



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 10:09 AM UTC

PDB ID : 1CD1 / pdb\_00001cd1  
Title : CD1(MOUSE) ANTIGEN PRESENTING MOLECULE  
Authors : Zeng, Z.H.; Segelke, B.W.; Wilson, I.A.  
Deposited on : 1997-04-02  
Resolution : 2.67 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

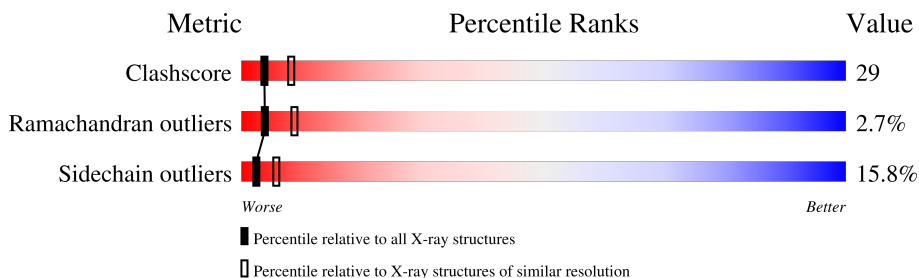
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)

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  $\geq 3$ , 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	315	 24% 37% 23% 13%
1	C	315	 25% 38% 19% 5% 13%
2	B	99	 25% 44% 28% 13%
2	D	99	 31% 44% 22% 13%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6026 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 CD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	2192	1396	378	405	13	0	0	0
1	C	273	2192	1396	378	405	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASP	conflict	UNP P11609
C	201	HIS	ASP	conflict	UNP P11609

- Molecule 2 is a protein called CD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	821	524	138	152	7	0	0	0
2	D	99	821	524	138	152	7	0	0	0





## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	59.34Å 76.20Å 103.40Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	10.00 – 2.67	Depositor
% Data completeness (in resolution range)	83.7 (10.00-2.67)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.192 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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	2.29	81/2257 (3.6%)	1.94	64/3069 (2.1%)
1	C	2.30	93/2257 (4.1%)	1.92	53/3069 (1.7%)
2	B	2.29	33/847 (3.9%)	1.93	25/1148 (2.2%)
2	D	2.29	28/847 (3.3%)	1.95	19/1148 (1.7%)
All	All	2.29	235/6208 (3.8%)	1.93	161/8434 (1.9%)

The worst 5 of 235 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	VAL	CA-CB	-10.82	1.42	1.54
2	D	8	GLN	N-CA	9.99	1.58	1.46
1	C	237	PHE	CA-C	-9.35	1.40	1.52
2	D	67	HIS	ND1-CE1	9.15	1.41	1.32
1	C	190	VAL	CA-C	8.85	1.64	1.52

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	GLN	N-CA-C	12.45	126.97	110.53
1	A	273	GLN	N-CA-C	10.45	125.98	110.52
2	B	59	ASP	N-CA-C	-10.10	101.20	112.72
1	C	94	TYR	CA-C-N	-9.74	107.66	119.84
1	C	94	TYR	C-N-CA	-9.74	107.66	119.84

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	2192	0	2097	126	0
1	C	2192	0	2097	139	0
2	B	821	0	796	43	0
2	D	821	0	796	41	0
All	All	6026	0	5786	339	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 29.

The worst 5 of 339 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:C:198:SER:HB2	1:C:201:HIS:HE1	1.26	1.00
1:C:102:ALA:HB2	1:C:116:LEU:HD23	1.43	0.97
1:C:9:THR:HG23	1:C:105:GLU:HG2	1.47	0.96
1:C:88:MET:HG3	1:C:92:GLU:HA	1.47	0.93
1:C:168:CYS:HB3	1:C:169:PRO:HD3	1.50	0.92

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	271/315 (86%)	229 (84%)	33 (12%)	9 (3%)	<b>3</b> <b>6</b>
1	C	271/315 (86%)	232 (86%)	33 (12%)	6 (2%)	<b>5</b> <b>12</b>
2	B	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	<b>3</b> <b>7</b>
2	D	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	<b>5</b> <b>13</b>
All	All	736/828 (89%)	635 (86%)	81 (11%)	20 (3%)	<b>4</b> <b>9</b>

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	199	SER
2	B	97	ARG
2	D	29	GLN
1	A	91	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	238/274 (87%)	198 (83%)	40 (17%)	2 5
1	C	238/274 (87%)	197 (83%)	41 (17%)	2 5
2	B	94/94 (100%)	82 (87%)	12 (13%)	4 9
2	D	94/94 (100%)	82 (87%)	12 (13%)	4 9
All	All	664/736 (90%)	559 (84%)	105 (16%)	2 6

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	26	THR
1	C	118	VAL
2	D	44	LYS
1	C	30	VAL
1	C	79	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	31	HIS
1	C	227	GLN
1	C	36	GLN
1	C	201	HIS
1	C	14	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 oligosaccharides 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

### 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.