



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2016 – 07:44 PM EDT

PDB ID : 1BD2
Title : COMPLEX BETWEEN HUMAN T-CELL RECEPTOR B7, VIRAL PEPTIDE (TAX) AND MHC CLASS I MOLECULE HLA-A 0201
Authors : Ding, Y.-H.; Smith, K.J.; Garboczi, D.N.; Utz, U.; Biddison, W.E.; Wiley, D.C.
Deposited on : 1998-05-12
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

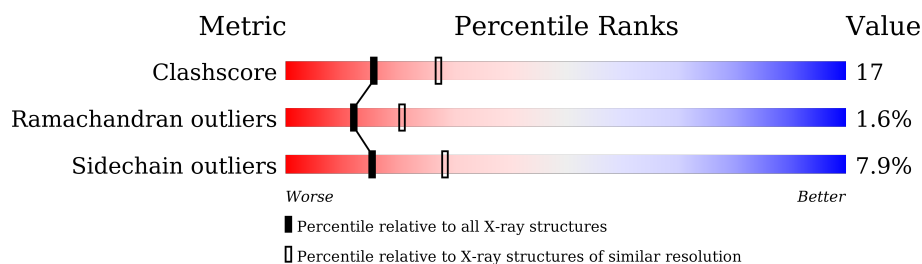
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	
2	B	100	
3	C	9	
4	D	204	
5	E	244	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6378 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-A 0201.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2186	1369	392	416	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			805	512	138	152	3			

- Molecule 3 is a protein called TAX PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			77	56	9	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	190	Total	C	N	O	S	0	0	0
			1421	899	230	285	7			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	56	ALA	GLU	CONFLICT	GB 338766
D	?	-	LYS	DELETION	GB 338766
D	93	MET	GLY	CONFLICT	GB 338766
D	94	GLU	ALA	CONFLICT	GB 338766
D	?	-	THR	DELETION	GB 338766
D	102	GLN	SER	CONFLICT	GB 338766
D	105	VAL	THR	CONFLICT	GB 338766
D	108	GLN	THR	CONFLICT	GB 338766

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Chain	Residue	Modelled	Actual	Comment	Reference
D	113	THR	GLN	CONFLICT	GB 338766
D	114	ILE	VAL	CONFLICT	GB 338766
D	115	ASN	THR	CONFLICT	GB 338766
D	116	PRO	LEU	CONFLICT	GB 338766
D	117	ASN	ASP	CONFLICT	GB 338766

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1850	1172	318	353	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	96	TYR	PHE	CONFLICT	GB 3002925
E	98	GLY	ARG	CONFLICT	GB 3002925
E	99	GLY	GLN	CONFLICT	GB 3002925
E	100	GLY	PRO	CONFLICT	GB 3002925
E	101	PHE	SER	CONFLICT	GB 3002925
E	?	-	ASN	DELETION	GB 3002925
E	107	TYR	PHE	CONFLICT	GB 3002925
E	117	THR	LEU	CONFLICT	GB 3002925
E	192	ALA	CYS	CONFLICT	GB 3002925
E	206	ASP	ASN	CONFLICT	GB 3002925

- Molecule 6 is water.

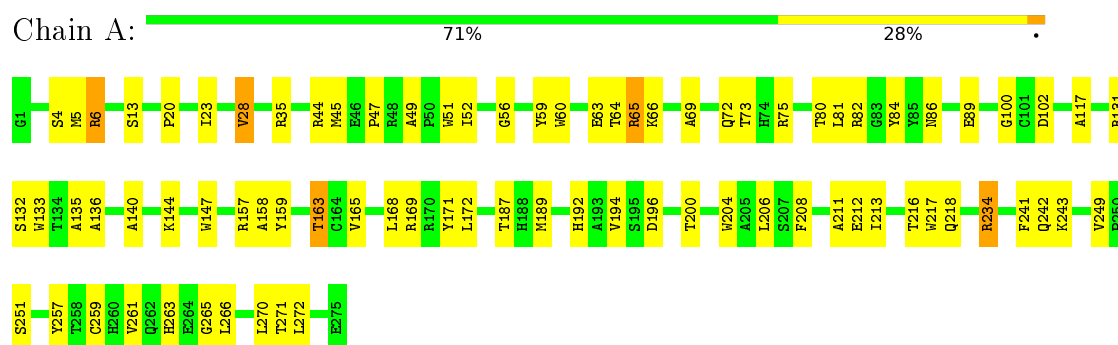
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	5	Total	O	0	0
			5	5		
6	D	13	Total	O	0	0
			13	13		
6	E	12	Total	O	0	0
			12	12		

3 Residue-property plots [i](#)

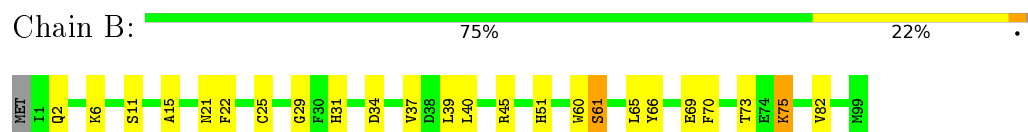
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-A 0201



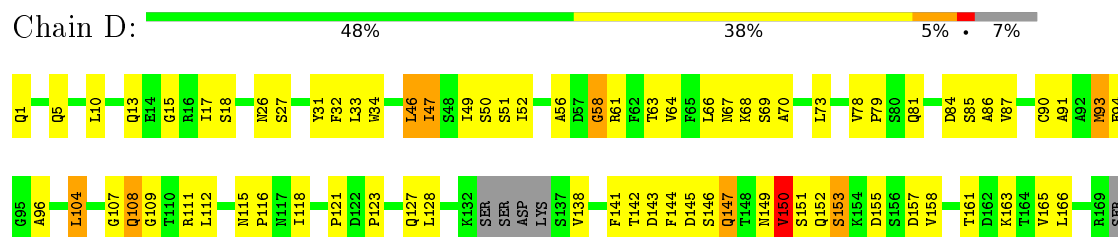
• Molecule 2: BETA-2 MICROGLOBULIN



• Molecule 3: TAX PEPTIDE

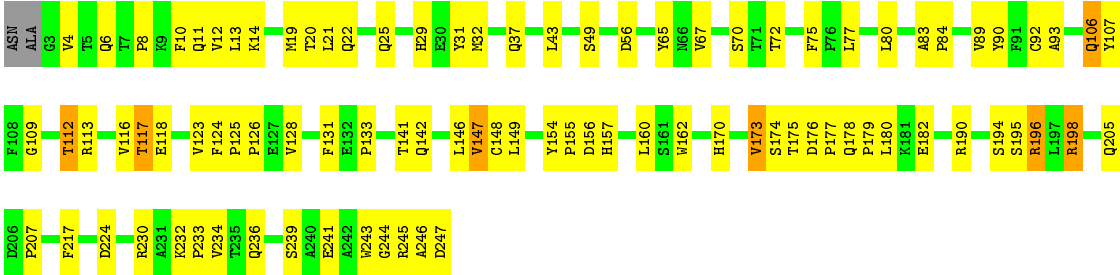


• Molecule 4: T CELL RECEPTOR ALPHA





● Molecule 5: T CELL RECEPTOR BETA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.80 Å 73.30 Å 217.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.6 (8.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.238 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6378	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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	0.47	0/2250	0.69	2/3058 (0.1%)
2	B	0.45	0/828	0.70	0/1121
3	C	0.56	0/80	0.88	0/108
4	D	0.55	0/1452	0.86	4/1980 (0.2%)
5	E	0.50	0/1905	0.75	0/2604
All	All	0.50	0/6515	0.75	6/8871 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	196	SER	N-CA-C	5.61	126.15	111.00
4	D	199	PRO	N-CA-C	5.59	126.64	112.10
4	D	187	PHE	N-CA-C	-5.29	96.70	111.00
4	D	199	PRO	N-CA-CB	5.16	109.49	103.30
1	A	28	VAL	N-CA-C	-5.14	97.13	111.00

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	2186	0	2005	60	0
2	B	805	0	756	17	0
3	C	77	0	79	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1421	0	1274	80	0
5	E	1850	0	1699	58	0
6	A	9	0	0	1	0
6	B	5	0	0	0	0
6	D	13	0	0	4	0
6	E	12	0	0	0	0
All	All	6378	0	5813	208	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 17.

The worst 5 of 208 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)
4:D:17:ILE:HG13	4:D:78:VAL:HG22	1.40	1.01
1:A:82:ARG:NH1	1:A:89:GLU:HG3	1.78	0.97
1:A:131:ARG:HE	1:A:157:ARG:HH12	1.18	0.88
4:D:151:SER:OG	4:D:195:ASN:HB2	1.73	0.87
1:A:131:ARG:NE	1:A:157:ARG:HH12	1.78	0.81

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	273/275 (99%)	250 (92%)	22 (8%)	1 (0%)	39	61
2	B	97/100 (97%)	91 (94%)	5 (5%)	1 (1%)	19	34
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	184/204 (90%)	161 (88%)	14 (8%)	9 (5%)	3	3
5	E	240/244 (98%)	224 (93%)	14 (6%)	2 (1%)	24	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	801/832 (96%)	733 (92%)	55 (7%)	13 (2%)	12	21

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	192	ALA
4	D	195	ASN
4	D	199	PRO
4	D	58	GLY
5	E	246	ALA

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	219/231 (95%)	208 (95%)	11 (5%)	30	53
2	B	89/95 (94%)	85 (96%)	4 (4%)	34	59
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	149/184 (81%)	131 (88%)	18 (12%)	6	11
5	E	191/209 (91%)	172 (90%)	19 (10%)	10	18
All	All	656/727 (90%)	604 (92%)	52 (8%)	15	28

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	104	LEU
4	D	187	PHE
5	E	198	ARG
4	D	108	GLN
4	D	150	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	67	ASN
4	D	183	ASN
5	E	86	GLN
4	D	55	ASN
5	E	106	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 ⓘ

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.