

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 1D6E

Title: CRYSTAL STRUCTURE OF HLA-DR4 COMPLEX WITH PEP-

TIDOMIMETIC AND SEB

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Deposited on : 1999-10-13

Resolution : 2.45 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.orgA 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 : 2.35.1

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)

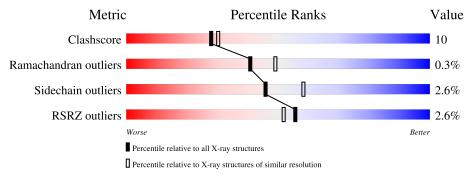
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.45 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
10100110	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 chain						
1	A	181	82%		14% ••				
2	В	192	70%	22%	• 7%				
3	С	239	73%	19%	• 6%				
4	D	9	56%	33%	11%				

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mo	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPQ	D	4	_	-	X	_



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4911 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	177	Total 1456	C 945	N 237	O 269	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	179	Total 1484	C 941	N 260	O 278	S 5	0	0	0

• Molecule 3 is a protein called ENTEROTOXIN TYPE B.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	225	Total 1869	C 1199	N 299	O 361	S 10	0	0	0

• Molecule 4 is a protein called PEPTIDOMIMETIC INHIBITOR.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	D	0	Total	С	N	О	S	0	0	1
4	ט	9	64	43	11	9	1	0	0	1

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	В	12	Total O 12 12	0	0
5	С	15	Total O 15 15	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 82% • Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN Chain B: 22% • Molecule 3: ENTEROTOXIN TYPE B Chain C: 73% 19% • 6% • Molecule 4: PEPTIDOMIMETIC INHIBITOR Chain D: 56% 33% 11%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	80.83Å 102.33Å 102.64Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 - 2.45	Depositor
resolution (A)	19.95 - 2.45	EDS
% Data completeness	96.3 (19.95-2.45)	Depositor
(in resolution range)	96.4 (19.95-2.45)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.00 (at 2.44Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.198 , 0.226	Depositor
it, it free	0.194 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 42.6	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4911	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.69% 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, ACE, MPQ, TBG

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	Mol Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.42	0/1501	0.67	0/2047	
2	В	0.39	0/1524	0.64	0/2070	
3	С	0.41	0/1912	0.62	0/2574	
4	D	1.02	0/28	1.46	0/33	
All	All	0.41	0/4965	0.65	0/6724	

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	1456	0	1397	27	0
2	В	1484	0	1399	35	0
3	С	1869	0	1797	35	0
4	D	64	0	68	12	0
5	A	11	0	0	0	0
5	В	12	0	0	0	0
5	С	15	0	0	0	0
All	All	4911	0	4661	94	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 10.

The worst 5 of 94 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:113:THR:HG22	1:A:114:PRO:HA	1.52	0.91
3:C:58:LEU:HD13	3:C:60:ASN:ND2	1.90	0.86
2:B:37:TYR:CD1	2:B:38:VAL:HG22	2.20	0.77
3:C:183:GLU:HB2	3:C:237:LYS:HG2	1.67	0.76
2:B:13:HIS:HD2	2:B:28:ASP:OD1	1.69	0.76

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	175/181 (97%)	170 (97%)	5 (3%)	0	100	100
2	В	175/192~(91%)	168 (96%)	6 (3%)	1 (1%)	25	29
3	C	221/239~(92%)	205 (93%)	15 (7%)	1 (0%)	29	34
4	D	4/9 (44%)	4 (100%)	0	0	100	100
All	All	575/621 (93%)	547 (95%)	26 (4%)	2 (0%)	41	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	165	PRO
3	С	57	LYS

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	162/166~(98%)	158 (98%)	4 (2%)	47 60		
2	В	161/173 (93%)	159 (99%)	2 (1%)	71 81		
3	С	208/225 (92%)	200 (96%)	8 (4%)	33 43		
4	D	3/3 (100%)	3 (100%)	0	100 100		
All	All	534/567 (94%)	520 (97%)	14 (3%)	46 58		

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

Mol	Chain	Res	Type
3	С	73	LEU
3	С	127	ASP
3	С	228	VAL
3	С	155	VAL
3	С	194	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	81	HIS
2	В	134	ASN
3	С	142	ASN
3	С	60	ASN
2	В	13	HIS

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).

Mal	Type	Chain	Res	Link	Bond lengths			Bond angles		
Mol	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	gles $\# Z > 2$ 0 1 (10%)
4	TBG	D	8	4	6,7,8	1.03	0	7,10,12	0.79	0
4	ALC	D	2	4	9,11,12	0.87	0	10,13,15	2.94	1 (10%)
4	MPQ	D	4	4	11,11,12	1.75	1 (9%)	9,13,15	0.21	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	TBG	D	8	4	-	0/6/8/10	-
4	ALC	D	2	4	-	4/5/14/16	0/1/1/1
4	MPQ	D	4	4	-	2/5/8/10	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{ iny A})$
4	D	4	MPQ	CG-CA	-4.17	1.48	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
4	D	2	ALC	CG-CB-CA	8.96	126.56	114.52

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	ALC	N-CA-CB-CG
4	D	2	ALC	C-CA-CB-CG
4	D	2	ALC	CA-CB-CG-CD2
4	D	4	MPQ	CG-CA-N-CM
4	D	2	ALC	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 8 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4	MPQ	8	0

5.5 Carbohydrates (i)

There are no monosaccharides 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, 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></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	177/181 (97%)	-0.57	2 (1%) 80 80	18, 33, 54, 63	0
2	В	179/192 (93%)	-0.31	6 (3%) 45 41	20, 36, 65, 82	0
3	С	225/239 (94%)	-0.29	7 (3%) 49 45	21, 37, 70, 82	0
4	D	4/9 (44%)	-0.44	0 100 100	14, 17, 17, 21	0
All	All	585/621 (94%)	-0.38	15 (2%) 56 52	14, 35, 63, 82	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	58	LEU	4.8
3	С	193	GLU	4.8
2	В	165	PRO	4.3
3	С	56	THR	3.1
2	В	55	ARG	3.1

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	ALC	D	2	11/12	0.91	0.16	9,11,12,12	0
4	MPQ	D	4	11/12	0.92	0.18	13,15,17,20	0
4	TBG	D	8	8/9	0.96	0.12	24,25,28,28	0



6.3 Carbohydrates (i)

There are no monosaccharides 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.

