



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:49 AM GMT

PDB ID : 1QRN
Title : CRYSTAL STRUCTURE OF HUMAN A6 TCR COMPLEXED WITH HLA-A2 BOUND TO ALTERED HTLV-1 TAX PEPTIDE P6A
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Deposited on : 1999-06-14
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

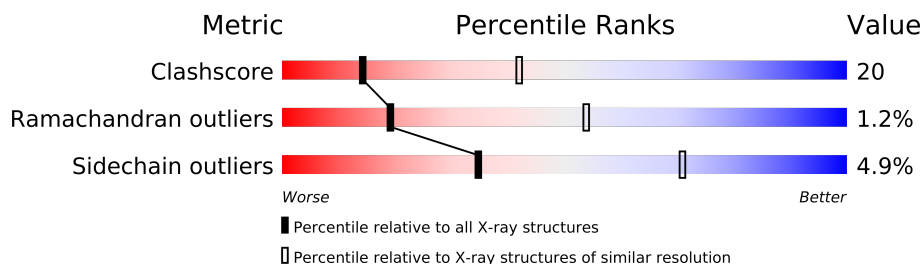
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	274	
2	B	100	
3	C	9	
4	D	200	
5	E	243	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6576 atoms, of which 0 are hydrogen and 0 are deuterium.

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-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	16	0	0
			2238	1398	408	423	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	-	CLONING ARTIFACT	UNP P61769

- Molecule 3 is a protein called TAX PEPTIDE P6A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			75	54	9	12			

- Molecule 4 is a protein called T-CELL RECEPTOR, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1504	943	247	308	6			

- Molecule 5 is a protein called T-CELL RECEPTOR, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1871	1177	329	357	8			

- Molecule 6 is water.

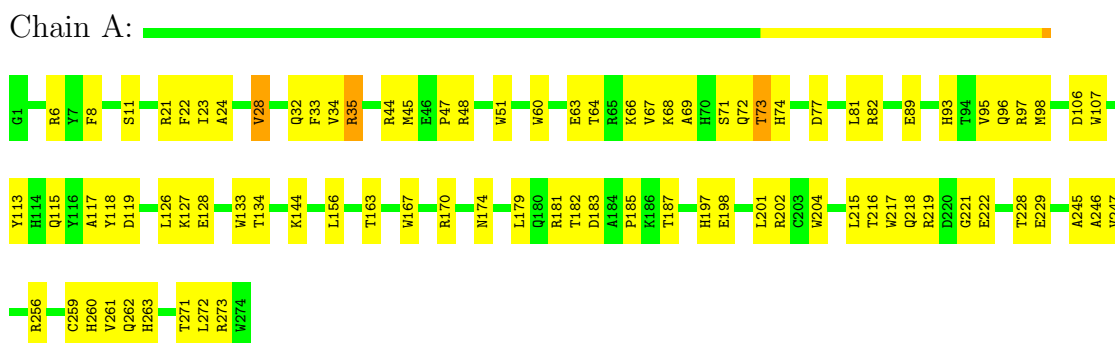
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total 18	O 18	0	0
6	B	16	Total 16	O 16	0	0
6	C	2	Total 2	O 2	0	0
6	D	6	Total 6	O 6	0	0
6	E	9	Total 9	O 9	0	0

3 Residue-property plots

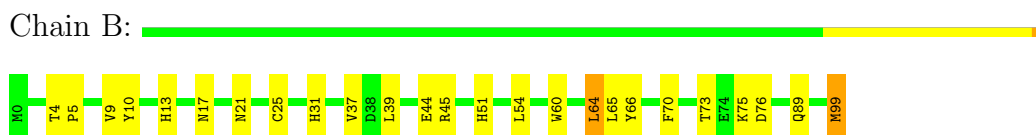
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

Note EDS was not executed.

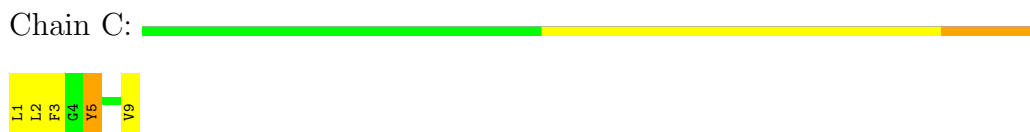
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN



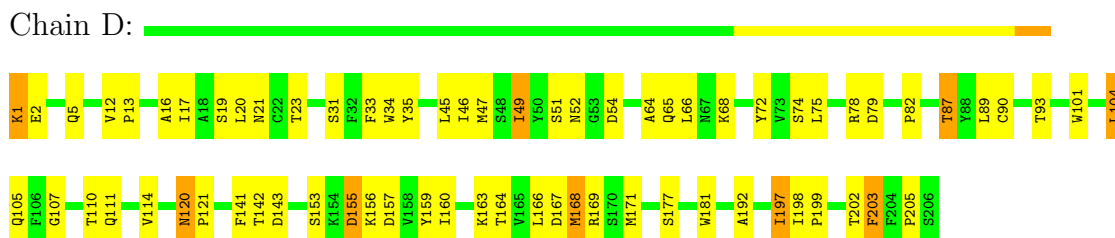
- Molecule 2: BETA-2 MICROGLOBULIN



- Molecule 3: TAX PEPTIDE P6A



- Molecule 4: T-CELL RECEPTOR, ALPHA CHAIN



- Molecule 5: T-CELL RECEPTOR, BETA CHAIN



P178	G101	G3
L185	R102	Q6
S188	P103	T7
R189	E105	P8
S193	Q106	
S194	G109	Q11
R195	P110	V12
L196	T112	L13
P197	R113	K14
V198	L114	T15
S199	T115	
A200	V116	M19
	L116A	T20
	E117	L21
Q204	L118	Q25
N205	L119	D26
	K120	M27
N208	N121	
H209	V122	Y31
F210	F123	M32
R211	P124	S33
	P125	W34
E221		Y35
	V129	R36
W225		
T226	P132	M41
Q227		
K231	H139	R44
P232	T140	L45
V233	Q141	L46
	K142	
A239	A143	T55
	T144	D56
	L145	Q57
W242		
A245	G151	V60
D246	F152	P61
	Y153	
	P154	V67
	D155	S68
	H156	R69
	L159	D74
	S160	
	V161	L77
	W162	
	V163	Q86
	E167	V89
	S170	C92
	G171	
	V172	R95
	S173	P96
	T174	G97
	D175	L98
	P176	A99
	G177	G100

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.95Å 48.76Å 95.55Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6576	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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	0.37	0/2303	0.58	1/3125 (0.0%)
2	B	0.40	0/860	0.65	0/1162
3	C	0.46	0/77	0.77	0/103
4	D	0.35	0/1537	0.58	0/2094
5	E	0.34	0/1924	0.60	0/2628
All	All	0.36	0/6701	0.60	1/9112 (0.0%)

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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	VAL	N-CA-C	-5.10	97.24	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	5	TYR	Sidechain

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2090	77	0
2	B	837	0	803	20	0
3	C	75	0	77	9	0
4	D	1504	0	1375	58	0
5	E	1871	0	1740	105	0
6	A	18	0	0	0	0
6	B	16	0	0	2	0
6	C	2	0	0	0	0
6	D	6	0	0	1	0
6	E	9	0	0	2	0
All	All	6576	0	6085	246	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 246 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:MET:H	1:A:64:THR:HG22	1.13	1.09
5:E:159:LEU:HD12	5:E:160:SER:N	1.83	0.94
5:E:116(A):THR:HG22	5:E:118:ASP:H	1.33	0.92
1:A:219:ARG:HB2	1:A:222:GLU:HB2	1.55	0.88
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.59	0.84

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%)	248 (91%)	24 (9%)	0	100	100
2	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/200 (99%)	172 (87%)	20 (10%)	6 (3%)	7	22
5	E	241/243 (99%)	218 (90%)	19 (8%)	4 (2%)	14	42
All	All	816/826 (99%)	737 (90%)	69 (8%)	10 (1%)	19	54

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	156	LYS
5	E	170	SER
4	D	155	ASP
5	E	120	LYS
5	E	153	TYR

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	230/230 (100%)	223 (97%)	7 (3%)	53	87
2	B	95/95 (100%)	90 (95%)	5 (5%)	32	67
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	161/178 (90%)	151 (94%)	10 (6%)	26	60
5	E	196/208 (94%)	184 (94%)	12 (6%)	26	61
All	All	689/718 (96%)	655 (95%)	34 (5%)	35	71

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	49	ILE
4	D	120	ASN
5	E	174	THR
4	D	104	LEU
1	A	273	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	31	HIS
4	D	37	GLN
5	E	141	GLN
2	B	83	ASN
4	D	5	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.