

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	3CNI
Title	:	Crystal structure of a domain of a putative ABC type-2 transporter from
		Thermotoga maritima MSB8
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		Xu, X.; Que, Q.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Minor, W.;
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Deposited on	:	2008-03-25
Resolution	:	2.30 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 following versions of software and data (see references (1)) were used in the production of this report:

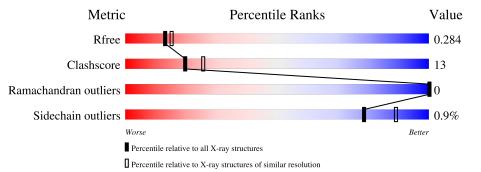
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643(2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Mol	Chain	Length	Quality of chain		
1	А	156	72%	21%	• 7%



3CNI

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1138 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 Putative ABC type-2 transporter.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	145	Total 1105	C 719	N 171	0 213	${ m Se} 2$	0	2	0

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Ca 2 2	0	0

• Molecule 3 is water.

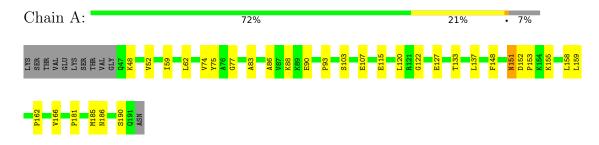
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	31	Total O 31 31	0	0



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.

• Molecule 1: Putative ABC type-2 transporter





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants	65.60Å 65.60Å 141.19Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.80 - 2.30	Depositor
Resolution (A)	29.75 - 2.30	EDS
% Data completeness	99.4 (56.80-2.30)	Depositor
(in resolution range)	99.5(29.75-2.30)	EDS
R _{merge}	0.05	Depositor
R _{sym}	0.05	Depositor
$< I/\sigma(I) > 1$	$3.57 (at 2.31 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.204 , 0.227	Depositor
It, Itfree	0.274 , 0.284	DCC
R_{free} test set	403 reflections $(4.72%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	62.1	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 61.1	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1138	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.86% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: CA

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).

ſ	Mol	Chain	Bond	lengths	Bond angles		
	NIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
	1	А	1.03	0/1127	0.90	1/1524~(0.1%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	88	LYS	CD-CE-NZ	5.75	124.93	111.70

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	А	1105	0	1104	28	0
2	А	2	0	0	0	0
3	А	31	0	0	0	0
All	All	1138	0	1104	28	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 13.

All (28) 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:A:62:LEU:O	1:A:62:LEU:HD13	1.84	0.77
1:A:48:LYS:O	1:A:93:PRO:HD2	1.92	0.69
1:A:59:ILE:HD11	1:A:148[A]:PHE:HD1	1.61	0.66
1:A:103:SER:O	1:A:107:GLU:HG3	1.99	0.62
1:A:152:ASP:HB2	1:A:155:LYS:HG3	1.82	0.62
1:A:59:ILE:HD11	1:A:148[A]:PHE:CD1	2.35	0.61
1:A:75:TYR:CE2	1:A:83:ALA:HB2	2.39	0.57
1:A:151:ASN:HD22	1:A:151:ASN:N	2.04	0.55
1:A:62:LEU:HD13	1:A:62:LEU:C	2.25	0.55
1:A:75:TYR:CD2	1:A:83:ALA:HB2	2.43	0.54
1:A:86:ALA:O	1:A:90:GLU:HB2	2.07	0.53
1:A:152:ASP:HB3	1:A:153:PRO:HD2	1.90	0.53
1:A:186:ASN:O	1:A:190:SER:HB3	2.09	0.52
1:A:120:LEU:HD11	1:A:181:PRO:HB3	1.93	0.50
1:A:52:VAL:HA	1:A:77:GLY:O	2.16	0.46
1:A:74:VAL:HG21	1:A:90:GLU:HG2	1.99	0.44
1:A:133:THR:O	1:A:137[A]:LEU:HG	2.17	0.44
1:A:59:ILE:CD1	1:A:148[A]:PHE:CD1	3.02	0.43
1:A:122:GLY:O	1:A:127:GLU:HG2	2.18	0.42
1:A:59:ILE:HD13	1:A:148[B]:PHE:CG	2.54	0.42
1:A:158:LEU:O	1:A:162:PRO:HD3	2.20	0.42
1:A:62:LEU:C	1:A:62:LEU:CD1	2.88	0.42
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.83	0.42
1:A:151:ASN:N	1:A:151:ASN:ND2	2.65	0.42
1:A:115:GLU:HA	1:A:166:VAL:O	2.20	0.41
1:A:181:PRO:O	1:A:185:MSE:HG2	2.21	0.41

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	Percent	tiles
1	А	145/156~(93%)	143 (99%)	2(1%)	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 side chain 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	А	113/130~(87%)	112~(99%)	1 (1%)	78 89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	А	69	ASN
1	А	144	GLN
1	А	151	ASN
1	А	191	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)

Of 2 ligands modelled in this entry, 2 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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

