



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:21 PM GMT

PDB ID : 4OM7
Title : Crystal structure of TIR domain of TLR6
Authors : Park, H.H; Jang, T.H
Deposited on : 2014-01-26
Resolution : 2.20 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

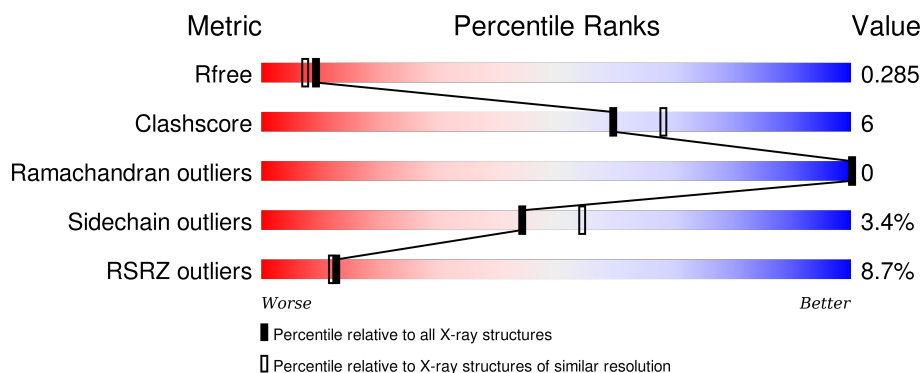
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	179	<div> <div>7%</div> <div>67%</div> <div>12%</div> <div>20%</div> </div>
1	B	179	<div> <div>7%</div> <div>68%</div> <div>12%</div> <div>20%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2431 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 Toll-like receptor 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1202	786	203	209	4			
1	B	143	Total	C	N	O	S	0	0	0
			1202	786	203	209	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	797	MET	-	EXPRESSION TAG	UNP Q9Y2C9
A	798	LYS	-	EXPRESSION TAG	UNP Q9Y2C9
A	799	LEU	-	EXPRESSION TAG	UNP Q9Y2C9
A	800	THR	-	EXPRESSION TAG	UNP Q9Y2C9
A	801	LEU	-	EXPRESSION TAG	UNP Q9Y2C9
A	802	VAL	-	EXPRESSION TAG	UNP Q9Y2C9
A	803	THR	-	EXPRESSION TAG	UNP Q9Y2C9
A	804	GLU	-	EXPRESSION TAG	UNP Q9Y2C9
A	805	ASN	-	EXPRESSION TAG	UNP Q9Y2C9
A	806	ASN	-	EXPRESSION TAG	UNP Q9Y2C9
A	807	ASP	-	EXPRESSION TAG	UNP Q9Y2C9
A	808	VAL	-	EXPRESSION TAG	UNP Q9Y2C9
A	809	LYS	-	EXPRESSION TAG	UNP Q9Y2C9
A	810	SER	-	EXPRESSION TAG	UNP Q9Y2C9
A	811	LEU	-	EXPRESSION TAG	UNP Q9Y2C9
A	812	GLU	-	EXPRESSION TAG	UNP Q9Y2C9
A	813	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
A	814	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
A	815	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
A	816	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
A	817	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
A	818	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
B	797	MET	-	EXPRESSION TAG	UNP Q9Y2C9
B	798	LYS	-	EXPRESSION TAG	UNP Q9Y2C9
B	799	LEU	-	EXPRESSION TAG	UNP Q9Y2C9

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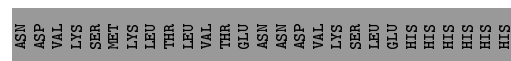
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Chain	Residue	Modelled	Actual	Comment	Reference
B	800	THR	-	EXPRESSION TAG	UNP Q9Y2C9
B	801	LEU	-	EXPRESSION TAG	UNP Q9Y2C9
B	802	VAL	-	EXPRESSION TAG	UNP Q9Y2C9
B	803	THR	-	EXPRESSION TAG	UNP Q9Y2C9
B	804	GLU	-	EXPRESSION TAG	UNP Q9Y2C9
B	805	ASN	-	EXPRESSION TAG	UNP Q9Y2C9
B	806	ASN	-	EXPRESSION TAG	UNP Q9Y2C9
B	807	ASP	-	EXPRESSION TAG	UNP Q9Y2C9
B	808	VAL	-	EXPRESSION TAG	UNP Q9Y2C9
B	809	LYS	-	EXPRESSION TAG	UNP Q9Y2C9
B	810	SER	-	EXPRESSION TAG	UNP Q9Y2C9
B	811	LEU	-	EXPRESSION TAG	UNP Q9Y2C9
B	812	GLU	-	EXPRESSION TAG	UNP Q9Y2C9
B	813	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
B	814	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
B	815	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
B	816	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
B	817	HIS	-	EXPRESSION TAG	UNP Q9Y2C9
B	818	HIS	-	EXPRESSION TAG	UNP Q9Y2C9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	10	Total O 10 10	0	0

- Molecule 1: Toll-like receptor 6



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.61Å 44.20Å 75.72Å 90.00° 118.90° 90.00°	Depositor
Resolution (Å)	31.82 – 2.20 31.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (31.82-2.20) 96.1 (31.82-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.233 , 0.285 0.233 , 0.285	Depositor DCC
R_{free} test set	943 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18216 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2431	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.90% 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](#)

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	0.48	0/1240	0.67	1/1681 (0.1%)
1	B	0.47	0/1240	0.66	0/1681
All	All	0.48	0/2480	0.66	1/3362 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770	ARG	NE-CZ-NH2	5.62	123.11	120.30

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	1202	0	1178	15	0
1	B	1202	0	1178	13	0
2	A	17	0	0	4	0
2	B	10	0	0	0	0
All	All	2431	0	2356	27	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 6.

All (27) 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:643:HIS:HB2	1:B:669:ILE:HG23	1.58	0.85
1:A:657:LYS:NZ	1:A:675:GLU:OE1	2.19	0.75
1:B:682:LYS:HD2	1:B:686:GLU:HB3	1.75	0.69
1:A:740:PRO:O	1:A:743:SER:OG	2.15	0.65
1:A:770:ARG:O	2:A:908:HOH:O	2.15	0.63
1:A:764:PRO:O	1:A:770:ARG:NH2	2.30	0.62
1:A:674:HIS:HA	1:A:678:PHE:CD1	2.36	0.60
1:A:741:GLN:NE2	2:A:917:HOH:O	2.36	0.59
1:A:643:HIS:HB2	1:A:669:ILE:HG23	1.84	0.58
1:B:674:HIS:HB2	1:B:687:ASN:HB3	1.85	0.58
1:A:770:ARG:HH21	1:A:770:ARG:CG	2.18	0.56
1:B:689:ILE:O	1:B:693:GLU:HG2	2.08	0.54
1:B:725:HIS:O	1:B:728:SER:HB3	2.08	0.53
1:A:686:GLU:OE1	2:A:911:HOH:O	2.19	0.51
1:A:678:PHE:CD1	1:A:687:ASN:HB3	2.48	0.49
1:A:747:LYS:HG3	1:B:717:TYR:CZ	2.50	0.46
1:A:758:ARG:NH2	1:A:760:TYR:OH	2.50	0.45
1:B:673:LEU:H	1:B:677:ASN:HB2	1.79	0.45
1:A:770:ARG:HH21	1:A:770:ARG:HG2	1.83	0.44
1:B:698:SER:HB2	1:B:723:LEU:HD11	2.00	0.44
1:A:704:PRO:O	1:A:708:GLN:HG2	2.17	0.43
1:B:728:SER:O	1:B:728:SER:OG	2.37	0.43
1:B:696:TYR:CE2	1:B:697:LYS:HE2	2.54	0.42
1:B:766:GLU:H	1:B:766:GLU:CD	2.21	0.42
1:B:750:LYS:HD2	1:B:750:LYS:HA	1.86	0.41
1:B:682:LYS:HE3	1:B:687:ASN:OD1	2.21	0.41
1:A:682:LYS:HA	2:A:911:HOH:O	2.20	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	A	141/179 (79%)	139 (99%)	2 (1%)	0	100	100
1	B	141/179 (79%)	140 (99%)	1 (1%)	0	100	100
All	All	282/358 (79%)	279 (99%)	3 (1%)	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	133/169 (79%)	127 (96%)	6 (4%)	34	41
1	B	133/169 (79%)	130 (98%)	3 (2%)	58	71
All	All	266/338 (79%)	257 (97%)	9 (3%)	44	54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	673	LEU
1	A	702	LEU
1	A	716	LEU
1	A	737	GLU
1	A	741	GLN
1	A	770	ARG
1	B	678	PHE
1	B	702	LEU
1	B	778	ARG

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 [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](#)

There are no ligands in this entry.

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	143/179 (79%)	0.56	12 (8%)	14 13	21, 38, 67, 87	0
1	B	143/179 (79%)	0.71	13 (9%)	11 11	24, 41, 70, 90	0
All	All	286/358 (79%)	0.64	25 (8%)	13 12	21, 40, 70, 90	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	679	VAL	13.4
1	B	678	PHE	9.9
1	B	680	PRO	9.4
1	B	677	ASN	6.1
1	B	676	ARG	5.7
1	B	675	GLU	4.5
1	A	679	VAL	4.2
1	B	666	LYS	3.9
1	B	682	LYS	3.7
1	B	681	GLY	3.4
1	A	675	GLU	3.4
1	A	782	ASN	3.3
1	B	758	ARG	3.2
1	B	668	ASP	3.2
1	A	766	GLU	3.1
1	A	714	TYR	3.0
1	A	681	GLY	2.7
1	A	680	PRO	2.6
1	B	667	GLU	2.6
1	B	765	LYS	2.4
1	A	700	PHE	2.4
1	A	716	LEU	2.3
1	A	647	SER	2.3
1	A	718	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	717	TYR	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 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.