



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:32 pm GMT

PDB ID : 1A7L  
Title : DOMINANT B-CELL EPITOPE FROM THE PRES2 REGION OF HEPATITIS B VIRUS IN THE FORM OF AN INSERTED PEPTIDE SEGMENT IN MALTODEXTRIN-BINDING PROTEIN  
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Deposited on : 1998-03-16  
Resolution : 2.90 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

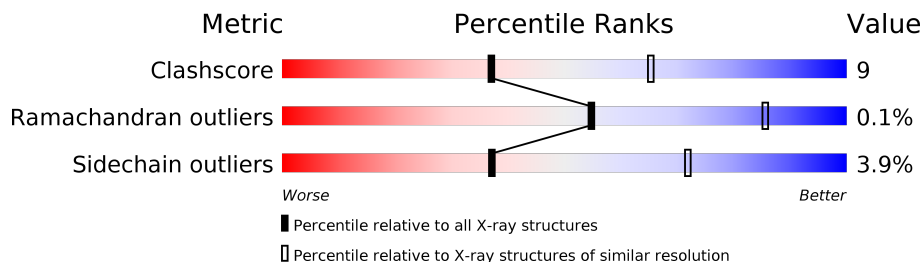
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	389	
1	B	389	
1	C	389	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAL	A	400	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAL	B	400	X	-	-	-
2	MAL	C	400	X	-	-	-

## 2 Entry composition [i](#)

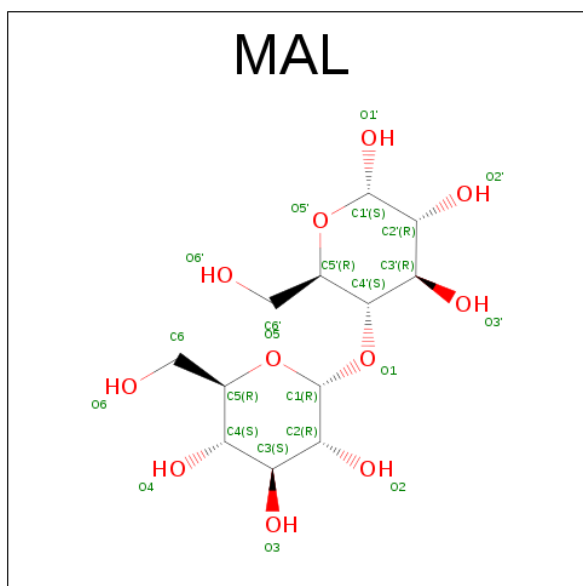
There are 3 unique types of molecules in this entry. The entry contains 8750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALE-B363.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2936	1888	480	560	8			
1	B	372	Total	C	N	O	S	0	0	0
			2893	1864	472	551	6			
1	C	362	Total	C	N	O	S	0	0	0
			2805	1807	455	537	6			

- Molecule 2 is SUGAR (MALTOSE) (three-letter code: MAL) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			22	11	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is water.

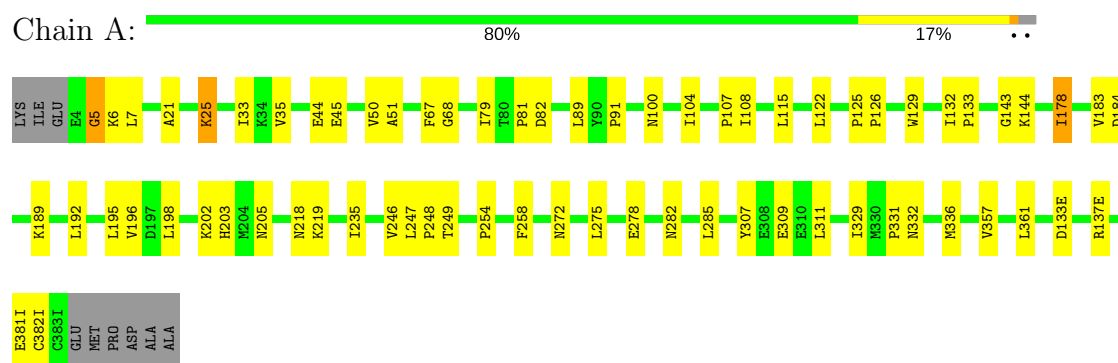
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	17	Total 17	O 17	0	0
3	C	11	Total 11	O 11	0	0

### 3 Residue-property plots [i](#)

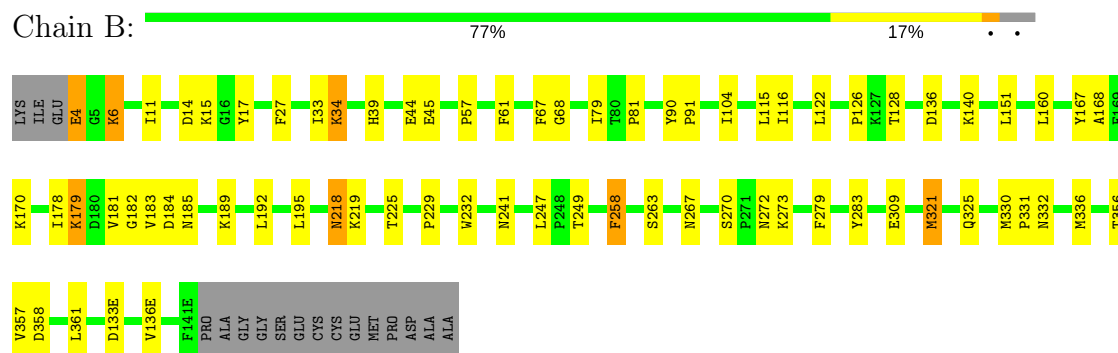
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

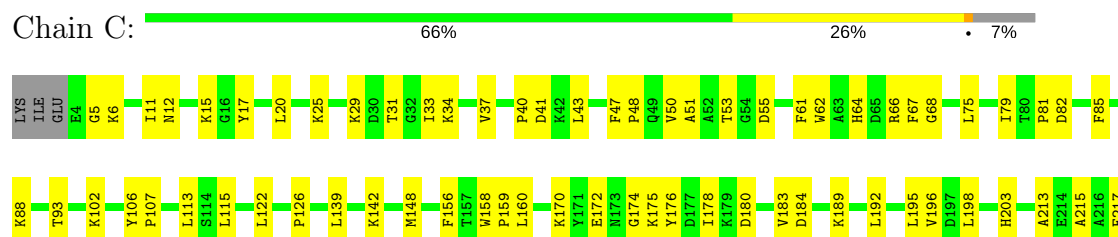
#### • Molecule 1: MALE-B363



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#### • Molecule 1: MALE-B363



N218	K219	G220	E221	T222	A223	N224	P229	N232	S238	N246	T249	P254	S255	K256	P257	F258	V259	G260	S263	S270	P271	N272	K273	L280	E291	K295	E309	E310	L311	A318	K321	E322	N323	K326	K330	P331	N332	I333	P334	Q335	K336	W340	
V343	V347	L361	S365I	GLN	ASP	PRO	ARG	VAL	ARG	GLY	LEU	TYR	PHE	PRO	ALA	GLY	SER	GLU	CYS	CYS	GLU	MET	PRO	ASP	ALA	ALA																	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.60Å 71.30Å 123.20Å 90.00° 94.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	98.0 (10.00-2.90)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.192 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP



## 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: MAL

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	0.39	1/3009 (0.0%)	0.57	0/4085
1	B	0.36	0/2965	0.58	0/4025
1	C	0.34	0/2874	0.55	0/3902
All	All	0.37	1/8848 (0.0%)	0.57	0/12012

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	GLY	N-CA	-8.37	1.33	1.46

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	2936	0	2891	44	0
1	B	2893	0	2856	43	0
1	C	2805	0	2770	63	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
2	C	22	0	18	4	0
3	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	0	0	0
3	C	11	0	0	1	0
All	All	8750	0	8579	153	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 9.

The worst 5 of 153 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:79:ILE:HG22	1:A:81:PRO:HD3	1.44	0.96
1:B:79:ILE:HG22	1:B:81:PRO:HD3	1.45	0.95
1:B:321:MET:O	1:B:325:GLN:HG2	1.78	0.82
1:C:331:PRO:HG2	1:C:336:MET:SD	2.21	0.81
2:C:400:MAL:C5	2:C:400:MAL:C3	2.58	0.81

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	378/389 (97%)	367 (97%)	11 (3%)	0	100	100
1	B	370/389 (95%)	358 (97%)	12 (3%)	0	100	100
1	C	360/389 (92%)	346 (96%)	13 (4%)	1 (0%)	44	77
All	All	1108/1167 (95%)	1071 (97%)	36 (3%)	1 (0%)	55	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	172	GLU

### 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	302/310 (97%)	291 (96%)	11 (4%)	40	75
1	B	298/310 (96%)	287 (96%)	11 (4%)	39	74
1	C	289/310 (93%)	276 (96%)	13 (4%)	32	66
All	All	889/930 (96%)	854 (96%)	35 (4%)	37	72

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	LYS
1	B	258	PHE
1	C	309	GLU
1	B	185	ASN
1	B	218	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	86	GLN
1	B	100	ASN
1	B	272	ASN
1	B	72	GLN
1	B	325	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MAL	A	400	-	24,24,24	0.78	1 (4%)	35,35,35	0.69	0
2	MAL	B	400	-	24,24,24	0.91	1 (4%)	35,35,35	0.64	0
2	MAL	C	400	-	21,21,24	1.06	1 (4%)	24,28,35	0.71	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
2	MAL	A	400	-	1/1/10/10	0/8/48/48	0/2/2/2
2	MAL	B	400	-	1/1/10/10	0/8/48/48	0/2/2/2
2	MAL	C	400	-	1/1/7/10	0/16/36/48	0/1/1/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	MAL	C4-C5	2.00	1.57	1.53
2	B	400	MAL	C4-C5	2.11	1.57	1.53
2	C	400	MAL	O5-C1	3.39	1.46	1.40

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	400	MAL	C1'
2	A	400	MAL	C1'
2	C	400	MAL	C1'

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	MAL	4	0

## 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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.