

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 2, 2021 – 12:59 PM EDT

PDB ID : 3LKB

Title : Crystal structure of a branched chain amino acid ABC transporter from Ther-

mus thermophilus with bound valine

Authors: Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center

for Structural Genomics (NYSGXRC)

Deposited on : 2010-01-27

Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.23.2

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)

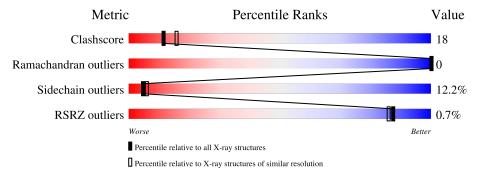
Validation Pipeline (wwPDB-VP) : 2.23.2

# 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 2.40 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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% 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	392	67%	25%	5% •	
1	В	392	71%	23%	• •	

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	VAL	A	393	-	-	X	-
2	VAL	В	393	-	-	X	-



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6089 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 Probable branched-chain amino acid ABC transporter, amino acid binding protein.

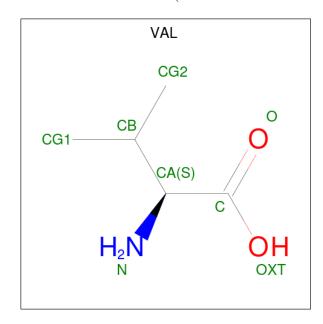
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	382	Total 2968	C 1893		O 547	S 7	0	0	0
1	В	382	Total 2968	C 1893		O 547	S 7	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5SL42
A	2	SER	-	expression tag	UNP Q5SL42
A	293	ALA	VAL	engineered mutation	UNP Q5SL42
A	295	ALA	SER	engineered mutation	UNP Q5SL42
A	385	GLU	-	expression tag	UNP Q5SL42
A	386	GLY	-	expression tag	UNP Q5SL42
A	387	HIS	-	expression tag	UNP Q5SL42
A	388	HIS	-	expression tag	UNP Q5SL42
A	389	HIS	-	expression tag	UNP Q5SL42
A	390	HIS	-	expression tag	UNP Q5SL42
A	391	HIS	-	expression tag	UNP Q5SL42
A	392	HIS	-	expression tag	UNP Q5SL42
В	1	MET	-	expression tag	UNP Q5SL42
В	2	SER	-	expression tag	UNP Q5SL42
В	293	ALA	VAL	engineered mutation	UNP Q5SL42
В	295	ALA	SER	engineered mutation	UNP Q5SL42
В	385	GLU	-	expression tag	UNP Q5SL42
В	386	GLY	-	expression tag	UNP Q5SL42
В	387	HIS	-	expression tag	UNP Q5SL42
В	388	HIS	-	expression tag	UNP Q5SL42
В	389	HIS	-	expression tag	UNP Q5SL42
В	390	HIS	-	expression tag	UNP Q5SL42
В	391	HIS	-	expression tag	UNP Q5SL42
В	392	HIS	-	expression tag	UNP Q5SL42

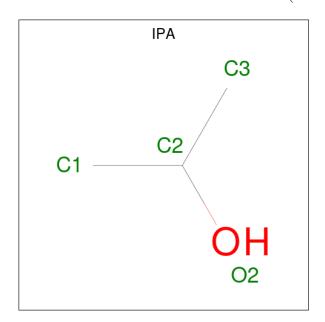


 $\bullet$  Molecule 2 is VALINE (three-letter code: VAL) (formula:  $\mathrm{C}_5\mathrm{H}_{11}\mathrm{NO}_2).$ 



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total 7			0	0
2	В	1	Total 7	C 5	O 1	0	0

 $\bullet$  Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $C_3H_8O$ ).



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

Continued on next page...



 $Continued\ from\ previous\ page...$ 

Mo	ol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3		В	1	Total 4	C 3	O 1	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	В	1	Total Na 1 1	0	0

• Molecule 5 is water.

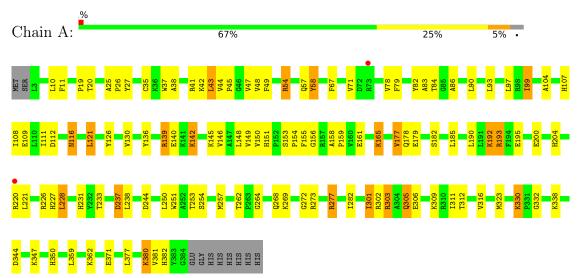
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	61	Total O 61 61	0	0
5	В	68	Total O 68 68	0	0



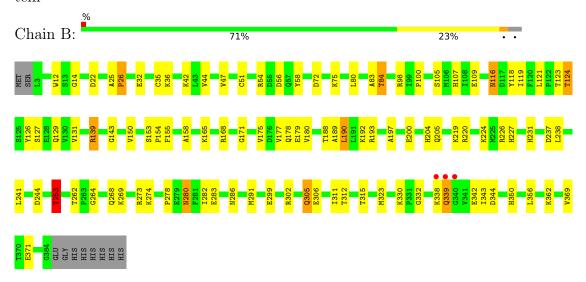
# 3 Residue-property plots (i)

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 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: Probable branched-chain amino acid ABC transporter, amino acid binding protein



• Molecule 1: Probable branched-chain amino acid ABC transporter, amino acid binding protein





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	76.71Å 83.18Å 122.00Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 - 2.40	Depositor
Resolution (A)	47.74 - 2.40	EDS
% Data completeness	99.8 (47.74-2.40)	Depositor
(in resolution range)	99.8 (47.74-2.40)	EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.35 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
D D.	0.174 , 0.236	Depositor
$R, R_{free}$	0.179 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40 , 40.8	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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: IPA, NA

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		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.99	$2/3035 \ (0.1\%)$	0.89	4/4118 (0.1%)	
1	В	1.01	0/3035	0.85	3/4118 (0.1%)	
All	All	1.00	$2/6070 \ (0.0\%)$	0.87	7/8236 (0.1%)	

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	A	254	SER	CB-OG	-5.42	1.35	1.42
1	A	130	VAL	CB-CG2	-5.38	1.41	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	226	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	303	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	В	56	ASP	CB-CG-OD1	5.30	123.07	118.30
1	В	253	THR	CB-CA-C	-5.28	97.35	111.60
1	A	237	ASP	CB-CG-OD1	-5.03	113.77	118.30

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	2968	0	2956	115	0
1	В	2968	0	2956	96	0
2	A	7	0	8	11	0
2	В	7	0	8	20	0
3	A	4	0	8	3	0
3	В	4	0	8	3	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
5	A	61	0	0	4	0
5	В	68	0	0	0	0
All	All	6089	0	5944	210	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 18.

The worst 5 of 210 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:84:THR:CG2	2:B:393:VAL:HG21	1.45	1.43
1:A:257:MET:CE	1:A:359:LEU:HD22	1.69	1.20
1:A:257:MET:HE3	1:A:359:LEU:HD22	1.26	1.14
1:B:84:THR:HG23	2:B:393:VAL:HG21	1.16	1.11
1:B:126:TYR:OH	2:B:393:VAL:HG23	1.50	1.10

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	Perce	ntiles
1	A	380/392 (97%)	373 (98%)	7 (2%)	0	100	100
1	В	380/392 (97%)	368 (97%)	12 (3%)	0	100	100
All	All	760/784 (97%)	741 (98%)	19 (2%)	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	306/315 (97%)	270 (88%)	36 (12%)	5 7		
1	В	306/315 (97%)	267 (87%)	39 (13%)	4 5		
All	All	612/630 (97%)	537 (88%)	75 (12%)	5 6		

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	219	LYS
1	В	339	GLN
1	В	224	LYS
1	В	274	LYS
1	A	269	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	87	ASN
1	В	382	HIS
1	В	178	GLN
1	В	280	ASN
1	В	116	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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IPA	A	4571	-	3,3,3	0.61	0	3,3,3	0.16	0
2	VAL	В	393	-	4,6,7	1.82	1 (25%)	6,7,9	1.32	1 (16%)
3	IPA	В	4571	-	3,3,3	0.55	0	3,3,3	0.43	0
2	VAL	A	393	-	4,6,7	2.10	1 (25%)	6,7,9	2.90	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

$\mathbf{Mol}$	Type	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
2	VAL	В	393	-	-	1/5/6/8	-
2	VAL	A	393	_	-	0/5/6/8	ı

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	A	393	VAL	CG2-CB	-3.45	1.40	1.52
2	В	393	VAL	CG2-CB	-3.12	1.41	1.52

#### All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	393	VAL	CB-CA-C	-5.87	105.02	112.94
2	A	393	VAL	O-C-CA	-3.91	114.53	124.78
2	В	393	VAL	O-C-CA	-2.81	117.42	124.78



There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms	
2	В	393	VAL	C-CA-CB-CG2	

There are no ring outliers.

4 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4571	IPA	3	0
2	В	393	VAL	20	0
3	В	4571	IPA	3	0
2	A	393	VAL	11	0

## 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)

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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9	
1	A	382/392 (97%)	-0.58	2 (0%)	91 8	89	5, 14, 29, 40	0
1	В	$382/392 \ (97\%)$	-0.51	3 (0%)	86	84	3, 15, 30, 45	0
All	All	764/784 (97%)	-0.54	5 (0%)	87	86	3, 15, 30, 45	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	339	GLN	4.3
1	В	338	LYS	2.6
1	В	340	GLY	2.1
1	A	220	ARG	2.1
1	A	73	ARG	2.1

## 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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
2	VAL	В	393	7/8	0.83	0.25	4,7,11,15	0
2	VAL	A	393	7/8	0.87	0.22	11,15,18,21	0
3	IPA	В	4571	4/4	0.91	0.23	18,26,26,29	0
3	IPA	A	4571	4/4	0.95	0.25	28,30,30,32	0
4	NA	В	394	1/1	0.95	0.10	22,22,22,22	0
4	NA	A	394	1/1	0.99	0.06	8,8,8,8	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

