



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 02:34 PM EST

PDB ID : 7SR3  
Title : Single chain trimer HLA-A\*02:01 (H98L, Y108C) with HPV.16 E7 peptide YMLDLQPETTDL  
Authors : Finton, K.A.K.; Rupert, P.B.  
Deposited on : 2021-11-07  
Resolution : 2.49 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](mailto: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>.

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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	:	2.31.2
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)	:	2.31.2

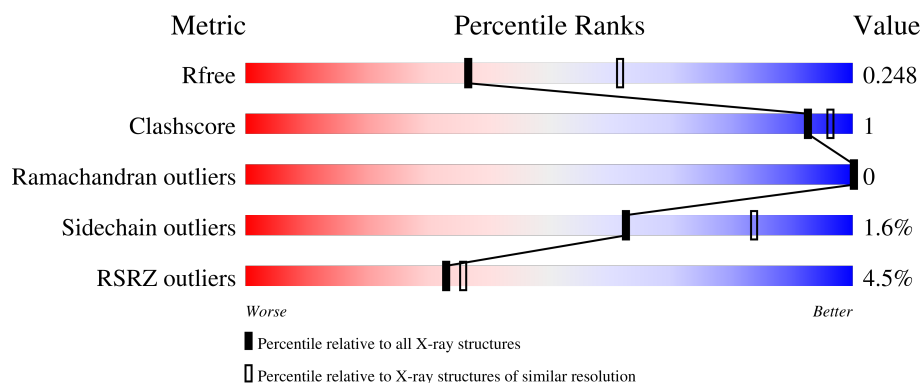
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	427	<div> <div>4%</div> <div>79%</div> <div>17%</div> </div>
1	C	427	<div> <div>5%</div> <div>79%</div> <div>18%</div> </div>
2	B	116	<div> <div>%</div> <div>92%</div> <div>.</div> </div>
2	D	116	<div> <div>3%</div> <div>90%</div> <div>8%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7255 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 Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2754	1743	482	517	12			
1	C	352	Total	C	N	O	S	0	0	0
			2714	1714	481	507	12			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	linker	UNP P03129
A	14	CYS	-	linker	UNP P03129
A	14A	GLY	-	linker	UNP P03129
A	14B	GLY	-	linker	UNP P03129
A	14C	SER	-	linker	UNP P03129
A	14D	GLY	-	linker	UNP P03129
A	14E	GLY	-	linker	UNP P03129
A	14F	GLY	-	linker	UNP P03129
A	14G	GLY	-	linker	UNP P03129
A	14H	SER	-	linker	UNP P03129
A	14I	GLY	-	linker	UNP P03129
A	14J	GLY	-	linker	UNP P03129
A	14K	GLY	-	linker	UNP P03129
A	14L	GLY	-	linker	UNP P03129
A	14M	SER	-	linker	UNP P03129
A	124	GLY	-	linker	UNP P16213
A	125	GLY	-	linker	UNP P16213
A	126	GLY	-	linker	UNP P16213
A	127	GLY	-	linker	UNP P16213
A	128	SER	-	linker	UNP P16213
A	129	GLY	-	linker	UNP P16213
A	130	GLY	-	linker	UNP P16213
A	131	GLY	-	linker	UNP P16213
A	132	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
A	133	SER	-	linker	UNP P16213
A	134	GLY	-	linker	UNP P16213
A	135	GLY	-	linker	UNP P16213
A	136	GLY	-	linker	UNP P16213
A	137	GLY	-	linker	UNP P16213
A	138	SER	-	linker	UNP P16213
A	139	GLY	-	linker	UNP P16213
A	140	GLY	-	linker	UNP P16213
A	141	GLY	-	linker	UNP P16213
A	142	GLY	-	linker	UNP P16213
A	143	SER	-	linker	UNP P16213
A	217	LEU	HIS	engineered mutation	UNP A0A678ZGP6
A	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
A	419	HIS	-	expression tag	UNP A0A678ZGP6
A	420	HIS	-	expression tag	UNP A0A678ZGP6
A	421	HIS	-	expression tag	UNP A0A678ZGP6
A	422	HIS	-	expression tag	UNP A0A678ZGP6
A	423	HIS	-	expression tag	UNP A0A678ZGP6
A	424	HIS	-	expression tag	UNP A0A678ZGP6
C	13	GLY	-	linker	UNP P03129
C	14	CYS	-	linker	UNP P03129
C	14A	GLY	-	linker	UNP P03129
C	14B	GLY	-	linker	UNP P03129
C	14C	SER	-	linker	UNP P03129
C	14D	GLY	-	linker	UNP P03129
C	14E	GLY	-	linker	UNP P03129
C	14F	GLY	-	linker	UNP P03129
C	14G	GLY	-	linker	UNP P03129
C	14H	SER	-	linker	UNP P03129
C	14I	GLY	-	linker	UNP P03129
C	14J	GLY	-	linker	UNP P03129
C	14K	GLY	-	linker	UNP P03129
C	14L	GLY	-	linker	UNP P03129
C	14M	SER	-	linker	UNP P03129
C	124	GLY	-	linker	UNP P16213
C	125	GLY	-	linker	UNP P16213
C	126	GLY	-	linker	UNP P16213
C	127	GLY	-	linker	UNP P16213
C	128	SER	-	linker	UNP P16213
C	129	GLY	-	linker	UNP P16213
C	130	GLY	-	linker	UNP P16213
C	131	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
C	132	GLY	-	linker	UNP P16213
C	133	SER	-	linker	UNP P16213
C	134	GLY	-	linker	UNP P16213
C	135	GLY	-	linker	UNP P16213
C	136	GLY	-	linker	UNP P16213
C	137	GLY	-	linker	UNP P16213
C	138	SER	-	linker	UNP P16213
C	139	GLY	-	linker	UNP P16213
C	140	GLY	-	linker	UNP P16213
C	141	GLY	-	linker	UNP P16213
C	142	GLY	-	linker	UNP P16213
C	143	SER	-	linker	UNP P16213
C	217	LEU	HIS	engineered mutation	UNP A0A678ZGP6
C	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
C	419	HIS	-	expression tag	UNP A0A678ZGP6
C	420	HIS	-	expression tag	UNP A0A678ZGP6
C	421	HIS	-	expression tag	UNP A0A678ZGP6
C	422	HIS	-	expression tag	UNP A0A678ZGP6
C	423	HIS	-	expression tag	UNP A0A678ZGP6
C	424	HIS	-	expression tag	UNP A0A678ZGP6

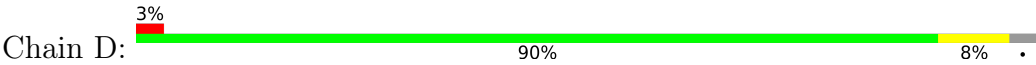
- Molecule 2 is a protein called VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			818	505	141	168	4			
2	D	113	Total	C	N	O	S	0	0	0
			834	514	143	173	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	24	Total	O	0	0
			24	24		
3	C	49	Total	O	0	0
			49	49		
3	D	21	Total	O	0	0
			21	21		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.09Å 118.09Å 262.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.99 – 2.49 48.99 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.99-2.49) 99.6 (48.99-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19.1 _4122	Depositor
R, $R_{free}$	0.225 , 0.248 0.225 , 0.248	Depositor DCC
$R_{free}$ test set	3215 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.15 % 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 9.2646e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.24	0/2831	0.49	0/3861
1	C	0.24	0/2788	0.50	0/3797
2	B	0.25	0/831	0.52	0/1127
2	D	0.24	0/847	0.52	0/1148
All	All	0.24	0/7297	0.50	0/9933

There are no bond length outliers.

There are no bond angle outliers.

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	2754	0	2453	8	0
1	C	2714	0	2418	6	0
2	B	818	0	746	2	0
2	D	834	0	771	4	0
3	A	41	0	0	0	0
3	B	24	0	0	0	0
3	C	49	0	0	1	0
3	D	21	0	0	0	0
All	All	7255	0	6388	20	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 (20) 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:A:13:GLY:H	1:A:286:THR:HG22	1.51	0.75
1:C:2:MET:HE1	1:C:210:VAL:HB	1.77	0.66
2:B:68:ARG:NH2	2:B:91:ASP:OD2	2.27	0.63
1:C:175:GLN:NE2	3:C:501:HOH:O	2.33	0.62
2:D:68:ARG:NH2	2:D:91:ASP:OD2	2.29	0.61
1:A:97:THR:O	1:A:121:ARG:NH1	2.34	0.60
1:A:250:TRP:O	1:A:312:ARG:NH1	2.34	0.60
2:D:69:PHE:CE2	2:D:84:MET:HG2	2.49	0.48
1:C:276:TRP:HB2	1:C:287:LYS:HG3	1.97	0.46
1:C:97:THR:O	1:C:121:ARG:NH1	2.50	0.45
1:A:250:TRP:HB3	1:A:312:ARG:HD3	1.98	0.44
1:C:84:TRP:CE2	1:C:260:ALA:HB2	2.53	0.44
2:D:34:ASN:O	2:D:73:ARG:NH1	2.45	0.44
1:A:308:VAL:O	1:A:312:ARG:HG3	2.18	0.44
1:A:79:SER:HB3	1:A:87:TYR:CZ	2.54	0.42
1:C:171:VAL:HG11	1:C:322:LEU:HD13	2.00	0.42
2:D:38:TRP:CZ3	2:D:82:LEU:HB2	2.55	0.42
1:A:84:TRP:CE2	1:A:260:ALA:HB2	2.54	0.42
1:A:171:VAL:HG11	1:A:322:LEU:HD13	2.02	0.42
2:B:38:TRP:CZ3	2:B:82:LEU:HB2	2.55	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	344/427 (81%)	336 (98%)	8 (2%)	0	100	100
1	C	340/427 (80%)	332 (98%)	8 (2%)	0	100	100
2	B	108/116 (93%)	106 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	109/116 (94%)	107 (98%)	2 (2%)	0	100	100
All	All	901/1086 (83%)	881 (98%)	20 (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	268/351 (76%)	264 (98%)	4 (2%)	65	85
1	C	261/351 (74%)	256 (98%)	5 (2%)	57	80
2	B	84/97 (87%)	83 (99%)	1 (1%)	71	88
2	D	88/97 (91%)	87 (99%)	1 (1%)	73	89
All	All	701/896 (78%)	690 (98%)	11 (2%)	62	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	PHE
1	A	154	SER
1	A	157	ARG
1	A	178	ARG
2	B	23	SER
1	C	11	ASP
1	C	94	PHE
1	C	154	SER
1	C	241	MET
1	C	331	HIS
2	D	23	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	197	GLN
1	A	284	GLN
1	C	175	GLN
1	C	298	GLN
1	C	331	HIS

### 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	356/427 (83%)	0.18	16 (4%) 33 36	24, 40, 76, 106	0
1	C	352/427 (82%)	0.25	22 (6%) 20 21	24, 41, 90, 120	1 (0%)
2	B	112/116 (96%)	-0.12	1 (0%) 84 86	22, 31, 66, 94	0
2	D	113/116 (97%)	-0.08	3 (2%) 54 58	22, 32, 70, 89	0
All	All	933/1086 (85%)	0.14	42 (4%) 33 36	22, 38, 80, 120	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	TRP	7.1
1	A	13	GLY	5.0
1	C	412	PRO	4.9
1	C	402	CYS	4.4
1	A	347	TRP	4.3
1	A	400	TYR	3.8
1	C	359	THR	3.8
1	C	400	TYR	3.7
1	A	283	ALA	3.3
1	C	416	ARG	3.3
1	C	357	THR	3.3
1	C	330	THR	3.2
1	C	361	GLN	3.2
1	C	387	TRP	3.1
1	C	346	CYS	3.0
1	A	414	THR	2.8
1	C	358	LEU	2.8
1	C	13	GLY	2.7
1	A	360	TRP	2.7
1	A	227	CYS	2.7
1	A	284	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	413	LEU	2.7
2	B	75	ASN	2.7
2	D	75	ASN	2.6
1	A	331	HIS	2.6
1	A	14	CYS	2.5
1	A	229	ASN	2.5
1	C	227	CYS	2.5
1	A	279	ALA	2.4
1	C	7	PRO	2.4
1	A	12	LEU	2.3
1	A	371	THR	2.3
1	C	12	LEU	2.3
1	C	410	PRO	2.2
1	C	414	THR	2.2
1	C	229	ASN	2.2
1	A	228	TYR	2.1
2	D	7	VAL	2.1
1	C	413	LEU	2.1
1	C	388	ALA	2.1
2	D	76	THR	2.1
1	C	373	LEU	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.