



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2016 – 08:22 AM EST

PDB ID : 4MJ6
Title : Crystal Structure of HLA-A*1101 in complex with H7-22, an influenza A(H7N9) virus epitope
Authors : Liu, J.; Tan, S.; Zhao, M.; Qi, J.; Gao, G.F.
Deposited on : 2013-09-03
Resolution : 2.57 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.

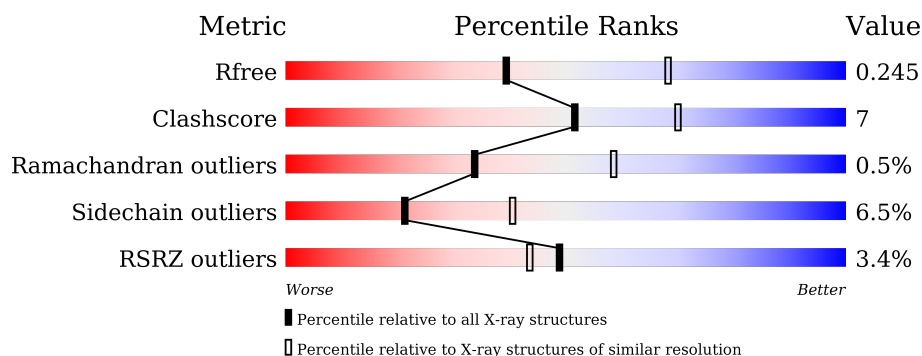
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	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

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X-RAY DIFFRACTION

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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	274	<div> <div>3%</div> <div>80%</div> <div>19%</div> </div>
2	B	100	<div> <div>3%</div> <div>79%</div> <div>20%</div> </div>
3	C	11	<div> <div>27%</div> <div>18%</div> <div>45%</div> <div>18%</div> <div>18%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3262 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 HLA class I histocompatibility antigen, A-11 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2235	1389	407	430	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	S	0	0	0
			92	59	15	15	3			

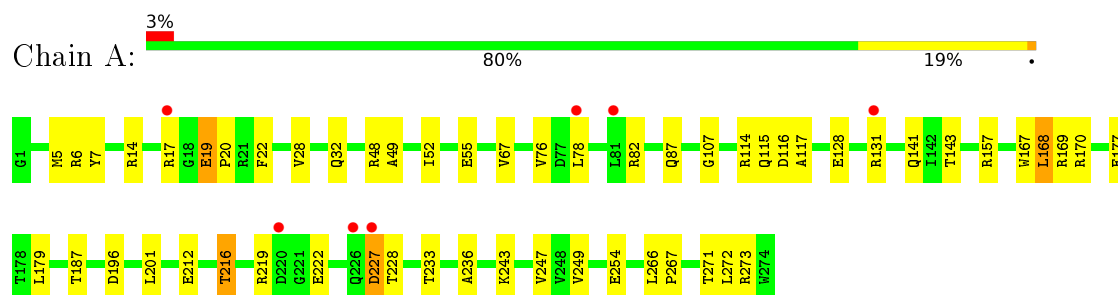
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	33	Total	O	0	0
			33	33		
4	C	2	Total	O	0	0
			2	2		

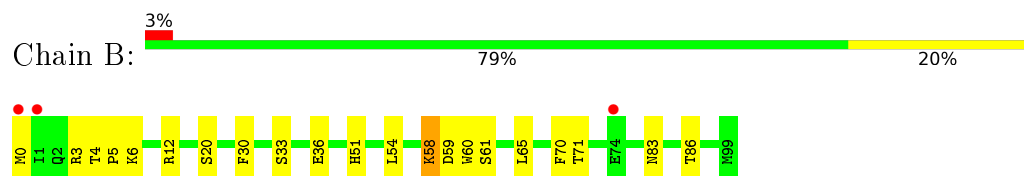
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

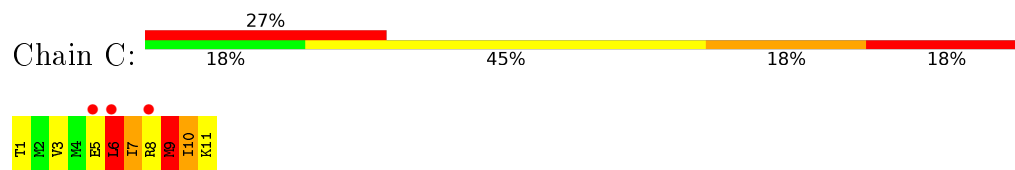
- Molecule 1: HLA class I histocompatibility antigen, A-11 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.99Å 65.05Å 109.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.84 – 2.57 39.22 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.84-2.57) 98.5 (39.22-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.186 , 0.247 0.185 , 0.245	Depositor DCC
R_{free} test set	629 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3262	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.28	0/2296	0.47	0/3117
2	B	0.27	0/860	0.44	0/1162
3	C	0.73	0/91	0.86	0/117
All	All	0.30	0/3247	0.47	0/4396

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
3	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	6	LEU	Peptide
3	C	7	ILE	Peptide

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	2235	0	2085	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	837	0	803	12	0
3	C	92	0	110	6	0
4	A	63	0	0	8	0
4	B	33	0	0	1	0
4	C	2	0	0	0	0
All	All	3262	0	2998	42	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 7.

All (42) 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)
2:B:4:THR:HA	2:B:86:THR:HG21	1.68	0.76
2:B:71:THR:O	4:B:102:HOH:O	2.07	0.72
1:A:212:GLU:OE2	4:A:353:HOH:O	2.08	0.70
1:A:32:GLN:OE1	4:A:312:HOH:O	2.13	0.67
1:A:273:ARG:NH1	4:A:337:HOH:O	2.28	0.66
1:A:19:GLU:HG2	1:A:20:PRO:HD2	1.81	0.63
1:A:107:GLY:O	1:A:169:ARG:NH1	2.32	0.62
1:A:5:MET:HB2	1:A:168:LEU:HG	1.84	0.59
1:A:115:GLN:NE2	4:A:350:HOH:O	2.35	0.54
1:A:55:GLU:OE1	1:A:170:ARG:NE	2.41	0.53
1:A:82:ARG:HG2	1:A:87:GLN:HB2	1.91	0.51
2:B:36:GLU:HB3	2:B:83:ASN:HB3	1.93	0.49
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.93	0.49
1:A:228:THR:HG21	4:A:305:HOH:O	2.13	0.48
1:A:187:THR:HB	1:A:272:LEU:HD11	1.96	0.47
3:C:6:LEU:HB2	3:C:8:ARG:H	1.79	0.47
1:A:227:ASP:HB3	1:A:247:VAL:HG23	1.96	0.47
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.97	0.46
1:A:48:ARG:NH2	4:A:320:HOH:O	2.33	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.51	0.45
1:A:14:ARG:HB2	1:A:17:ARG:HB2	1.99	0.45
1:A:7:TYR:CE1	3:C:1:THR:HG22	2.51	0.45
2:B:20:SER:HA	2:B:71:THR:HG22	1.99	0.44
2:B:3:ARG:NH1	2:B:61:SER:HB3	2.32	0.43
2:B:5:PRO:HB3	2:B:30:PHE:HB3	2.00	0.42
1:A:196:ASP:N	1:A:196:ASP:OD1	2.52	0.42
1:A:131:ARG:HH22	1:A:157:ARG:HH12	1.67	0.42
1:A:233:THR:OG1	1:A:243:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:ILE:C	3:C:9:MET:N	2.72	0.42
2:B:58:LYS:HD2	2:B:59:ASP:N	2.35	0.42
3:C:3:VAL:O	3:C:5:GLU:N	2.52	0.42
3:C:10:ILE:HG13	3:C:10:ILE:H	1.55	0.41
2:B:6:LYS:HB2	2:B:6:LYS:HE3	1.76	0.41
1:A:143:THR:HG23	3:C:11:LYS:HA	2.01	0.41
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.41
2:B:51:HIS:HA	2:B:65:LEU:O	2.20	0.41
1:A:128:GLU:OE1	4:A:346:HOH:O	2.21	0.41
1:A:216:THR:OG1	4:A:307:HOH:O	2.12	0.41
1:A:22:PHE:HE2	1:A:67:VAL:HG22	1.86	0.41
1:A:236:ALA:HB1	2:B:12:ARG:HG3	2.02	0.40
1:A:266:LEU:HA	1:A:267:PRO:HD2	1.88	0.40
1:A:271:THR:O	1:A:272:LEU:HD23	2.22	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	272/274 (99%)	262 (96%)	9 (3%)	1 (0%)	39	63
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	9/11 (82%)	3 (33%)	5 (56%)	1 (11%)	0	0
All	All	379/385 (98%)	362 (96%)	15 (4%)	2 (0%)	34	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	9	MET
1	A	227	ASP

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	231/231 (100%)	215 (93%)	16 (7%)	19	37
2	B	95/95 (100%)	92 (97%)	3 (3%)	46	73
3	C	11/11 (100%)	8 (73%)	3 (27%)	0	1
All	All	337/337 (100%)	315 (94%)	22 (6%)	21	40

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	19	GLU
1	A	76	VAL
1	A	78	LEU
1	A	114	ARG
1	A	116	ASP
1	A	141	GLN
1	A	167	TRP
1	A	168	LEU
1	A	177	GLU
1	A	201	LEU
1	A	216	THR
1	A	219	ARG
1	A	222	GLU
1	A	249	VAL
1	A	254	GLU
2	B	0	MET
2	B	58	LYS
2	B	70	PHE
3	C	6	LEU
3	C	9	MET
3	C	10	ILE

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](#)

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 [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, 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	274/274 (100%)	0.10	7 (2%) 59 55	16, 33, 67, 100	0
2	B	100/100 (100%)	-0.13	3 (3%) 54 49	16, 29, 57, 87	0
3	C	11/11 (100%)	0.87	3 (27%) 1 0	28, 48, 98, 107	0
All	All	385/385 (100%)	0.06	13 (3%) 49 43	16, 32, 71, 107	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	ARG	3.8
1	A	81	LEU	3.3
1	A	227	ASP	2.9
3	C	8	ARG	2.7
3	C	6	LEU	2.5
3	C	5	GLU	2.5
2	B	1	ILE	2.4
1	A	78	LEU	2.4
1	A	131	ARG	2.4
1	A	220	ASP	2.3
2	B	0	MET	2.2
1	A	226	GLN	2.1
2	B	74	GLU	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.