



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:46 am BST

PDB ID : 1SEB
Title : COMPLEX OF THE HUMAN MHC CLASS II GLYCOPROTEIN HLA-DR1
AND THE BACTERIAL SUPERANTIGEN SEB
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Stauffer, C.; Strominger, J.L.; Wiley, D.C.
Deposited on : 1995-11-26
Resolution : 2.70 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

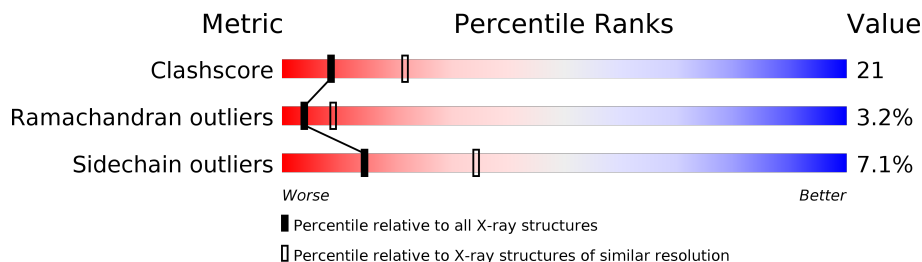
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	
1	E	181	
2	B	192	
2	F	192	
3	C	13	
3	G	13	
4	D	234	
4	H	234	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9396 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
			Total	C	N	O	S			
1	A	181	1483	960	241	277	5	0	0	0
1	E	181	1483	960	241	277	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	192	1556	980	277	293	6	0	0	0
2	F	192	1556	980	277	293	6	0	0	0

- Molecule 3 is a protein called ENDOGENOUS PEPTIDE MODEL, POLY-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	13	65	39	13	13	0	0	0
3	G	13	65	39	13	13	0	0	0

- Molecule 4 is a protein called ENTEROTOXIN TYPE B.

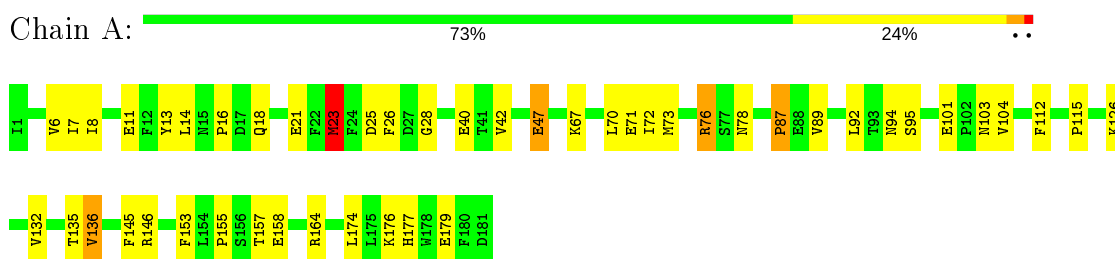
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	206	1594	1024	249	311	10	0	0	0
4	H	206	1594	1024	249	311	10	0	0	0

3 Residue-property plots

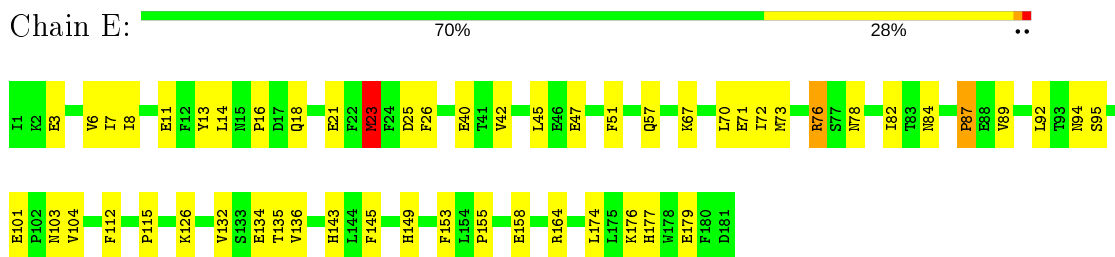
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

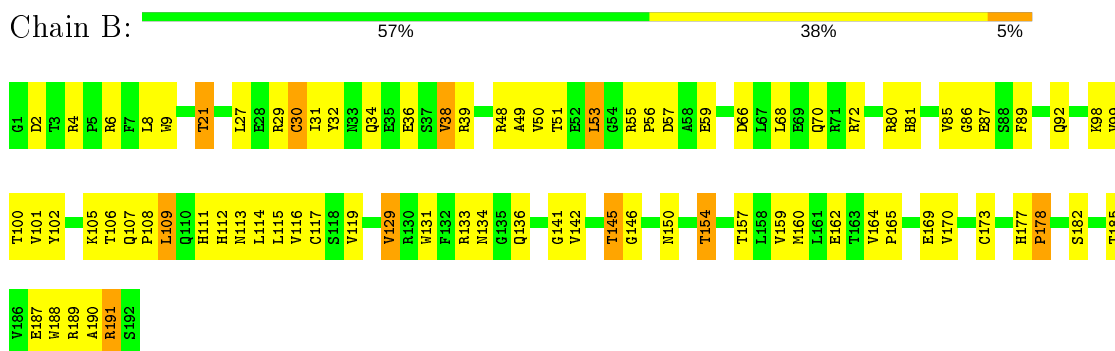
- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN



- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN



- Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN

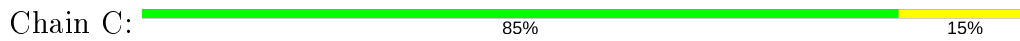


- Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN

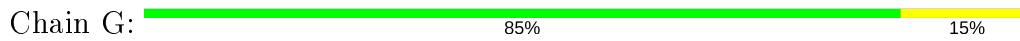




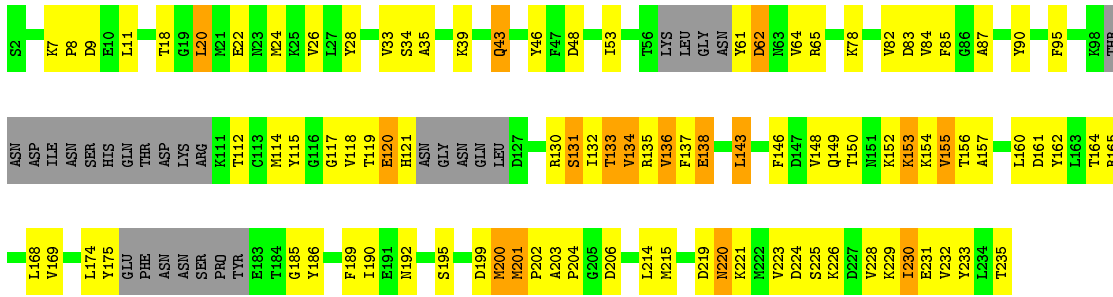
- Molecule 3: ENDOGENOUS PEPTIDE MODEL, POLY-ALA



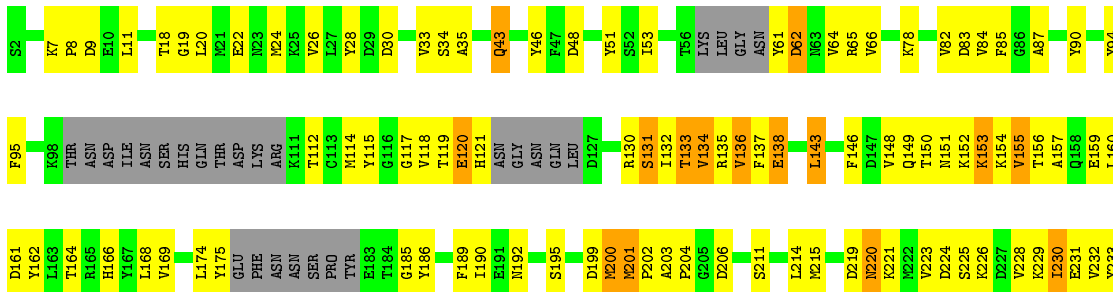
- Molecule 3: ENDOGENOUS PEPTIDE MODEL, POLY-ALA



- Molecule 4: ENTEROTOXIN TYPE B



- Molecule 4: ENTEROTOXIN TYPE B



T234
T235

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.00Å 114.70Å 149.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.257 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9396	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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	0.92	0/1528	1.05	2/2084 (0.1%)
1	E	0.93	1/1528 (0.1%)	1.06	2/2084 (0.1%)
2	B	0.87	2/1596 (0.1%)	1.04	4/2170 (0.2%)
2	F	0.89	3/1596 (0.2%)	1.19	7/2170 (0.3%)
4	D	0.69	0/1627	0.92	2/2206 (0.1%)
4	H	0.78	1/1627 (0.1%)	0.92	2/2206 (0.1%)
All	All	0.85	7/9502 (0.1%)	1.03	19/12920 (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
2	F	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	19	GLY	C-N	14.42	1.67	1.34
2	F	93	ARG	C-N	8.46	1.53	1.34
2	F	129	VAL	CB-CG2	-6.10	1.40	1.52
2	B	129	VAL	CB-CG2	-6.09	1.40	1.52
1	E	84	ASN	C-N	-5.83	1.20	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	93	ARG	O-C-N	-19.70	91.19	122.70
2	F	93	ARG	CA-C-N	13.94	147.87	117.20
2	F	93	ARG	C-N-CA	11.14	149.56	121.70
2	F	38	VAL	CB-CA-C	-6.21	99.60	111.40
2	B	38	VAL	CB-CA-C	-6.20	99.61	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	93	ARG	Mainchain

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	1483	0	1414	40	0
1	E	1483	0	1414	40	0
2	B	1556	0	1475	67	0
2	F	1556	0	1475	75	0
3	C	65	0	15	2	0
3	G	65	0	15	2	0
4	D	1594	0	1407	90	0
4	H	1594	0	1407	92	0
All	All	9396	0	8622	371	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 21.

The worst 5 of 371 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)
4:D:82:VAL:HG11	4:D:118:VAL:HB	1.27	1.12
4:H:82:VAL:HG11	4:H:118:VAL:HB	1.27	1.09
1:A:157:THR:O	2:F:112:HIS:HE1	1.41	1.02
4:D:203:ALA:HB1	4:D:204:PRO:HD2	1.44	1.00
2:B:51:THR:CA	2:F:52:GLU:OE2	2.11	0.98

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	179/181 (99%)	176 (98%)	3 (2%)	0	100	100
1	E	179/181 (99%)	176 (98%)	3 (2%)	0	100	100
2	B	190/192 (99%)	178 (94%)	7 (4%)	5 (3%)	5	13
2	F	190/192 (99%)	178 (94%)	7 (4%)	5 (3%)	5	13
4	D	196/234 (84%)	163 (83%)	20 (10%)	13 (7%)	1	2
4	H	196/234 (84%)	163 (83%)	20 (10%)	13 (7%)	1	2
All	All	1130/1214 (93%)	1034 (92%)	60 (5%)	36 (3%)	4	9

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	62	ASP
4	D	136	VAL
4	D	153	LYS
4	H	62	ASP
4	H	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	164/166 (99%)	151 (92%)	13 (8%)	12	28
1	E	164/166 (99%)	151 (92%)	13 (8%)	12	28
2	B	169/173 (98%)	160 (95%)	9 (5%)	22	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	169/173 (98%)	160 (95%)	9 (5%)	22	48
4	D	159/220 (72%)	146 (92%)	13 (8%)	11	26
4	H	159/220 (72%)	146 (92%)	13 (8%)	11	26
All	All	984/1118 (88%)	914 (93%)	70 (7%)	14	34

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

Mol	Chain	Res	Type
4	D	200	MET
1	E	76	ARG
4	H	143	LEU
4	D	201	MET
1	E	23	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	43	GLN
1	E	143	HIS
2	F	150	ASN
2	B	156	GLN
2	F	156	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	19:GLY	C	20:LEU	N	1.67

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.