



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 PM GMT

PDB ID : 4I5B
Title : Structure of human MHC class II protein HLA-DR1 carrying an influenza hemagglutinin peptide partially filling the binding groove
Authors : Schulze, M.-S.E.D.
Deposited on : 2012-11-28
Resolution : 2.12 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

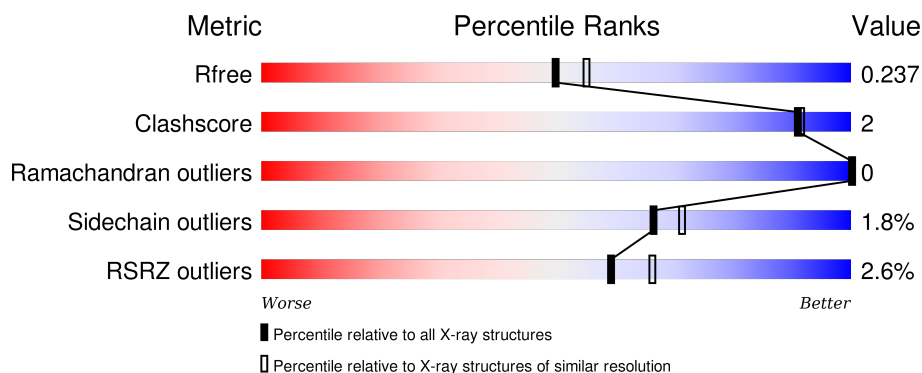
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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	187	<div> <div>5%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	D	187	<div> <div>5%</div> <div>93%</div> <div>7%</div> </div>
2	B	192	<div> <div>4%</div> <div>94%</div> <div>6%</div> </div>
2	E	192	<div> <div>4%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
3	C	12	<div> <div>8%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	12	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment representing 83%, a yellow segment representing 8%, and a grey segment representing 8%. The percentages are labeled below the corresponding segments.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6518 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	180	Total	C	N	O	S	0	0	0
			1481	958	241	276	6			
1	D	187	Total	C	N	O	S	0	0	0
			1531	990	248	287	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	CYS	VAL	CONFLICT	UNP P01903
D	65	CYS	VAL	CONFLICT	UNP P01903

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1578	991	284	298	5			
2	E	190	Total	C	N	O	S	0	0	0
			1563	983	282	293	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	SER	CYS	CONFLICT	UNP P04229
E	30	SER	CYS	CONFLICT	UNP P04229

- Molecule 3 is a protein called truncated hemagglutinin peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	S	0	0	0
			92	59	17	15	1			
3	F	11	Total	C	N	O	S	0	0	0
			83	53	15	14	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total 71	O 71	0	0
4	B	57	Total 57	O 57	0	0
4	C	3	Total 3	O 3	0	0
4	D	29	Total 29	O 29	0	0
4	E	28	Total 28	O 28	0	0
4	F	2	Total 2	O 2	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



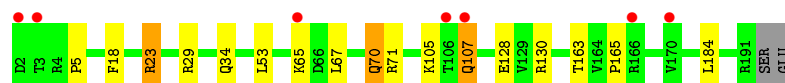
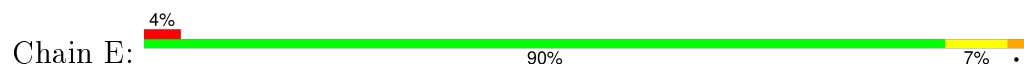
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



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




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



- Molecule 3: truncated hemagglutinin peptide



- Molecule 3: truncated hemagglutinin peptide

Chain F:  83% 8% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.81Å 111.38Å 211.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.12 49.28 – 2.12	Depositor EDS
% Data completeness (in resolution range)	91.4 (49.28-2.12) 91.4 (49.28-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.94 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.237 0.198 , 0.237	Depositor DCC
R_{free} test set	2965 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58721 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6518	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.44	0/1526	0.58	0/2079
1	D	0.40	0/1579	0.57	0/2153
2	B	0.45	0/1618	0.57	0/2197
2	E	0.41	0/1603	0.54	0/2177
3	C	0.37	0/91	0.65	0/120
3	F	0.30	0/82	0.60	0/109
All	All	0.42	0/6499	0.57	0/8835

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

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	1481	0	1415	6	0
1	D	1531	0	1463	8	0
2	B	1578	0	1506	5	0
2	E	1563	0	1495	10	0
3	C	92	0	108	0	0
3	F	83	0	95	1	0
4	A	71	0	0	0	0
4	B	57	0	0	0	0
4	C	3	0	0	0	0
4	D	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	28	0	0	0	0
4	F	2	0	0	0	0
All	All	6518	0	6082	27	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 2.

All (27) 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:D:132:VAL:HG12	1:D:151:LEU:HD13	1.73	0.70
2:E:18:PHE:HB2	2:E:23:ARG:HB2	1.81	0.62
2:E:163:THR:HG23	2:E:165:PRO:HD3	1.82	0.61
2:E:70:GLN:C	2:E:70:GLN:HE21	2.11	0.54
1:D:174:LEU:HD21	1:D:176:LYS:HD3	1.93	0.50
2:E:70:GLN:HG3	2:E:71:ARG:N	2.26	0.50
1:A:73:MET:HE1	2:B:53:LEU:HB3	1.94	0.49
2:B:25:ARG:CZ	2:B:27:LEU:HD11	2.43	0.48
2:E:128:GLU:HG2	2:E:130:ARG:NH1	2.30	0.47
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.97	0.46
1:D:138:LEU:HB2	1:D:146:ARG:HG3	1.97	0.46
1:D:141:GLU:OE1	2:E:29:ARG:NH2	2.47	0.45
1:A:2:LYS:HB2	1:A:2:LYS:HE3	1.74	0.45
2:E:107:GLN:HB2	2:E:107:GLN:HE21	1.42	0.44
1:D:118:ASN:HB2	1:D:166:GLU:HB2	1.99	0.44
1:D:110:ASP:OD1	1:D:146:ARG:HB3	2.18	0.44
1:D:176:LYS:HD2	1:D:176:LYS:HA	1.78	0.44
2:E:67:LEU:HD21	3:F:314:LEU:HD13	2.00	0.44
1:D:8:ILE:HB	1:D:25:ASP:HB3	2.00	0.43
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.54	0.43
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.81	0.43
2:E:53:LEU:HD23	2:E:53:LEU:HA	1.92	0.42
2:E:65:LYS:HB3	2:E:65:LYS:NZ	2.35	0.42
1:A:91:VAL:HG23	1:A:176:LYS:HB3	2.01	0.41
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.56	0.41
2:B:40:PHE:HB2	2:B:47:TYR:CE1	2.56	0.41
2:B:9:TRP:CH2	2:B:30:SER:HB3	2.57	0.40

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	178/187 (95%)	177 (99%)	1 (1%)	0	100	100
1	D	185/187 (99%)	184 (100%)	1 (0%)	0	100	100
2	B	190/192 (99%)	187 (98%)	3 (2%)	0	100	100
2	E	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
3	C	10/12 (83%)	10 (100%)	0	0	100	100
3	F	9/12 (75%)	9 (100%)	0	0	100	100
All	All	760/782 (97%)	751 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	165/171 (96%)	163 (99%)	2 (1%)	78	83
1	D	171/171 (100%)	169 (99%)	2 (1%)	78	83
2	B	174/174 (100%)	172 (99%)	2 (1%)	80	85
2	E	172/174 (99%)	165 (96%)	7 (4%)	37	36
3	C	11/11 (100%)	11 (100%)	0	100	100
3	F	10/11 (91%)	10 (100%)	0	100	100
All	All	703/712 (99%)	690 (98%)	13 (2%)	66	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	129	THR
2	B	23	ARG
2	B	34	GLN
1	D	23	MET
1	D	92	LEU
2	E	5	PRO
2	E	23	ARG
2	E	34	GLN
2	E	70	GLN
2	E	105	LYS
2	E	107	GLN
2	E	184	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	107	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 ⓘ

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 ⓘ

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	180/187 (96%)	-0.14	1 (0%) 90 92	15, 23, 40, 53	0
1	D	187/187 (100%)	0.18	9 (4%) 34 43	19, 30, 52, 67	0
2	B	192/192 (100%)	-0.16	2 (1%) 84 87	16, 26, 45, 63	0
2	E	190/192 (98%)	0.19	7 (3%) 45 54	17, 31, 50, 62	0
3	C	12/12 (100%)	-0.05	1 (8%) 14 19	21, 25, 47, 56	0
3	F	11/12 (91%)	0.13	0 100 100	28, 32, 44, 55	0
All	All	772/782 (98%)	0.02	20 (2%) 59 66	15, 28, 48, 67	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	PRO	4.2
1	D	184	SER	3.7
1	D	185	PRO	3.6
1	D	182	ALA	3.6
2	E	2	ASP	3.5
1	D	100	ARG	3.4
1	D	99	LEU	2.7
1	A	51	PHE	2.7
2	B	3	THR	2.6
1	D	37	ALA	2.6
2	E	166	ARG	2.5
2	E	3	THR	2.5
2	E	106	THR	2.5
1	D	186	LEU	2.5
2	E	170	VAL	2.3
1	D	2	LYS	2.3
2	B	191	ARG	2.2
2	E	65	LYS	2.2
3	C	319	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	107	GLN	2.0

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.