Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2016 – 10:54 AM EST

PDB ID	:	5TSC
Title	:	The crystal structure of Lpg2147 from Legionella pneumophila
Authors	:	Valleau, D.; Xu, X.; Cui, H.; Joachimiak, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2016-10-28
Resolution	:	2.01 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 ①) were used in the production of this report:

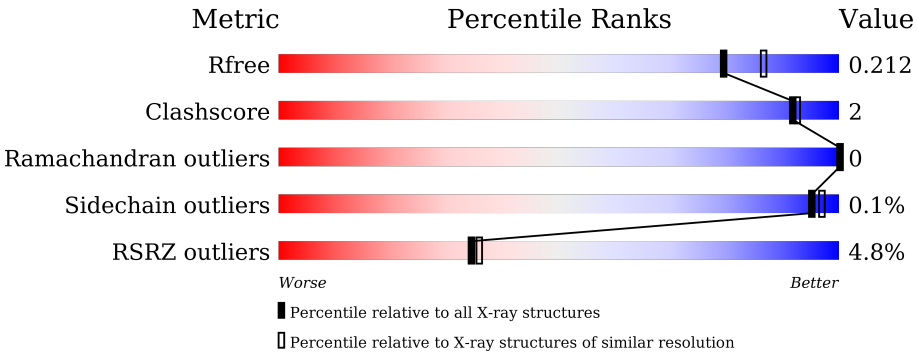
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

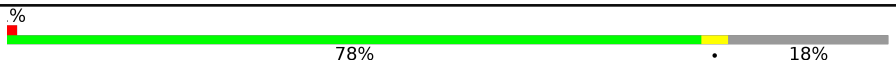
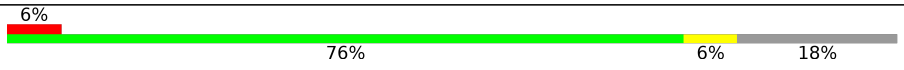
The reported resolution of this entry is 2.01 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	463	
1	B	463	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6535 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	2	0
			3032	1919	495	601	17			
1	B	378	Total	C	N	O	S	0	3	0
			3038	1924	496	601	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q5ZTL4
A	74	ALA	CYS	engineered mutation	UNP Q5ZTL4
B	0	GLY	-	expression tag	UNP Q5ZTL4
B	74	ALA	CYS	engineered mutation	UNP Q5ZTL4

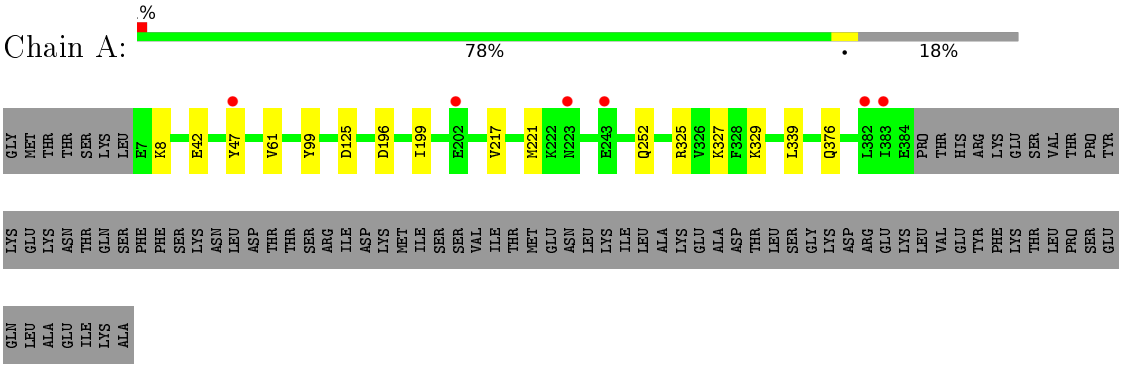
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	237	Total	O	0	0
			237	237		
2	B	228	Total	O	0	0
			228	228		

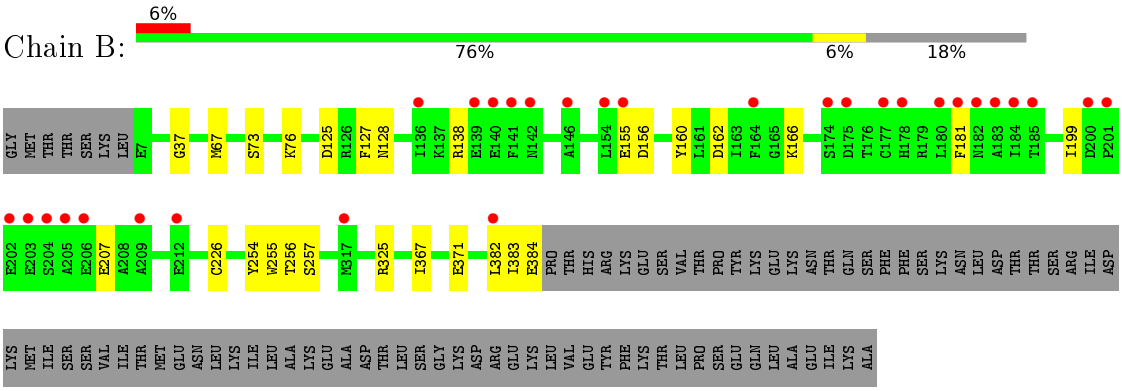
3 Residue-property plots (i)

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.93Å 68.37Å 71.66Å 117.13° 98.77° 90.28°	Depositor
Resolution (Å)	36.02 – 2.01 36.02 – 2.01	Depositor EDS
% Data completeness (in resolution range)	93.0 (36.02-2.01) 78.7 (36.02-2.01)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.02 (at 2.01Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1496: ???)	Depositor
R, R_{free}	0.174 , 0.210 0.173 , 0.212	Depositor DCC
R_{free} test set	1945 reflections (3.85%)	DCC
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,k,-k-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6535	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

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	0.32	0/3096	0.48	0/4176
1	B	0.32	0/3105	0.49	0/4187
All	All	0.32	0/6201	0.48	0/8363

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	GLN	Peptide

5.2 Too-close contacts

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	3032	0	2985	9	0
1	B	3038	0	2998	16	0
2	A	237	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	228	0	0	0	0
All	All	6535	0	5983	25	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 (25) 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:128:ASN:O	1:B:226:CYS:HB3	2.08	0.54
1:A:125:ASP:HB2	1:A:325:ARG:HG2	1.92	0.52
1:B:199:ILE:HG23	1:B:207:GLU:HB3	1.95	0.48
1:B:73:SER:HB3	1:B:76:LYS:HB2	1.97	0.47
1:B:383:ILE:O	1:B:384:GLU:HB2	2.13	0.47
1:A:8:LYS:HA	1:A:339:LEU:HD12	1.97	0.46
1:B:255:TRP:CD1	1:B:256:THR:HG23	2.51	0.46
1:A:196:ASP:HB3	1:A:199:ILE:HG23	1.99	0.45
1:A:99:TYR:HB3	1:A:327:LYS:HB3	1.99	0.45
1:B:127:PHE:CE1	1:B:226:CYS:HB2	2.53	0.44
1:A:99:TYR:CZ	1:A:329:LYS:HE3	2.53	0.44
1:B:181:PHE:CD2	1:B:181:PHE:O	2.71	0.44
1:B:37:GLY:HA2	1:B:67:MET:SD	2.58	0.44
1:B:162:ASP:OD2	1:B:166:LYS:HB2	2.18	0.44
1:B:254:TYR:HB3	1:B:257[A]:SER:HB3	2.00	0.43
1:A:217:VAL:O	1:A:221:MET:HG2	2.18	0.43
1:A:47:TYR:CD2	1:A:61:VAL:HG22	2.54	0.42
1:B:383:ILE:O	1:B:384:GLU:CB	2.68	0.42
1:A:42:GLU:OE2	1:A:376:GLN:NE2	2.52	0.41
1:B:160:TYR:CZ	1:B:162:ASP:HA	2.54	0.41
1:B:138:ARG:NH2	1:B:156:ASP:OD1	2.38	0.41
1:B:367:ILE:O	1:B:371:GLU:HG3	2.19	0.41
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.86	0.41
1:A:125:ASP:OD2	1:A:327:LYS:NZ	2.48	0.40
1:B:125:ASP:HB2	1:B:325:ARG:HG2	2.04	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	378/463 (82%)	372 (98%)	6 (2%)	0	100	100
1	B	379/463 (82%)	368 (97%)	11 (3%)	0	100	100
All	All	757/926 (82%)	740 (98%)	17 (2%)	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	337/414 (81%)	337 (100%)	0	100	100
1	B	338/414 (82%)	337 (100%)	1 (0%)	94	96
All	All	675/828 (82%)	674 (100%)	1 (0%)	95	97

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

Mol	Chain	Res	Type
1	B	155	GLU

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	OWAB(Å^2)	Q<0.9
1	A	378/463 (81%)	-0.30	6 (1%) 74 75	9, 26, 57, 108	0
1	B	378/463 (81%)	0.15	30 (7%) 15 16	10, 29, 91, 123	0
All	All	756/926 (81%)	-0.08	36 (4%) 34 36	9, 28, 84, 123	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	GLU	5.5
1	B	185	THR	4.8
1	B	201	PRO	4.7
1	B	174	SER	4.6
1	B	178	HIS	4.4
1	B	175	ASP	4.2
1	B	202	GLU	4.1
1	B	177	CYS	4.1
1	B	206	GLU	4.0
1	B	184	ILE	3.7
1	B	155	GLU	3.7
1	A	382	LEU	3.6
1	B	200	ASP	3.6
1	B	164	PHE	3.5
1	B	139	GLU	3.5
1	B	154	LEU	3.2
1	B	182	ASN	3.1
1	B	212	GLU	3.1
1	B	140	GLU	3.1
1	B	180	LEU	2.9
1	B	136	ILE	2.9
1	B	205	ALA	2.9
1	B	141	PHE	2.8
1	B	382	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	183	ALA	2.7
1	A	383	ILE	2.7
1	B	146	ALA	2.5
1	A	47	TYR	2.4
1	A	202	GLU	2.4
1	B	209	ALA	2.4
1	B	204	SER	2.4
1	A	223	ASN	2.3
1	B	317	MET	2.2
1	A	243	GLU	2.1
1	B	181	PHE	2.1
1	B	142	ASN	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.