wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 05:48 am BST

PDB ID	:	1AKJ
Title	:	COMPLEX OF THE HUMAN MHC CLASS I GLYCOPROTEIN HLA-A2 AND THE T CELL CORECEPTOR CD8
Authors	:	Tormo, J.; Stuart, D.I.; Jones, E.Y.
Deposited on	:	1997-05-21
Resolution	:	2.65 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 (1)) were used in the production of this report:

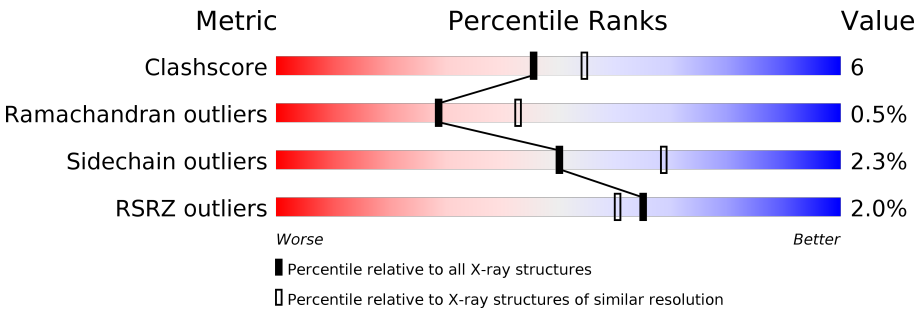
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.65 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	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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% 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	276	% 83% 17% •
2	B	99	% 83% 16% •
3	C	9	78% 22%
4	D	120	3% 80% 14% • 5%
4	E	120	5% 71% 23% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5065 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 MHC CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2254	1408	410	427	9	0	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	98	821	522	139	157	3	0	0	0

- Molecule 3 is a protein called HIV REVERSE TRANSCRIPTASE EPITOPE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	70	46	12	12	0	0	0

- Molecule 4 is a protein called T-CELL CORECEPTOR CD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	114	906	583	153	166	4	0	0	0
4	E	114	906	583	153	166	4	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	52	52	52	0	0
5	B	20	20	20	0	0

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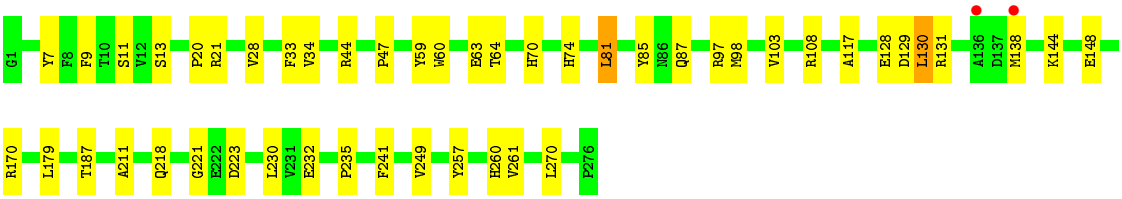
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	1	1	1	0	0
			Total	O		
5	D	21	21	21	0	0
			Total	O		
5	E	14	14	14	0	0

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 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.

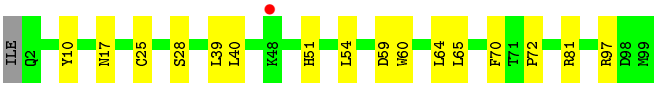
• Molecule 1: MHC CLASS I HISTOCOMPATIBILITY ANTIGEN (HLA-A*0201) (ALPHA CHAIN)

Chain A:



• Molecule 2: BETA 2-MICROGLOBULIN

Chain B:

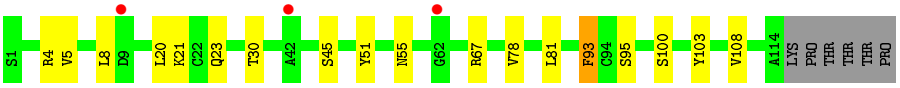


• Molecule 3: HIV REVERSE TRANSCRIPTASE EPITOPE

Chain C:

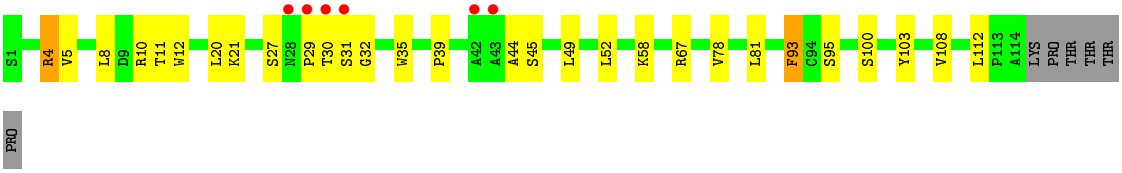
• Molecule 4: T-CELL CORECEPTOR CD8

Chain D:



• Molecule 4: T-CELL CORECEPTOR CD8

Chain E:


S1
R4
V5
L8
D9
R10
T11
W12
L20
K21
S27
N28
P29
T30
S31
G32
W35
P39
A42
A43
A44
S45
L49
L52
K58
R67
V78
L81
F93
C94
S95
S100
Y103
V108
L112
P113
A114
LYS
PRO
THR
THR
THR
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.90Å 89.60Å 116.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.65 19.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-2.65) 96.5 (19.96-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.67Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.276 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5065	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.34	0/2320	0.62	0/3149
2	B	0.34	0/844	0.59	0/1141
3	C	0.37	0/71	0.55	0/94
4	D	0.35	0/931	0.60	0/1263
4	E	0.38	0/931	0.61	0/1263
All	All	0.35	0/5097	0.61	0/6910

There are no bond length outliers.

There are no bond angle outliers.

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	2254	0	2103	30	0
2	B	821	0	780	12	0
3	C	70	0	78	2	0
4	D	906	0	885	10	0
4	E	906	0	885	17	0
5	A	52	0	0	0	0
5	B	20	0	0	1	0
5	C	1	0	0	0	0
5	D	21	0	0	0	0
5	E	14	0	0	1	0
All	All	5065	0	4731	62	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 6.

The worst 5 of 62 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:28:VAL:HG11	1:A:179:LEU:HD13	1.80	0.63
4:E:10:ARG:HH11	4:E:10:ARG:HG2	1.64	0.62
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.36	0.59
4:D:21:LYS:HG2	4:D:78:VAL:HG22	1.87	0.55
2:B:17:ASN:HA	2:B:72:PRO:O	2.06	0.55

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	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
2	B	96/99 (97%)	90 (94%)	6 (6%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	112/120 (93%)	101 (90%)	11 (10%)	0	100	100
4	E	112/120 (93%)	101 (90%)	8 (7%)	3 (3%)	5	6
All	All	601/624 (96%)	565 (94%)	33 (6%)	3 (0%)	29	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	32	GLY
4	E	30	THR
4	E	31	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	232/232 (100%)	227 (98%)	5 (2%)	52	70
2	B	93/94 (99%)	92 (99%)	1 (1%)	73	85
3	C	8/8 (100%)	8 (100%)	0	100	100
4	D	100/106 (94%)	97 (97%)	3 (3%)	41	59
4	E	100/106 (94%)	97 (97%)	3 (3%)	41	59
All	All	533/546 (98%)	521 (98%)	12 (2%)	50	68

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	70	PHE
4	D	45	SER
4	E	4	ARG
1	A	223	ASP
4	D	93	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	2	GLN
4	E	99	ASN
4	D	13	ASN
1	A	218	GLN
4	E	13	ASN

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)

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	276/276 (100%)	-0.47	2 (0%)	87	87	7, 21, 42, 52	0
2	B	98/99 (98%)	-0.45	1 (1%)	82	81	9, 21, 42, 55	0
3	C	9/9 (100%)	-0.45	0	100	100	15, 20, 25, 27	0
4	D	114/120 (95%)	-0.10	3 (2%)	56	52	11, 28, 48, 57	0
4	E	114/120 (95%)	0.06	6 (5%)	26	23	14, 32, 52, 76	0
All	All	611/624 (97%)	-0.30	12 (1%)	65	60	7, 25, 47, 76	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	30	THR	4.4
4	E	29	PRO	4.1
4	E	31	SER	3.6
4	D	9	ASP	3.3
2	B	48	LYS	3.3

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.