

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 22, 2020 - 10:20 am BST

PDB ID	:	5IEH
$\operatorname{Title}$	:	Structure of HLA-B*40:02 in complex with the phosphorylated endogenous
		peptide REF(p)SKEPEL
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Deposited on		
$\operatorname{Resolution}$	:	1.50  Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

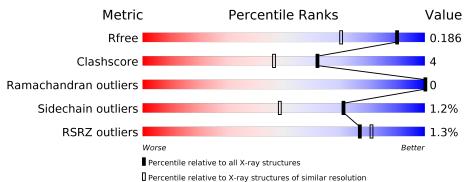
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\rm CCP4$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on 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 <=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	А	277	% 91%	9%
2	В	100	2% 92%	6% •
3	С	9	89%	11%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6825 atoms, of which 3009 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, B-40 alpha chain.

Mol	Chain	Residues			Atoms	5			ZeroOcc	AltConf	Trace
1	А	276	Total 4380	C 1406	Н 2121	N 410	0 437	S 6	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q04826
А	44	ALA	ARG	$\operatorname{conflict}$	UNP Q04826

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

Mol	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace
2	В	98	Total 1609	C 524	Н 785	N 139	0 158	S 3	0	1	0

There is a discrepancy between the modelled and reference sequences:

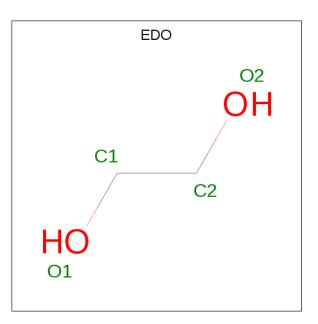
Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called Inner centromere protein.

Mol	Chain	Residues		ŀ	4ton	ns			ZeroOcc	AltConf	Trace
3	С	9	Total 195	$\begin{array}{c} \mathrm{C} \\ 59 \end{array}$	Н 97	N 16	O 22	Р 1	0	2	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total C 10 2	Н 6	O 2	0	0

• Molecule 5 is water.

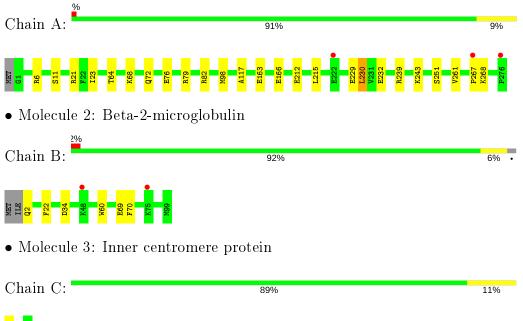
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	460	Total O 460 460	0	0
5	В	152	Total O 152 152	0	0
5	С	19	Total O 19 19	0	0



# 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 the various outlier classes 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 (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, B-40 alpha chain







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	51.04Å $82.25$ Å $110.08$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	24.86 - 1.50	Depositor
	55.04 - 1.20	EDS
% Data completeness	$100.0\ (24.86-1.50)$	Depositor
(in resolution range)	99.7(55.04-1.20)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.62 (at 1.20 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10	Depositor
B B.	0.161 , $0.183$	Depositor
$R, R_{free}$	0.163 , $0.186$	DCC
$R_{free}$ test set	7178 reflections $(4.96\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.40 , $42.4$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6825	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

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

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		
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.45	0/2328	0.67	0/3166	
2	В	0.42	0/850	0.61	0/1149	
3	С	0.52	0/94	0.84	0/120	
All	All	0.44	0/3272	0.66	0/4435	

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	А	2259	2121	2123	22	0
2	В	824	785	785	5	0
3	С	98	97	97	2	0
4	В	4	6	6	0	0
5	А	460	0	0	12	1
5	В	152	0	0	5	1
5	С	19	0	0	0	0
All	All	3816	3009	3011	27	1

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 4.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:OE1	5:A:301:HOH:O	1.91	0.87
1:A:232:GLU:OE1	5:A:302:HOH:O	1.93	0.85
1:A:166:GLU:OE1	5:A:303:HOH:O	1.99	0.79
1:A:79:ARG:NH1	5:A:306:HOH:O	2.15	0.78
1:A:212:GLU:OE1	5:A:304:HOH:O	2.04	0.75

The worst 5 of 27 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:539:HOH:O	5:B:305:HOH:O[3_544]	2.11	0.09

### 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	Perce	ntiles
1	А	276/277~(100%)	272~(99%)	4 (1%)	0	100	100
2	В	97/100~(97%)	97~(100%)	0	0	100	100
3	С	7/9~(78%)	6 (86%)	1 (14%)	0	100	100
All	All	380/386~(98%)	375~(99%)	5(1%)	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.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	238/237~(100%)	235~(99%)	3 (1%)	69 44
2	В	94/95~(99%)	93~(99%)	1 (1%)	73 53
3	С	10/8~(125%)	10 (100%)	0	100 100
All	All	342/340~(101%)	338~(99%)	4 (1%)	71 48

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	6	ARG
1	А	230	LEU
1	А	239	ARG
2	В	70	PHE

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)

1 non-standard protein/DNA/RNA residue is 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	Dec	Link	Bond lengths			Bond angles		
	туре	Chain	$\mathbf{Res}$	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SEP	С	4	3	$8,\!9,\!10$	1.34	1 (12%)	8,12,14	0.83	0

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
	3	SEP	С	4	3	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	С	4	SEP	P-O1P	2.86	1.59	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

#### 5.6 Ligand geometry (i)

1 ligand is 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	Bos	Res Link Bond lengths			Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	EDO	В	101	-	$^{3,3,3}$	0.32	0	$^{2,2,2}$	0.48	0

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
4	EDO	В	101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 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, 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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	276/277 (99%)	0.02	3 (1%) 80 84	7, 13, 25, 30	2(0%)
2	В	98/100~(98%)	0.16	2 (2%) 65 70	8, 19, 27, 29	0
3	С	8/9 (88%)	-0.20	0 100 100	10, 14, 16, 19	0
All	All	382/386~(98%)	0.05	5 (1%) 77 81	7, 14, 26, 30	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	48	LYS	4.9
1	А	276	PRO	2.4
1	А	222	GLU	2.2
1	А	267	PRO	2.2
2	В	75	LYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	$Q{<}0.9$
3	SEP	C	4	10/11	0.97	0.08	$10,\!13,\!23,\!25$	0

### 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.



### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
4	EDO	В	101	4/4	0.94	0.09	$18,\!23,\!27,\!31$	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

