



wwPDB EM Map/Model Validation Report ⓘ

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PDB ID : 3J0A
EMDB ID: : EMD-5287
Title : Homology model of human Toll-like receptor 5 fitted into an electron microscopy single particle reconstruction
Authors : Modis, Y.; Zhou, K.; Kanai, R.; Lee, P.; Wang, H.W.
Deposited on : 2011-06-02
Resolution : 26.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

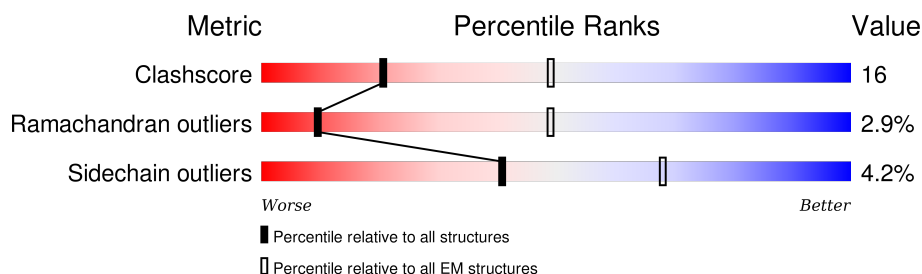
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 26.00 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	844	 60% 31% • 6%
1	B	844	 46% 26% • 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11828 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	797	Total	C	N	O	S	0	0
			6437	4155	1081	1176	25		
1	B	632	Total	C	N	O	S	0	0
			5055	3272	839	927	17		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	859	GLY	-	EXPRESSION TAG	UNP O60602
A	860	SER	-	EXPRESSION TAG	UNP O60602
A	861	HIS	-	EXPRESSION TAG	UNP O60602
A	862	HIS	-	EXPRESSION TAG	UNP O60602
A	863	HIS	-	EXPRESSION TAG	UNP O60602
A	864	HIS	-	EXPRESSION TAG	UNP O60602
A	865	HIS	-	EXPRESSION TAG	UNP O60602
A	866	HIS	-	EXPRESSION TAG	UNP O60602
B	859	GLY	-	EXPRESSION TAG	UNP O60602
B	860	SER	-	EXPRESSION TAG	UNP O60602
B	861	HIS	-	EXPRESSION TAG	UNP O60602
B	862	HIS	-	EXPRESSION TAG	UNP O60602
B	863	HIS	-	EXPRESSION TAG	UNP O60602
B	864	HIS	-	EXPRESSION TAG	UNP O60602
B	865	HIS	-	EXPRESSION TAG	UNP O60602
B	866	HIS	-	EXPRESSION TAG	UNP O60602

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total	C	N	O	0
			168	98	7	63	
2	A	2	Total	C	N	O	0
			168	98	7	63	

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Mol	Chain	Residues	Atoms				AltConf
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	A	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0
2	B	2	Total 168	C 98	N 7	O 63	0




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	4241	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	52000	Depositor
Image detector	Gatan Ultra4000	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.87	7/6589 (0.1%)	0.61	1/8938 (0.0%)
1	B	0.75	2/5172 (0.0%)	0.59	3/7029 (0.0%)
All	All	0.82	9/11761 (0.1%)	0.61	4/15967 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	738	GLU	CD-OE1	-28.34	0.94	1.25
1	A	738	GLU	CD-OE2	9.38	1.35	1.25
1	A	582	ILE	C-O	7.25	1.37	1.23
1	A	738	GLU	CA-C	7.20	1.71	1.52
1	B	616	PHE	CE2-CZ	6.46	1.49	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	GLU	OE1-CD-OE2	-11.45	109.56	123.30
1	B	664	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	B	664	ARG	NH1-CZ-NH2	5.22	125.15	119.40
1	B	660	VAL	CG1-CB-CG2	-5.15	102.66	110.90

There are no chirality outliers.

There are no planarity outliers.

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	6437	0	6385	214	0
1	B	5055	0	5041	160	0
2	A	168	0	154	2	0
2	B	168	0	154	2	0
All	All	11828	0	11734	372	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 16.

The worst 5 of 372 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:514:LEU:HD13	1:B:538:LEU:HG	1.55	0.87
1:A:748:ILE:HG23	1:A:754:ILE:HD11	1.58	0.86
1:A:123:GLU:HG2	1:A:149:ARG:HB3	1.58	0.85
1:B:123:GLU:HG2	1:B:149:ARG:HB3	1.58	0.85
1:A:707:VAL:HG13	1:A:711:LEU:HD23	1.64	0.78

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 PDB entries followed by that with respect to all EM entries.

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	791/844 (94%)	621 (78%)	151 (19%)	19 (2%)	7	47
1	B	628/844 (74%)	471 (75%)	135 (22%)	22 (4%)	4	39
All	All	1419/1688 (84%)	1092 (77%)	286 (20%)	41 (3%)	9	43

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	397	THR
1	B	182	ILE
1	B	506	VAL
1	A	181	GLN

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 PDB entries followed by that with respect to all EM entries.

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	727/770 (94%)	697 (96%)	30 (4%)	37	71
1	B	576/770 (75%)	551 (96%)	25 (4%)	35	70
All	All	1303/1540 (85%)	1248 (96%)	55 (4%)	41	70

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	571	LEU
1	B	40	GLN
1	B	460	PHE
1	A	650	LEU
1	A	738	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	ASN
1	B	80	GLN
1	B	505	GLN
1	A	743	ASN
1	A	804	GLN

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 ⓘ

28 carbohydrates are modelled in this entry.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1037	1,2	14,14,15	1.51	2 (14%)	15,19,21	1.29	2 (13%)
2	FUC	A	1038	2	10,10,11	1.69	3 (30%)	13,14,16	2.05	4 (30%)
2	NAG	A	1245	1,2	14,14,15	1.66	3 (21%)	15,19,21	1.72	4 (26%)
2	FUC	A	1246	2	10,10,11	1.39	1 (10%)	13,14,16	1.25	1 (7%)
2	NAG	A	1342	1,2	14,14,15	1.39	4 (28%)	15,19,21	1.09	0
2	FUC	A	1343	2	10,10,11	1.60	3 (30%)	13,14,16	1.87	4 (30%)
2	NAG	A	1422	1,2	14,14,15	1.93	2 (14%)	15,19,21	1.39	2 (13%)
2	FUC	A	1423	2	10,10,11	1.69	2 (20%)	13,14,16	1.50	2 (15%)
2	NAG	A	1595	1,2	14,14,15	1.37	2 (14%)	15,19,21	1.42	2 (13%)
2	FUC	A	1596	2	10,10,11	1.90	3 (30%)	13,14,16	2.04	2 (15%)
2	NAG	A	2046	1,2	14,14,15	1.76	4 (28%)	15,19,21	1.26	1 (6%)
2	FUC	A	2047	2	10,10,11	1.61	3 (30%)	13,14,16	1.50	3 (23%)
2	NAG	A	2598	1,2	14,14,15	1.43	2 (14%)	15,19,21	1.08	1 (6%)
2	FUC	A	2599	2	10,10,11	1.83	3 (30%)	13,14,16	2.26	6 (46%)
2	NAG	B	1037	1,2	14,14,15	1.60	2 (14%)	15,19,21	1.39	3 (20%)
2	FUC	B	1038	2	10,10,11	1.61	2 (20%)	13,14,16	1.36	3 (23%)
2	NAG	B	1245	1,2	14,14,15	1.91	3 (21%)	15,19,21	1.11	1 (6%)
2	FUC	B	1246	2	10,10,11	1.70	3 (30%)	13,14,16	1.74	3 (23%)
2	NAG	B	1342	1,2	14,14,15	1.56	3 (21%)	15,19,21	1.36	2 (13%)
2	FUC	B	1343	2	10,10,11	1.60	2 (20%)	13,14,16	1.68	2 (15%)
2	NAG	B	1422	1,2	14,14,15	1.96	2 (14%)	15,19,21	1.38	2 (13%)
2	FUC	B	1423	2	10,10,11	1.69	2 (20%)	13,14,16	1.49	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1595	1,2	14,14,15	1.76	4 (28%)	15,19,21	1.13	1 (6%)
2	FUC	B	1596	2	10,10,11	1.95	3 (30%)	13,14,16	2.74	5 (38%)
2	NAG	B	2046	1,2	14,14,15	1.25	1 (7%)	15,19,21	1.21	3 (20%)
2	FUC	B	2047	2	10,10,11	1.47	3 (30%)	13,14,16	1.20	2 (15%)
2	NAG	B	2598	1,2	14,14,15	1.69	3 (21%)	15,19,21	1.49	3 (20%)
2	FUC	B	2599	2	10,10,11	1.79	3 (30%)	13,14,16	2.06	3 (23%)

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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1037	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1038	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1245	1,2	-	1/6/23/26	0/1/1/1
2	FUC	A	1246	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1342	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1343	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1422	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1423	2	-	0/0/17/20	0/1/1/1
2	NAG	A	1595	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	1596	2	-	0/0/17/20	0/1/1/1
2	NAG	A	2046	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	2047	2	-	0/0/17/20	0/1/1/1
2	NAG	A	2598	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	2599	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1037	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1038	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1245	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1246	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1342	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1343	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1422	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1423	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1595	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	1596	2	-	0/0/17/20	0/1/1/1
2	NAG	B	2046	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	2047	2	-	0/0/17/20	0/1/1/1
2	NAG	B	2598	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	2599	2	-	0/0/17/20	0/1/1/1

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2047	FUC	C2-C3	2.02	1.55	1.52
2	A	2598	NAG	C3-C2	2.03	1.57	1.52
2	A	1342	NAG	C1-C2	2.03	1.55	1.52
2	A	1422	NAG	O5-C5	2.04	1.47	1.43
2	A	1245	NAG	C8-C7	2.05	1.54	1.50

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1245	NAG	C2-N2-C7	-3.80	118.16	123.11
2	B	2598	NAG	C2-N2-C7	-3.59	118.44	123.11
2	B	1342	NAG	C2-N2-C7	-3.34	118.76	123.11
2	B	1595	NAG	C2-N2-C7	-3.06	119.13	123.11
2	A	1422	NAG	O7-C7-C8	-2.99	116.56	122.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1245	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1342	NAG	1	0
2	A	2598	NAG	1	0
2	B	1342	NAG	1	0
2	B	2598	NAG	1	0

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 ⓘ

There are no chain breaks in this entry.