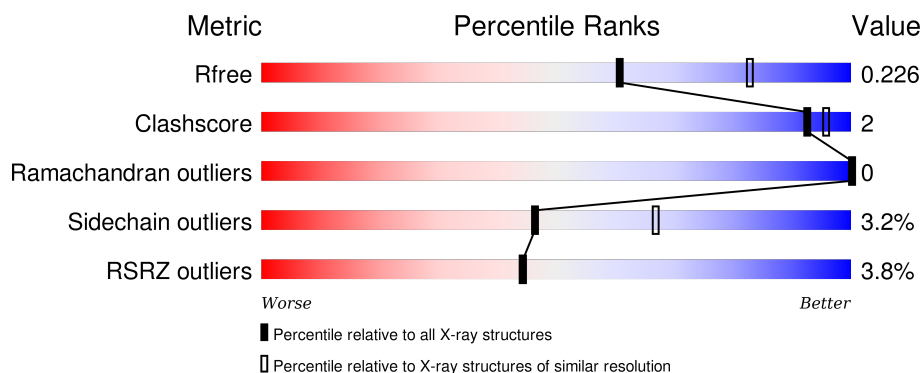
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

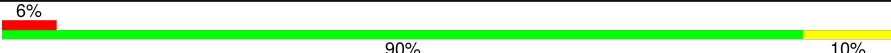
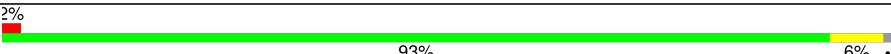
The reported resolution of this entry is 2.41 Å.

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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	264	
1	B	264	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	267	-	-	-	X
2	BR	B	266	-	-	-	X
2	BR	B	267	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4395 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 Endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2172	1417	347	400	8			
1	B	262	Total	C	N	O	S	0	0	1
			2144	1400	339	397	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	CYS	ASP	ENGINEERED MUTATION	UNP Q9S5X8
A	259	HIS	-	EXPRESSION TAG	UNP Q9S5X8
A	260	HIS	-	EXPRESSION TAG	UNP Q9S5X8
A	261	HIS	-	EXPRESSION TAG	UNP Q9S5X8
A	262	HIS	-	EXPRESSION TAG	UNP Q9S5X8
A	263	HIS	-	EXPRESSION TAG	UNP Q9S5X8
A	264	HIS	-	EXPRESSION TAG	UNP Q9S5X8
B	188	CYS	ASP	ENGINEERED MUTATION	UNP Q9S5X8
B	259	HIS	-	EXPRESSION TAG	UNP Q9S5X8
B	260	HIS	-	EXPRESSION TAG	UNP Q9S5X8
B	261	HIS	-	EXPRESSION TAG	UNP Q9S5X8
B	262	HIS	-	EXPRESSION TAG	UNP Q9S5X8
B	263	HIS	-	EXPRESSION TAG	UNP Q9S5X8
B	264	HIS	-	EXPRESSION TAG	UNP Q9S5X8

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

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

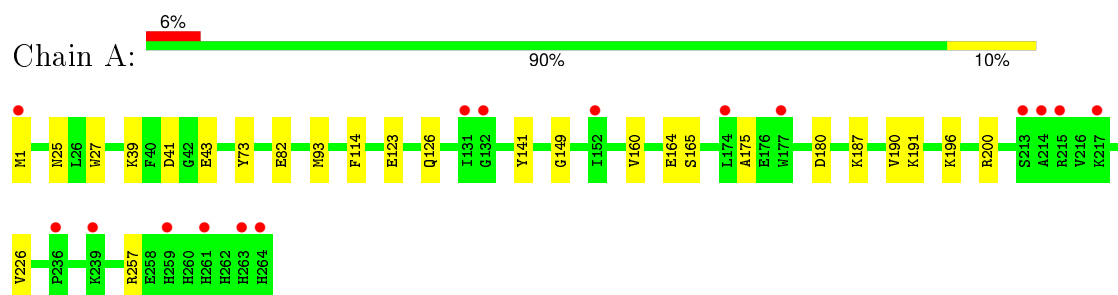
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	44	Total 44	O 44	0	0

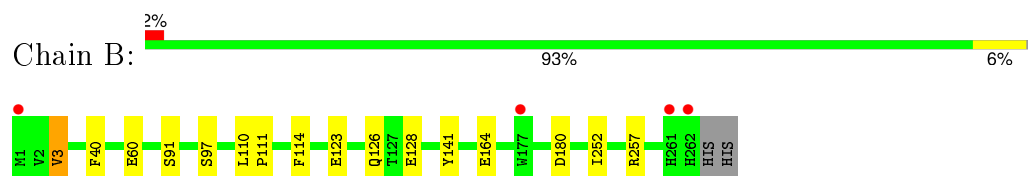
3 Residue-property plots [i](#)

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: Endoglucanase



• Molecule 1: Endoglucanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	114.03 Å 114.03 Å 98.82 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.18 – 2.41 37.34 – 2.41	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.18-2.41) 97.6 (37.34-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.42 Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.176 , 0.216 0.193 , 0.226	Depositor DCC
R_{free} test set	1404 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.2	EDS
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27582 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4395	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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](#)

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

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	0.46	0/2247	0.69	0/3051
1	B	0.50	0/2216	0.69	0/3009
All	All	0.48	0/4463	0.69	0/6060

There are no bond length outliers.

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	2172	0	2059	9	0
1	B	2144	0	2039	8	0
2	A	3	0	0	0	0
2	B	4	0	0	2	0
3	A	28	0	0	0	0
3	B	44	0	0	0	0
All	All	4395	0	4098	17	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 (17) 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:123:GLU:H	1:B:126:GLN:HE21	1.44	0.64
1:B:114:PHE:HB3	1:B:141:TYR:HB3	1.83	0.61
1:A:39:LYS:HE2	1:A:41:ASP:HB3	1.89	0.54
1:B:3:VAL:HG13	1:B:40:PHE:HB3	1.90	0.54
1:A:123:GLU:H	1:A:126:GLN:HE21	1.57	0.53
1:A:141:TYR:CE1	1:A:191:LYS:HB3	2.47	0.50
1:B:97:SER:HB2	2:B:267:BR:BR	2.66	0.50
1:B:123:GLU:H	1:B:126:GLN:NE2	2.09	0.50
1:A:114:PHE:HB3	1:A:141:TYR:HB3	1.97	0.47
1:A:93:MET:O	1:A:200:ARG:HD3	2.15	0.46
1:A:160:VAL:HB	1:A:196:LYS:HB3	2.01	0.42
1:B:110:LEU:HA	1:B:111:PRO:HD3	1.97	0.42
1:B:97:SER:CB	2:B:267:BR:BR	3.23	0.42
1:A:73:TYR:O	1:A:226:VAL:HB	2.21	0.41
1:B:91:SER:O	1:B:257:ARG:NH1	2.54	0.41
1:A:149:GLY:HA3	1:A:175:ALA:HB2	2.02	0.41
1:A:25:ASN:OD1	1:A:27:TRP:HB3	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	262/264 (99%)	254 (97%)	8 (3%)	0	100	100
1	B	260/264 (98%)	251 (96%)	9 (4%)	0	100	100
All	All	522/528 (99%)	505 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	234/234 (100%)	225 (96%)	9 (4%)	40	59
1	B	231/234 (99%)	225 (97%)	6 (3%)	54	74
All	All	465/468 (99%)	450 (97%)	15 (3%)	46	67

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	43	GLU
1	A	82	GLU
1	A	164	GLU
1	A	165	SER
1	A	180	ASP
1	A	187	LYS
1	A	190	VAL
1	A	257	ARG
1	B	3	VAL
1	B	60	GLU
1	B	128	GLU
1	B	164	GLU
1	B	180	ASP
1	B	252	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	126	GLN
1	A	143	ASN
1	A	144	ASN
1	A	201	HIS
1	B	126	GLN
1	B	143	ASN

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](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - 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.

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

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	264/264 (100%)	0.08	16 (6%) 25 24	30, 46, 76, 148	0
1	B	262/264 (99%)	-0.19	4 (1%) 76 75	27, 41, 65, 78	0
All	All	526/528 (99%)	-0.05	20 (3%) 44 44	27, 43, 72, 148	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	HIS	8.2
1	A	214	ALA	5.0
1	A	263	HIS	4.5
1	B	262	HIS	4.1
1	A	1	MET	3.6
1	A	177	TRP	3.5
1	A	261	HIS	3.4
1	A	132	GLY	3.3
1	A	259	HIS	3.2
1	A	174	LEU	3.1
1	A	236	PRO	3.1
1	B	261	HIS	3.0
1	A	217	LYS	2.5
1	A	213	SER	2.5
1	B	177	TRP	2.4
1	B	1	MET	2.2
1	A	215	ARG	2.2
1	A	131	ILE	2.2
1	A	152	ILE	2.1
1	A	239	LYS	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](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BR	A	267	1/1	0.87	0.31	8.63	120,120,120,120	1
2	BR	B	266	1/1	0.72	0.27	6.01	65,65,65,65	1
2	BR	B	265	1/1	0.99	0.10	-1.37	48,48,48,48	1
2	BR	B	268	1/1	0.98	0.06	-	99,99,99,99	0
2	BR	A	266	1/1	0.51	0.39	-	53,53,53,53	1
2	BR	A	265	1/1	1.00	0.12	-	42,42,42,42	1
2	BR	B	267	1/1	0.75	0.31	-	44,44,44,44	1

6.5 Other polymers [i](#)

There are no such residues in this entry.