



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:42 AM GMT

PDB ID : 2IAM
Title : Structural basis for recognition of mutant self by a tumor-specific, MHC class II-restricted TCR
Authors : Deng, L.; Langley, R.J.; Mariuzza, R.A.
Deposited on : 2006-09-08
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
<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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

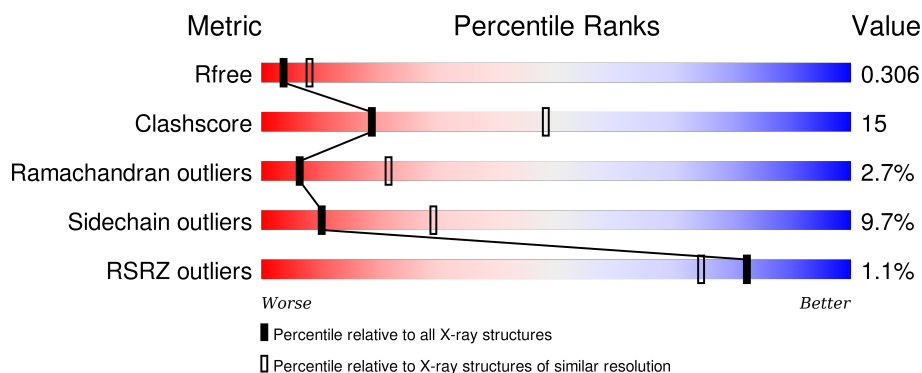
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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.

Mol	Chain	Length	Quality of chain
1	A	182	<div> <div>2%</div> <div>58% 33% 6% ..</div> </div>
2	B	190	<div> <div>2%</div> <div>65% 26% . . .</div> </div>
3	P	15	<div> <div>67% 27% 7%</div> </div>
4	C	202	<div> <div>61% 31% . . .</div> </div>
5	D	240	<div> <div>%</div> <div>63% 30% 5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6551 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 II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1473	954	239	275	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1487	936	264	281	6			

- Molecule 3 is a protein called 15-mer peptide from Triosephosphate isomerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	15	Total	C	N	O	0	0	0
			104	66	17	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	28	ILE	THR	ENGINEERED	UNP P60174

- Molecule 4 is a protein called CD4+ T cell receptor E8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	198	Total	C	N	O	S	0	0	0
			1546	967	260	312	7			

- Molecule 5 is a protein called CD4+ T cell receptor E8 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	239	Total	C	N	O	S	0	0	0
			1901	1206	324	362	9			

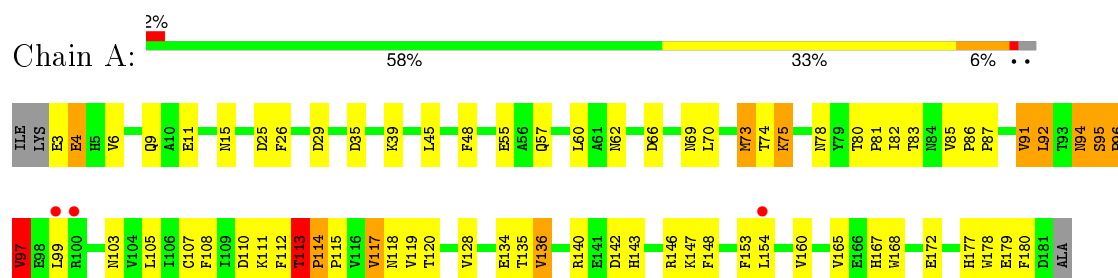
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total 17	O 17	0	0
6	B	7	Total 7	O 7	0	0
6	C	6	Total 6	O 6	0	0
6	D	9	Total 9	O 9	0	0
6	P	1	Total 1	O 1	0	0

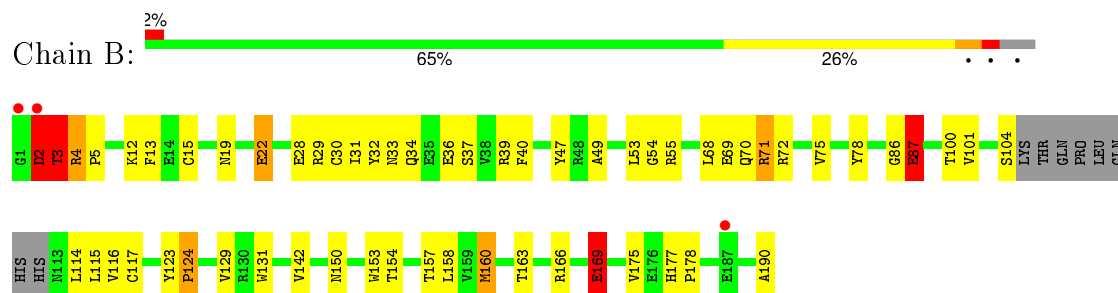
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

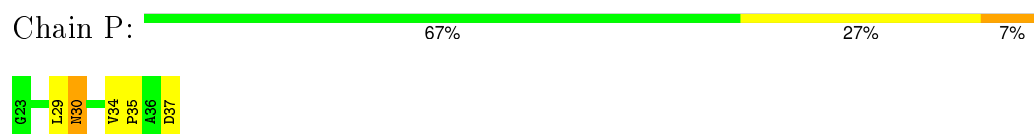
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



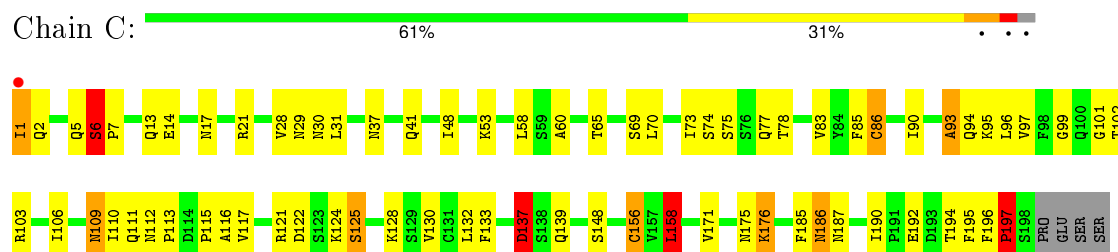
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



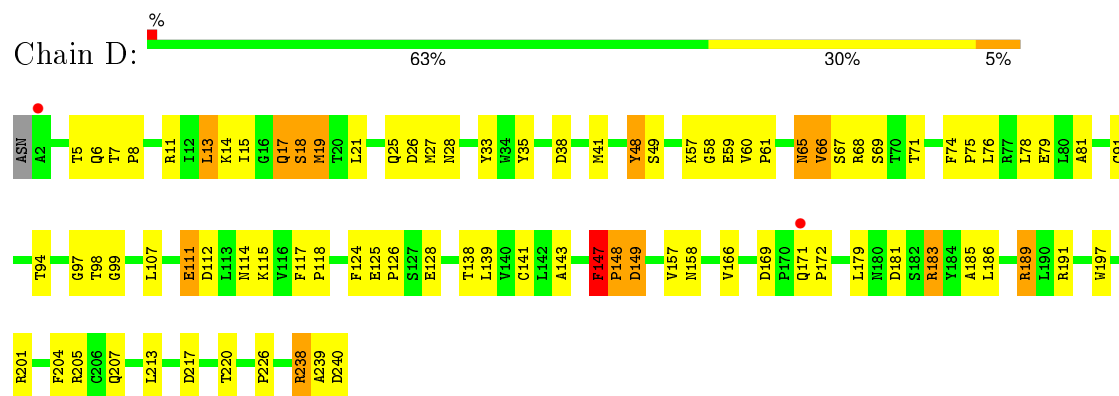
- Molecule 3: 15-mer peptide from Triosephosphate isomerase



- Molecule 4: CD4+ T cell receptor E8 alpha chain



- Molecule 5: CD4+ T cell receptor E8 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.39 Å 270.54 Å 97.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.91 – 2.80 41.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (41.91-2.80) 92.2 (41.91-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.279 0.244 , 0.306	Depositor DCC
R_{free} test set	1329 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 19.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 26375 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.91	3/1518 (0.2%)	0.91	3/2070 (0.1%)
2	B	1.32	3/1523 (0.2%)	0.92	1/2067 (0.0%)
3	P	1.09	0/104	1.19	0/139
4	C	0.91	1/1579 (0.1%)	0.96	4/2148 (0.2%)
5	D	0.96	4/1956 (0.2%)	0.94	2/2666 (0.1%)
All	All	1.03	11/6680 (0.2%)	0.94	10/9090 (0.1%)

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
1	A	0	1
2	B	0	3
4	C	0	2
5	D	0	3
All	All	0	9

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	GLU	CD-OE2	36.50	1.65	1.25
2	B	169	GLU	CD-OE1	9.63	1.36	1.25
5	D	111	GLU	CG-CD	7.62	1.63	1.51
4	C	86	CYS	CB-SG	-7.57	1.69	1.82
2	B	190	ALA	C-O	7.11	1.36	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	THR	C-N-CD	-7.39	104.34	120.60
5	D	183	ARG	NE-CZ-NH1	6.83	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	93	ALA	C-N-CA	-6.20	106.20	121.70
2	B	169	GLU	CG-CD-OE2	-5.57	107.16	118.30
5	D	147	PHE	C-N-CD	-5.47	108.56	120.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	THR	Peptide
2	B	123	TYR	Peptide
2	B	169	GLU	Sidechain
2	B	3	THR	Peptide
4	C	1	ILE	Peptide

5.2 Too-close contacts

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	1473	0	1407	48	0
2	B	1487	0	1419	46	0
3	P	104	0	109	7	0
4	C	1546	0	1474	53	0
5	D	1901	0	1800	56	0
6	A	17	0	0	1	0
6	B	7	0	0	0	0
6	C	6	0	0	0	0
6	D	9	0	0	1	0
6	P	1	0	0	0	0
All	All	6551	0	6209	196	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 15.

The worst 5 of 196 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)
2:B:169:GLU:OE2	2:B:169:GLU:CD	1.65	1.31
2:B:19:ASN:HD22	2:B:22:GLU:HG2	1.11	1.16
2:B:2:ASP:O	2:B:3:THR:HB	1.49	1.11
5:D:94:THR:HG22	5:D:99:GLY:HA2	1.34	1.04
1:A:82:ILE:HD13	1:A:114:PRO:HD3	1.48	0.93

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	177/182 (97%)	157 (89%)	15 (8%)	5 (3%)	6	21
2	B	178/190 (94%)	161 (90%)	12 (7%)	5 (3%)	6	21
3	P	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
4	C	196/202 (97%)	173 (88%)	17 (9%)	6 (3%)	5	17
5	D	237/240 (99%)	218 (92%)	13 (6%)	6 (2%)	7	24
All	All	801/829 (97%)	721 (90%)	58 (7%)	22 (3%)	6	21

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
2	B	2	ASP
2	B	87	GLU
2	B	169	GLU
4	C	6	SER

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	164/166 (99%)	145 (88%)	19 (12%)	7	20
2	B	163/171 (95%)	150 (92%)	13 (8%)	15	40
3	P	10/10 (100%)	9 (90%)	1 (10%)	9	27
4	C	178/182 (98%)	162 (91%)	16 (9%)	12	34
5	D	206/207 (100%)	185 (90%)	21 (10%)	9	26
All	All	721/736 (98%)	651 (90%)	70 (10%)	10	29

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	163	THR
4	C	97	VAL
5	D	179	LEU
3	P	30	ASN
4	C	41	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	30	ASN
4	C	5	GLN
5	D	65	ASN
2	B	150	ASN
2	B	156	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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](#)

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, 95th 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	OWAB(Å ²)	Q<0.9
1	A	179/182 (98%)	-0.18	3 (1%) 73 63	53, 68, 76, 79	0
2	B	182/190 (95%)	-0.15	3 (1%) 74 66	53, 66, 72, 75	0
3	P	15/15 (100%)	-0.33	0 100 100	45, 52, 69, 76	0
4	C	198/202 (98%)	-0.38	1 (0%) 91 88	43, 60, 84, 88	0
5	D	239/240 (99%)	-0.48	2 (0%) 87 81	45, 57, 71, 83	0
All	All	813/829 (98%)	-0.31	9 (1%) 82 74	43, 64, 77, 88	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ARG	4.9
2	B	1	GLY	3.1
1	A	154	LEU	2.8
4	C	1	ILE	2.7
5	D	171	GLN	2.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.