



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 08:58 PM EDT

PDB ID : 6APN
Title : HLA-A*0201 single chain trimer with HPV.16 E7 peptide LLMGTLGIV
Authors : Finton, K.A.K.
Deposited on : 2017-08-17
Resolution : 2.22 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

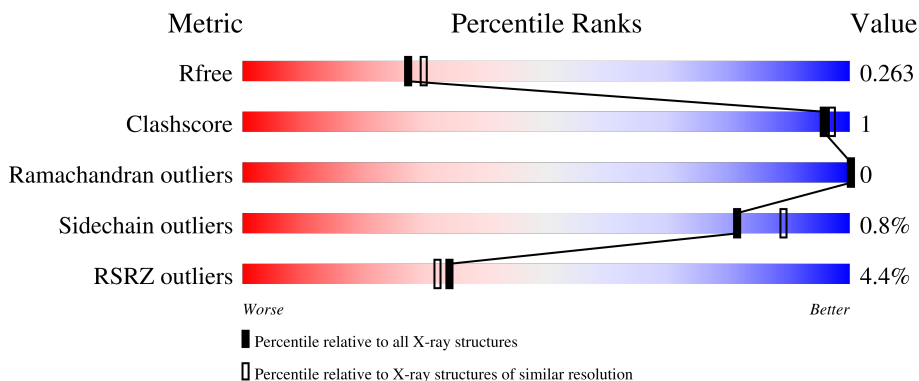
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 of 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 $\leq 5\%$. 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	446	 4% 85% 14%
1	B	446	 3% 81% 5% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6256 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 Beta-2-microglobulin--HLA-A*0201--HPV.16 E7 peptide LLMGTLGIV chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	3019	1906	535	566	12	0	2	0
1	B	383	3031	1910	536	574	11	0	1	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLY	-	linker	UNP P61769
A	125	GLY	-	linker	UNP P61769
A	126	GLY	-	linker	UNP P61769
A	127	GLY	-	linker	UNP P61769
A	128	SER	-	linker	UNP P61769
A	129	GLY	-	linker	UNP P61769
A	130	GLY	-	linker	UNP P61769
A	131	GLY	-	linker	UNP P61769
A	132	GLY	-	linker	UNP P61769
A	133	SER	-	linker	UNP P61769
A	134	GLY	-	linker	UNP P61769
A	135	GLY	-	linker	UNP P61769
A	136	GLY	-	linker	UNP P61769
A	137	GLY	-	linker	UNP P61769
A	138	SER	-	linker	UNP P61769
A	139	GLY	-	linker	UNP P61769
A	140	GLY	-	linker	UNP P61769
A	141	GLY	-	linker	UNP P61769
A	142	GLY	-	linker	UNP P61769
A	143	SER	-	linker	UNP P61769
A	144	GLY	-	linker	UNP P61769
A	227	ALA	TYR	conflict	UNP P01892
A	419	GLU	PRO	conflict	UNP P01892
A	420	ASN	SER	conflict	UNP P01892

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	421	LEU	-	expression tag	UNP P01892
A	422	TYR	-	expression tag	UNP P01892
A	423	PHE	-	expression tag	UNP P01892
A	424	GLN	-	expression tag	UNP P01892
A	425	GLY	-	expression tag	UNP P01892
A	426	HIS	-	expression tag	UNP P01892
A	427	HIS	-	expression tag	UNP P01892
A	428	HIS	-	expression tag	UNP P01892
A	429	HIS	-	expression tag	UNP P01892
A	430	HIS	-	expression tag	UNP P01892
A	431	HIS	-	expression tag	UNP P01892
A	432	GLY	-	expression tag	UNP P01892
A	433	LEU	-	expression tag	UNP P01892
A	434	ASN	-	expression tag	UNP P01892
A	435	ASP	-	expression tag	UNP P01892
A	436	ILE	-	expression tag	UNP P01892
A	437	PHE	-	expression tag	UNP P01892
A	438	GLU	-	expression tag	UNP P01892
A	439	ALA	-	expression tag	UNP P01892
A	440	GLN	-	expression tag	UNP P01892
A	441	LYS	-	expression tag	UNP P01892
A	442	ILE	-	expression tag	UNP P01892
A	443	GLU	-	expression tag	UNP P01892
A	444	TRP	-	expression tag	UNP P01892
A	445	HIS	-	expression tag	UNP P01892
A	446	GLU	-	expression tag	UNP P01892
B	124	GLY	-	linker	UNP P61769
B	125	GLY	-	linker	UNP P61769
B	126	GLY	-	linker	UNP P61769
B	127	GLY	-	linker	UNP P61769
B	128	SER	-	linker	UNP P61769
B	129	GLY	-	linker	UNP P61769
B	130	GLY	-	linker	UNP P61769
B	131	GLY	-	linker	UNP P61769
B	132	GLY	-	linker	UNP P61769
B	133	SER	-	linker	UNP P61769
B	134	GLY	-	linker	UNP P61769
B	135	GLY	-	linker	UNP P61769
B	136	GLY	-	linker	UNP P61769
B	137	GLY	-	linker	UNP P61769
B	138	SER	-	linker	UNP P61769
B	139	GLY	-	linker	UNP P61769

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	140	GLY	-	linker	UNP P61769
B	141	GLY	-	linker	UNP P61769
B	142	GLY	-	linker	UNP P61769
B	143	SER	-	linker	UNP P61769
B	144	GLY	-	linker	UNP P61769
B	227	ALA	TYR	conflict	UNP P01892
B	419	GLU	PRO	conflict	UNP P01892
B	420	ASN	SER	conflict	UNP P01892
B	421	LEU	-	expression tag	UNP P01892
B	422	TYR	-	expression tag	UNP P01892
B	423	PHE	-	expression tag	UNP P01892
B	424	GLN	-	expression tag	UNP P01892
B	425	GLY	-	expression tag	UNP P01892
B	426	HIS	-	expression tag	UNP P01892
B	427	HIS	-	expression tag	UNP P01892
B	428	HIS	-	expression tag	UNP P01892
B	429	HIS	-	expression tag	UNP P01892
B	430	HIS	-	expression tag	UNP P01892
B	431	HIS	-	expression tag	UNP P01892
B	432	GLY	-	expression tag	UNP P01892
B	433	LEU	-	expression tag	UNP P01892
B	434	ASN	-	expression tag	UNP P01892
B	435	ASP	-	expression tag	UNP P01892
B	436	ILE	-	expression tag	UNP P01892
B	437	PHE	-	expression tag	UNP P01892
B	438	GLU	-	expression tag	UNP P01892
B	439	ALA	-	expression tag	UNP P01892
B	440	GLN	-	expression tag	UNP P01892
B	441	LYS	-	expression tag	UNP P01892
B	442	ILE	-	expression tag	UNP P01892
B	443	GLU	-	expression tag	UNP P01892
B	444	TRP	-	expression tag	UNP P01892
B	445	HIS	-	expression tag	UNP P01892
B	446	GLU	-	expression tag	UNP P01892

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	100	Total O 100 100	0	0
2	B	106	Total O 106 106	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.36Å 65.09Å 130.32Å 90.00° 96.25° 90.00°	Depositor
Resolution (Å)	50.01 – 2.22 31.07 – 2.22	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.01-2.22) 90.5 (31.07-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.22Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.260 0.218 , 0.263	Depositor DCC
R_{free} test set	1887 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtrriage
Anisotropy	0.273	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6256	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.79 % 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 5.5198e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.46	0/3114	0.61	1/4235 (0.0%)
1	B	0.47	0/3116	0.62	0/4239
All	All	0.47	0/6230	0.61	1/8474 (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	208	ARG	NE-CZ-NH1	5.24	122.92	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	3019	0	2766	1	0
1	B	3031	0	2799	12	0
2	A	100	0	0	0	0
2	B	106	0	0	0	0
All	All	6256	0	5565	13	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 1.

All (13) 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:274:ARG:NH2	1:B:300:ARG:NH2	2.54	0.55
1:B:3:MET:HE3	1:B:299:LEU:HD22	1.90	0.53
1:B:64:LEU:HD23	1:B:69:ARG:HA	1.90	0.52
1:B:374:VAL:HG13	1:B:387:TRP:CZ2	2.45	0.52
1:B:274:ARG:NH2	1:B:300:ARG:HH22	2.08	0.51
1:B:2:LEU:HD11	1:B:188:MET:CE	2.40	0.51
1:B:48:ASN:HB3	1:B:89:LEU:HD11	1.95	0.49
1:B:84:TRP:CE2	1:B:260:ALA:HB2	2.49	0.48
1:B:330:THR:OG1	1:B:413:LEU:HD21	2.15	0.46
1:B:392:VAL:HG22	1:B:400:TYR:CZ	2.55	0.42
1:B:344:LEU:HD22	1:B:392:VAL:HG21	2.01	0.41
1:B:274:ARG:HH21	1:B:300:ARG:NH2	2.17	0.41
1:A:192:ALA:O	1:A:195:ILE:HG22	2.21	0.40

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	378/446 (85%)	374 (99%)	4 (1%)	0	100	100
1	B	378/446 (85%)	369 (98%)	9 (2%)	0	100	100
All	All	756/892 (85%)	743 (98%)	13 (2%)	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	A	303/363 (84%)	301 (99%)	2 (1%)	84	91
1	B	307/363 (85%)	304 (99%)	3 (1%)	76	85
All	All	610/726 (84%)	605 (99%)	5 (1%)	81	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	PHE
1	A	154	SER
1	B	56	PRO
1	B	94	PHE
1	B	324	ARG

Sometimes 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 monosaccharides 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

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	384/446 (86%)	0.24	20 (5%) 27 25	18, 31, 63, 88	17 (4%)
1	B	383/446 (85%)	0.08	14 (3%) 41 39	17, 28, 52, 80	26 (6%)
All	All	767/892 (85%)	0.16	34 (4%) 34 32	17, 30, 60, 88	43 (5%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	ALA	8.0
1	A	143	SER	6.1
1	A	371	THR	5.7
1	A	340	HIS	5.2
1	A	337	VAL	4.9
1	B	337	VAL	4.9
1	B	369	GLN	4.1
1	A	373	LEU	4.0
1	B	335	HIS	4.0
1	A	338	SER	3.1
1	A	343	THR	3.1
1	B	336	ALA	3.1
1	A	417	TRP	3.1
1	A	391	VAL	3.0
1	B	334	HIS	3.0
1	A	395	GLY	3.0
1	B	339	ASP	3.0
1	A	364	GLY	2.8
1	B	144	GLY	2.8
1	A	11	GLY	2.8
1	A	335	HIS	2.6
1	A	368	THR	2.6
1	A	288	HIS	2.5
1	B	248	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	339	ASP	2.4
1	B	256	TYR	2.4
1	A	392	VAL	2.4
1	B	338	SER	2.4
1	B	370	ASP	2.3
1	A	334	HIS	2.3
1	B	294	HIS	2.3
1	B	114	PRO	2.3
1	A	144	GLY	2.2
1	B	288	HIS	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 monosaccharides 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.