

wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 07:24 AM EDT

PDB ID : 1KTL

Title: The human non-classical major histocompatibility complex molecule HLA-E

Authors: Holmes, M.A.; Strong, R.K.

Deposited on : 2002-01-16

Resolution : 3.10 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

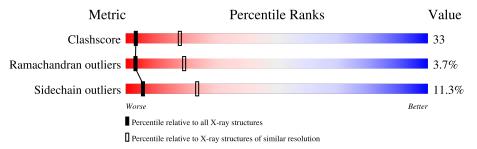
Validation Pipeline (wwPDB-VP) : 2.35

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 3.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain								
1	A	274	46%	45%	8% •						
1	С	274	49%	36%	12% •						
2	В	100	56%	37%	6% •						
2	D	100	42%	46%	10% •						
3	Р	9	33%	44% 11%	11%						
3	Q	9	33%	44% 11%	11%						



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6211 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, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total 2200	C 1376	11	O 428	S 7	0	0	0
1	С	274	Total 2212	C 1383		O 428	S 7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	ARG	engineered mutation	UNP P13747
A	256	ALA	ARG	conflict	UNP P13747
С	107	GLY	ARG	engineered mutation	UNP P13747
С	256	ALA	ARG	conflict	UNP P13747

• Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	100	Total 828	C 526	- 1	O 159	S 4	0	0	0
2	D	100	Total			O	S	0	0	0
	2 D	100	828	526	139	159	4	U		U

There are 2 discrepancies between the modelled and reference sequences:

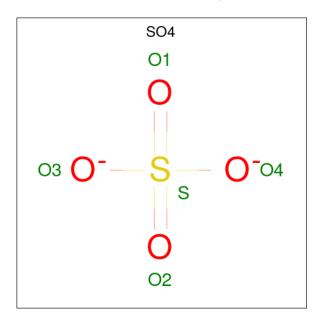
Chain	Residue	Modelled	Actual	Comment	Reference
В	1	MET	-	cloning artifact	UNP P01884
D	1	MET	-	cloning artifact	UNP P01884

• Molecule 3 is a protein called Peptide VTAPRTLLL.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	0	Total	С	N	О	0	0	0
)	3 P	9	69	45	12	12	0	U	U
9	0	0	Total	С	N	O N	0	0	
)	$\mathcal{S} \qquad \mathcal{Q}$	9	69	45	12	12	0	0	U

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total O 5 4	S 1	0	0

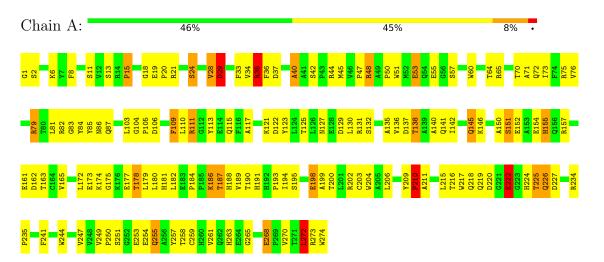


3 Residue-property plots (i)

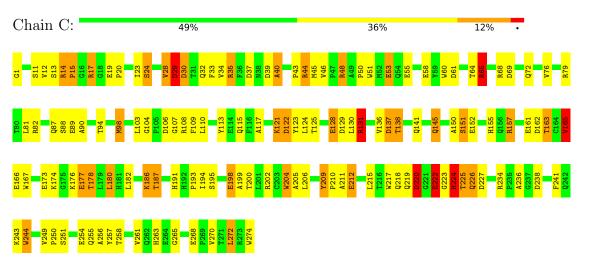
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, ALPHA CHAIN



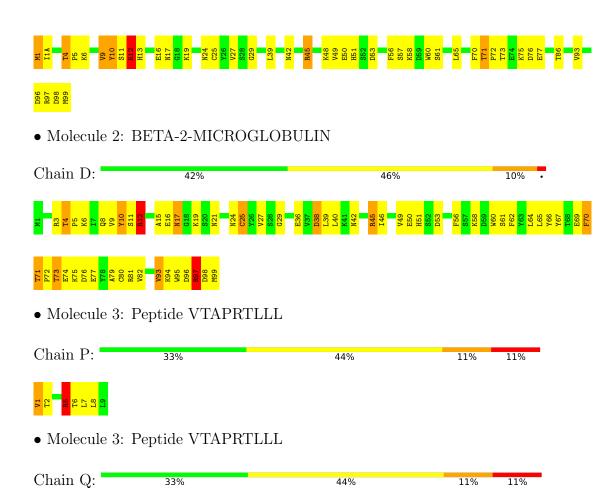
• Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, ALPHA CHAIN



• Molecule 2: BETA-2-MICROGLOBULIN

Chain B: 56% 37% 6%







4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	178.40Å 178.40Å 87.30Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 - 3.10	Depositor
% Data completeness	(Not available) (25.00-3.10)	Depositor
(in resolution range)	(110t available) (20.00 9.10)	Беровног
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6211	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP



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: SO4

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	Bo	nd lengths	Bond angles		
IVIOI	Wioi Chain		# Z > 5	RMSZ	# Z > 5	
1	A	1.30	3/2265~(0.1%)	1.24	$12/3082 \ (0.4\%)$	
1	С	1.24	$11/2278 \; (0.5\%)$	1.30	23/3099 (0.7%)	
2	В	1.40	4/851 (0.5%)	1.32	9/1152 (0.8%)	
2	D	1.28	3/851~(0.4%)	1.26	9/1152 (0.8%)	
3	Р	2.38	$5/69 \ (7.2\%)$	3.05	5/93 (5.4%)	
3	Q	1.44	1/69 (1.4%)	2.05	3/93 (3.2%)	
All	All	1.31	$27/6383 \ (0.4\%)$	1.32	61/8671 (0.7%)	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	С	0	3
3	Р	0	1
3	Q	0	1
All	All	0	7

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	С	1	GLY	C-O	9.59	1.39	1.23
3	P	5	ARG	CZ-NH1	-8.86	1.21	1.33
3	P	5	ARG	CG-CD	8.48	1.73	1.51
1	С	131	ARG	CZ-NH2	7.41	1.42	1.33
1	A	21	ARG	CZ-NH1	7.20	1.42	1.33

The worst 5 of 61 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	Р	5	ARG	NE-CZ-NH1	-17.62	111.49	120.30
3	Р	5	ARG	NE-CZ-NH2	12.52	126.56	120.30
1	С	157	ARG	CG-CD-NE	12.02	137.03	111.80
1	С	131	ARG	NE-CZ-NH2	10.97	125.78	120.30
1	A	79	ARG	NE-CZ-NH1	10.73	125.67	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	TYR	Mainchain,Sidechain
1	С	113	TYR	Sidechain
1	С	131	ARG	Sidechain
1	С	209	TYR	Sidechain
3	P	5	ARG	Sidechain

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	2200	0	2022	157	1
1	С	2212	0	2039	152	0
2	В	828	0	780	50	0
2	D	828	0	780	58	0
3	Р	69	0	83	21	0
3	Q	69	0	83	18	0
4	A	5	0	0	1	0
All	All	6211	0	5787	393	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 33.

The worst 5 of 393 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
2:B:1:MET:SD	2:B:1:MET:CE	2.10	1.39

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:115:GLN:HG2	1:A:125:THR:HG23	1.34	1.10
1:C:65:ARG:HH11	1:C:65:ARG:CB	1.69	1.06
1:A:65:ARG:HH21	1:C:145:GLN:NE2	1.56	1.02
1:A:263:HIS:HD2	1:A:265:GLY:H	1.10	1.00

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	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:A:111:ARG:NH1	1:A:268:GLU:OE2[5_555]	2.08	0.12

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	Percentile	s
1	A	272/274~(99%)	232 (85%)	25 (9%)	15 (6%)	2 11	
1	С	272/274 (99%)	231 (85%)	30 (11%)	11 (4%)	3 17	
2	В	98/100 (98%)	92 (94%)	6 (6%)	0	100 100	
2	D	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	7 31	
3	Р	7/9 (78%)	7 (100%)	0	0	100 100	
3	Q	7/9 (78%)	7 (100%)	0	0	100 100	
All	All	754/766~(98%)	654 (87%)	72 (10%)	28 (4%)	3 19	

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	A	222	GLU
1	A	224	HIS
1	A	226	GLN

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	С	29	ASP

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	229/234~(98%)	204 (89%)	25 (11%)	6 25
1	C	231/234 (99%)	202 (87%)	29 (13%)	4 18
2	В	93/95 (98%)	87 (94%)	6 (6%)	17 47
2	D	93/95 (98%)	83 (89%)	10 (11%)	6 25
3	Р	8/8 (100%)	6 (75%)	2 (25%)	0 2
3	Q	8/8 (100%)	5 (62%)	3 (38%)	0 0
All	All	662/674 (98%)	587 (89%)	75 (11%)	6 23

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	258	THR
3	Р	5	ARG
1	С	272	LEU
2	D	70	PHE
1	A	273	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	141	GLN
1	С	263	HIS
2	D	89	GLN
2	D	2	GLN
1	С	255	GLN



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)

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	275	-	4,4,4	1.02	0	6,6,6	0.30	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	275	SO4	1	0



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

