wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 11:26 am BST

PDB ID	:	1QRN
Title	:	CRYSTAL STRUCTURE OF HUMAN A6 TCR COMPLEXED WITH HLA-A2 BOUND TO ALTERED HTLV-1 TAX PEPTIDE P6A
Authors	:	Ding, Y.H.; Baker, B.M.; Garboczi, D.N.; Biddison, W.E.; Wiley, D.C.
Deposited on	:	1999-06-14
Resolution	:	2.80 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 (i)) were used in the production of this report:

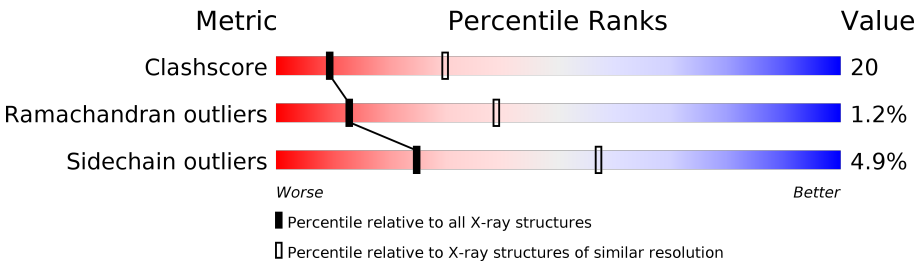
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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	68% 31% •
2	B	100	75% 23% •
3	C	9	44% 44% 11%
4	D	200	65% 31% 5%
5	E	243	58% 37% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6576 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, A-2 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2238	1398	408	423	9	16	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

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
			Total	C	N	O			
3	C	9	75	54	9	12	0	0	0

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

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

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

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

- Molecule 6 is water.

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

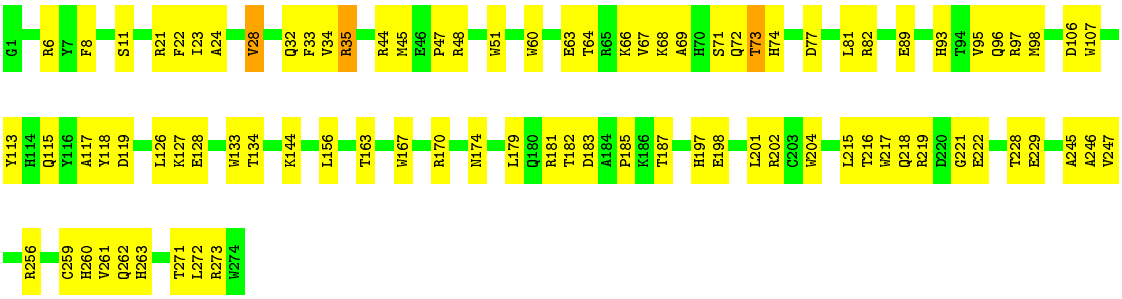
3 Residue-property plots (i)

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. 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.

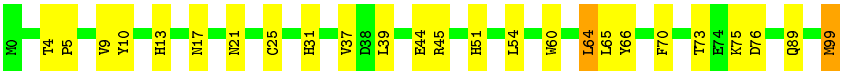
- Molecule 1: HLA CLASS I HISTOCOMPATIBILITY ANTIGEN, A-2 ALPHA CHAIN

Chain A:



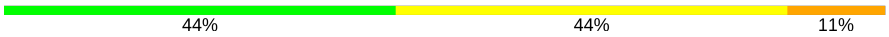
- Molecule 2: BETA-2 MICROGLOBULIN

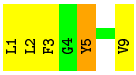
Chain B:



- Molecule 3: TAX PEPTIDE P6A

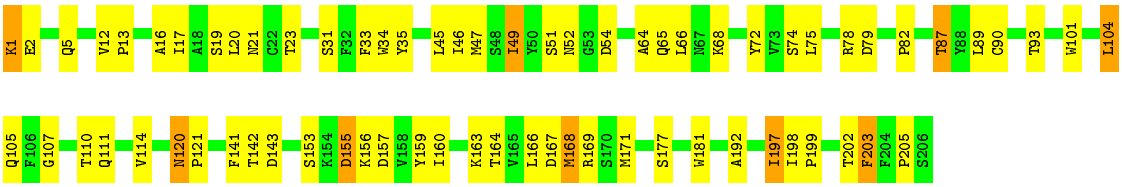
Chain C:





- Molecule 4: T-CELL RECEPTOR, ALPHA CHAIN

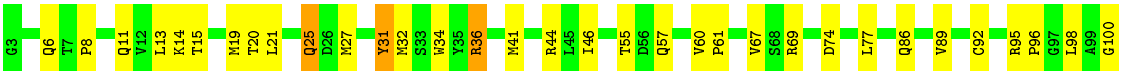
Chain D:

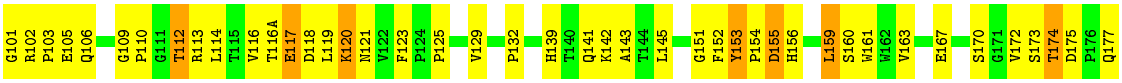


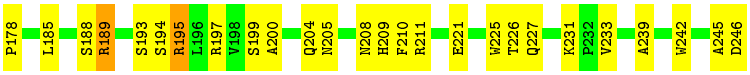
- Molecule 5: T-CELL RECEPTOR, BETA CHAIN

Chain E:

58%
37%
5%


G3
Q6
T7
P8
Q11
V12
L13
K14
T15
M19
T20
L21
Q25
D26
M27
Y31
M32
S33
W34
Y35
R36
M41
R44
L45
I46
T55
D56
Q57
V60
P61
V67
S68
R69
D74
L77
Q86
V89
C92
R95
P96
G97
L98
A99
G100


G101
R102
P103
E105
Q106
G109
P110
G111
T112
R113
L114
T115
V116
T116A
E117
D118
L119
K120
N121
V122
F123
P124
P125
V129
P132
H139
T140
Q141
K142
A143
T144
L145
G151
F152
Y153
P154
D155
H156
L159
S160
W161
W162
V163
E167
S170
G171
V172
S173
T174
D175
P176
Q177


P178
L185
S188
R189
S193
S194
R195
L196
R197
V198
S199
A200
Q204
N205
N208
H209
F210
R211
E221
W225
T226
Q227
K231
P232
V233
A239
W242
A245
D246

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore 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(^{o})	Ideal(^{o})
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 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	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

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 20.

The worst 5 of 246 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: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 (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	272/274 (99%)	248 (91%)	24 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/200 (99%)	172 (87%)	20 (10%)	6 (3%)	4	15
5	E	241/243 (99%)	218 (90%)	19 (8%)	4 (2%)	9	29
All	All	816/826 (99%)	737 (90%)	69 (8%)	10 (1%)	13	39

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 (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	230/230 (100%)	223 (97%)	7 (3%)	41	75
2	B	95/95 (100%)	90 (95%)	5 (5%)	22	54
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	161/178 (90%)	151 (94%)	10 (6%)	18	47
5	E	196/208 (94%)	184 (94%)	12 (6%)	18	48
All	All	689/718 (96%)	655 (95%)	34 (5%)	25	57

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

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Mol	Chain	Res	Type
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 (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 carbohydrates 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 (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.