

Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 08:32 pm BST

PDB ID	:	1TJB
Title	:	Crystal Structure of a High Affinity Lanthanide-Binding Peptide (LBT)
Authors	:	Nitz, M.; Sherawat, M.; Franz, K.J.; Peisach, E.; Allen, K.N.; Imperiali, B.
Deposited on		
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 following versions of software and data (see references (1)) were used in the production of this report:

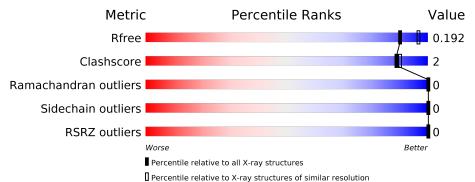
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11
Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	::	5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	А	18	100%							
1	В	18	89%	11%						



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 332 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 Lanthanide-Binding Peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	А	18	Total C N O 141 88 21 32	0	0	1
1	В	18	Total C N O 141 88 21 32	0	0	1

• Molecule 2 is TERBIUM(III) ION (three-letter code: TB) (formula: Tb).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Tb 1 1	0	0
2	А	1	Total Tb 1 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	3	Total Cl 3 3	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	26	Total O 26 26	0	0
4	В	19	Total O 19 19	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 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.

11%

• Molecule 1: Lanthanide-Binding Peptide

Chain A:

in A: 100%

There are no outlier residues recorded for this chain.

 \bullet Molecule 1: Lanthanide-Binding Peptide

Chain B:

89%





4 Data and refinement statistics (i)

Property	Value	Source		
Space group	C 1 2 1	Depositor		
Cell constants	52.16Å 22.27 Å 30.03 Å	Depositor		
a, b, c, α , β , γ	90.00° 103.89° 90.00°	Depositor		
Resolution (Å)	17.18 - 2.00	Depositor		
Resolution (A)	17.18 - 2.01	EDS		
% Data completeness	96.9 (17.18-2.00)	Depositor		
(in resolution range)	96.9(17.18-2.01)	EDS		
R _{merge}	0.11	Depositor		
R_{sym}	(Not available)	Depositor		
$< I/\sigma(I) > 1$	$7.65 (at 2.00 \text{\AA})$	Xtriage		
Refinement program	CNS	Depositor		
D D.	0.161 , 0.195	Depositor		
R, R_{free}	0.155 , 0.192	DCC		
R_{free} test set	210 reflections (9.35%)	wwPDB-VP		
Wilson B-factor (Å ²)	11.6	Xtriage		
Anisotropy	0.240	Xtriage		
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.40 , 58.7	EDS		
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.32$	Xtriage		
Estimated twinning fraction	No twinning to report.	Xtriage		
F_o, F_c correlation	0.95	EDS		
Total number of atoms	332	wwPDB-VP		
Average B, all atoms $(Å^2)$	14.0	wwPDB-VP		

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 28.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7506e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: CL, TB, NH2

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			
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.30	0/143	0.57	0/195		
1	В	0.29	0/143	0.56	0/195		
All	All	0.30	0/286	0.57	0/390		

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	А	141	0	114	0	0
1	В	141	0	114	1	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	3	0	0	0	0
4	А	26	0	0	0	0
4	В	19	0	0	0	0
All	All	332	0	228	1	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 (1)	close	$\operatorname{contacts}$	within	the	same	$\operatorname{asymmetric}$	unit	are	listed	below,	sorted	by	their	clash
magnit	ude.													

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:109:GLU:O	1:B:112:GLU:HB2	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	Percentiles
1	А	16/18~(89%)	15~(94%)	1 (6%)	0	100 100
1	В	16/18~(89%)	14 (88%)	2(12%)	0	100 100
All	All	32/36~(89%)	29~(91%)	3 (9%)	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	А	14/14~(100%)	14~(100%)	0	100 100		
1	В	14/14~(100%)	14 (100%)	0	100 100		
All	All	28/28~(100%)	28~(100%)	0	100 100		

There are no protein residues with a non-rotameric sidechain to report.



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 5 ligands modelled in this entry, 5 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)

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 $>$	#	$\#RSRZ{>}2$		$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	17/18~(94%)	-0.23	0	100	100	10, 12, 15, 23	0
1	В	17/18~(94%)	-0.08	0	100	100	10, 13, 17, 18	0
All	All	34/36~(94%)	-0.16	0	100	100	10, 13, 17, 23	0

There are no RSRZ outliers to report.

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. 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	CL	А	205	1/1	0.99	0.08	$13,\!13,\!13,\!13$	0
2	TB	А	201	1/1	1.00	0.01	$16,\!16,\!16,\!16$	0
3	CL	А	203	1/1	1.00	0.04	9,9,9,9	0
3	CL	А	204	1/1	1.00	0.10	11,11,11,11	0
2	TB	В	202	1/1	1.00	0.01	$18,\!18,\!18,\!18$	0



6.5 Other polymers (i)

There are no such residues in this entry.

