

wwPDB X-ray Structure Validation Summary Report (i)

Aug 2, 2023 – 02:57 AM EDT

PDB ID : 1D5M

Title : X-RAY CRYSTAL STRUCTURE OF HLA-DR4 COMPLEXED WITH PEP-

TIDE AND SEB

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Deposited on : 1999-10-07

Resolution : 2.00 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.34

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

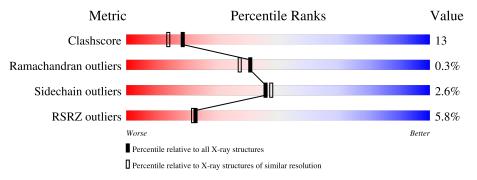
Validation Pipeline (wwPDB-VP) : 2.34

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 2.00 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	Similar resolution
	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of 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 chair	1	
1	A	181	78%	19%	
2	В	192	5% 67%	25%	• 6%
3	С	239	71%	22%	• 5%
4	D	9	56%	33%	11%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5076 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	178	Total 1464	C 949	N 238	O 272	S 5	0	0	0

• Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	181	Total 1499	C 948	N 263	O 283	S 5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	180	VAL	LEU	conflict	UNP P13760

• Molecule 3 is a protein called ENTEROTOXIN TYPE B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	С	226	Total 1884	C 1208	N 304	O 362	S 10	0	0	0

• Molecule 4 is a protein called INHIBITOR.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	D	0	Total	С	N	О	S	0	1	1
4	D	9	70	43	13	11	3	U	1	1

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
5	A	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 6 is water.

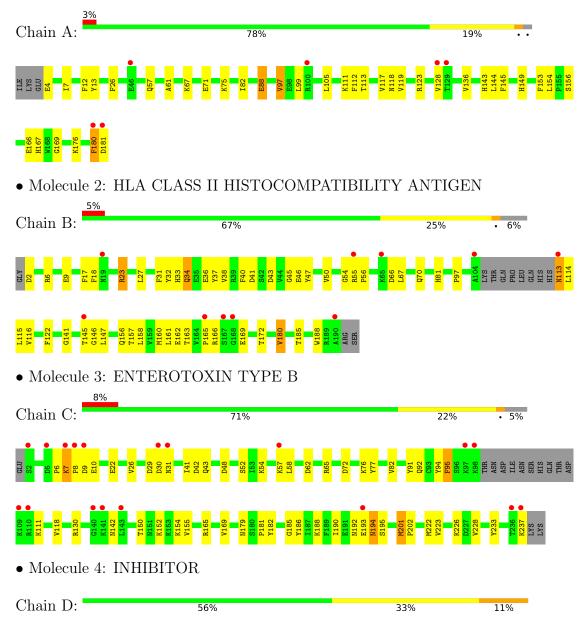
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	52	Total O 52 52	0	0
6	В	38	Total O 38 38	0	0
6	С	51	Total O 51 51	0	0
6	D	4	Total O 4 4	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	82.38Å 93.34Å 99.68Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 - 2.00	Depositor
rtesolution (A)	19.89 - 1.99	EDS
% Data completeness	92.9 (19.90-2.00)	Depositor
(in resolution range)	92.2 (19.89-1.99)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.22 (at 1.99Å)	Xtriage
Refinement program	CNS 0.9	Depositor
P. P.	0.236 , 0.260	Depositor
R, R_{free}	0.234 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 51.0	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ALC, NH2, NAG, CY1, ACE

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).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.44	1/1509 (0.1%)	0.68	$1/2058 \ (0.0\%)$	
2	В	0.35	0/1539	0.64	0/2091	
3	С	0.35	0/1927	0.59	0/2592	
4	D	0.57	0/36	1.19	0/44	
All	All	0.38	1/5011 (0.0%)	0.64	$1/6785 \ (0.0\%)$	

All (1) bond length outliers are listed below:

M	ol	Chain	Res	Type	Atoms	${f Z}$	Observed(Å)	$\operatorname{Ideal}(ext{\AA})$
1		A	97	VAL	CB-CG1	-6.57	1.39	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	88	GLU	N-CA-C	-5.16	97.07	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	1464	0	1400	45	0
2	В	1499	0	1407	52	0



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	С	1884	0	1821	41	0
4	D	70	0	76	5	0
5	A	14	0	13	0	0
6	A	52	0	0	0	0
6	В	38	0	0	1	0
6	С	51	0	0	0	0
6	D	4	0	0	1	0
All	All	5076	0	4717	127	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 13.

The worst 5 of 127 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:97:VAL:CG1	1:A:180:PHE:HE2	1.51	1.23
3:C:194:ASN:C	3:C:194:ASN:HD22	1.58	1.05
1:A:97:VAL:CG1	1:A:180:PHE:CE2	2.41	1.02
1:A:97:VAL:HG12	1:A:180:PHE:HE2	1.22	1.02
1:A:97:VAL:HG12	1:A:180:PHE:CE2	1.97	0.99

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	Perce	ntiles
1	A	176/181 (97%)	173 (98%)	2 (1%)	1 (1%)	25	19
2	В	177/192~(92%)	171 (97%)	6 (3%)	0	100	100
3	С	222/239 (93%)	211 (95%)	10 (4%)	1 (0%)	29	23
4	D	5/9 (56%)	5 (100%)	0	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	580/621 (93%)	560 (97%)	18 (3%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	95	PHE
1	A	136	VAL

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	163/166 (98%)	160 (98%)	3 (2%)	59 63
2	В	163/173~(94%)	157 (96%)	6 (4%)	34 32
3	С	210/225~(93%)	205 (98%)	5 (2%)	49 51
4	D	4/4 (100%)	4 (100%)	0	100 100
All	All	540/568~(95%)	526 (97%)	14 (3%)	46 48

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	113	ASN
2	В	180	VAL
3	С	201	MET
3	С	142	ASN
3	С	194	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	С	171	ASN
3	С	194	ASN
2	В	81	HIS



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Mol	Chain	Res	Type
2	В	113	ASN
2	В	120	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Tuno	Chain	Res	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CY1	D	808[B]	-	9,10,11	1.59	2 (22%)	5,11,13	1.97	1 (20%)
4	ALC	D	804	4	9,11,12	0.73	0	10,13,15	1.00	1 (10%)
4	CY1	D	808[A]	-	9,10,11	1.51	3 (33%)	5,11,13	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CY1	D	808[B]	-	-	0/5/9/11	-
4	ALC	D	804	4	-	0/5/14/16	0/1/1/1
4	CY1	D	808[A]	-	-	0/5/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
4	D	808[B]	CY1	CB-SG	3.12	1.93	1.80
4	D	808[B]	CY1	CD-SG	-2.76	1.77	1.82
4	D	808[A]	CY1	CD-SG	-2.35	1.78	1.82



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
4	D	808[A]	CY1	CD-NE	2.30	1.47	1.44
4	D	808[A]	CY1	CB-SG	2.14	1.89	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
4	D	808[B]	CY1	CB-SG-CD	3.97	108.56	102.02
4	D	804	ALC	CG-CB-CA	2.26	117.56	114.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	808[B]	CY1	2	0
4	D	808[A]	CY1	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type Cha		Chain	Chain Res		Во	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	NAG	A	1201	1	14,14,15	0.50	0	17,19,21	0.91	1 (5%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the



Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1201	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
5	A	1201	NAG	C4-C3-C2	-2.44	107.44	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1201	NAG	C3-C2-N2-C7
5	A	1201	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	178/181 (98%)	0.13	6 (3%) 45 44	11, 19, 35, 46	0
2	В	181/192 (94%)	0.42	10 (5%) 25 24	12, 23, 44, 53	0
3	С	226/239 (94%)	0.51	18 (7%) 12 11	13, 23, 47, 64	0
4	D	5/9 (55%)	0.13	0 100 100	8, 8, 16, 18	0
All	All	590/621 (95%)	0.36	34 (5%) 23 22	8, 22, 43, 64	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	8	PRO	5.8
3	С	110	ARG	5.4
2	В	65	LYS	5.1
2	В	190	ALA	4.7
2	В	104	ALA	4.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ m B ext{-}factors(\AA^2)$	Q<0.9
4	ALC	D	804	11/12	0.88	0.16	6,8,11,13	0
4	CY1	D	808[A]	11/12	0.91	0.22	7,14,15,16	6
4	CY1	D	808[B]	11/12	0.91	0.22	7,14,20,22	6



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	NAG	A	1201	14/15	0.74	0.21	34,37,39,43	0

6.5 Other polymers (i)

There are no such residues in this entry.

