



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:23 AM GMT

PDB ID : 3OV6  
Title : CD1c in complex with MPM (mannosyl-beta1-phosphomycoketide)  
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Deposited on : 2010-09-15  
Resolution : 2.50 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

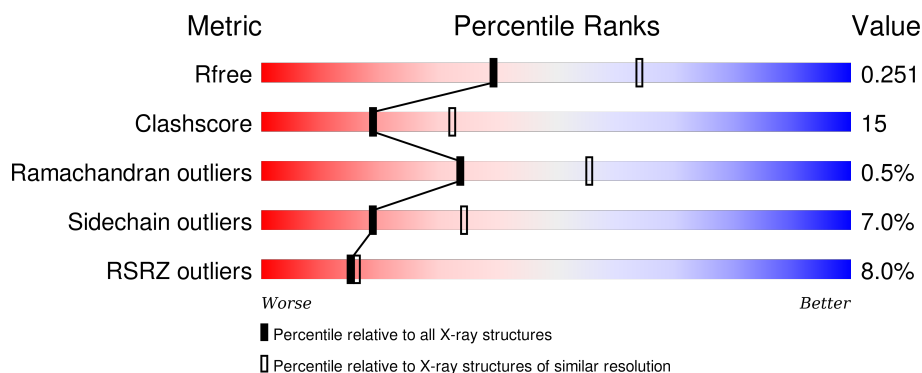
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	397	<div> <div>8%</div> <div>67%</div> <div>25%</div> <div>5%</div> </div>

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	NAG	A	1	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	D12	A	1104	-	-	X	-
4	MK0	A	1105	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3126 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 Beta-2-microglobulin, T-cell surface glycoprotein CD1c, T-cell surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	178	0	0
			3014	1926	517	559	12			

There are 26 discrepancies between the modelled and reference sequences:

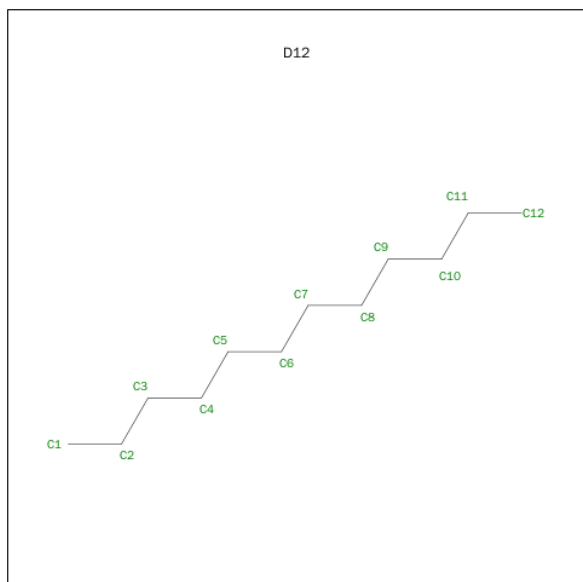
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	ALA	-	EXPRESSION TAG	UNP P61769
A	999	ASP	-	EXPRESSION TAG	UNP P61769
A	1000	PRO	-	EXPRESSION TAG	UNP P61769
A	1100	GLY	-	LINKER	UNP P61769
A	1101	GLY	-	LINKER	UNP P61769
A	1102	GLY	-	LINKER	UNP P61769
A	1103	GLY	-	LINKER	UNP P61769
A	1104	SER	-	LINKER	UNP P61769
A	1105	GLY	-	LINKER	UNP P61769
A	1106	GLY	-	LINKER	UNP P61769
A	1107	SER	-	LINKER	UNP P61769
A	1108	GLY	-	LINKER	UNP P61769
A	1109	SER	-	LINKER	UNP P61769
A	1110	GLY	-	LINKER	UNP P61769
A	1111	GLY	-	LINKER	UNP P61769
A	1112	GLY	-	LINKER	UNP P61769
A	1113	SER	-	LINKER	UNP P61769
A	1114	SER	-	LINKER	UNP P61769
A	52	GLN	ASN	ENGINEERED MUTATION	UNP P29017
A	57	GLN	ASN	ENGINEERED MUTATION	UNP P29017
A	108	GLY	LYS	ENGINEERED MUTATION	UNP P29017
A	128	GLN	ASN	ENGINEERED MUTATION	UNP P29017
A	241	GLN	ASN	ENGINEERED MUTATION	UNP P29016
A	242	GLY	TRP	ENGINEERED MUTATION	UNP P29016
A	279	HIS	-	EXPRESSION TAG	UNP P29016
A	280	HIS	-	EXPRESSION TAG	UNP P29016

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



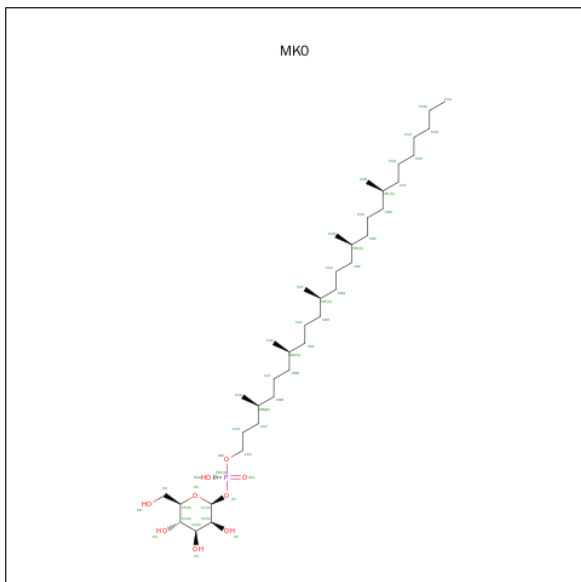
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			12	12		

- Molecule 4 is 1-O-[(S)-HYDROXY{[(4S,8S,16S,20S)-4,8,12,16,20-PENTAMETHYLHEPTACOSYL]OXY}PHOSPHORYL]-BETA-D-MANNOPYRANOSE (three-letter code: MK0) (formula: C<sub>38</sub>H<sub>77</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	48	38	9	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	1	0
			38	38		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.72Å 87.09Å 88.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.54 – 2.50 43.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.54-2.50) 91.3 (43.54-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.240 , 0.273 0.231 , 0.251	Depositor DCC
$R_{free}$ test set	686 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.0	EDS
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 13644 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, D12, MK0

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	0.54	0/3104	0.72	0/4211

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

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	3014	0	2858	84	0
2	A	14	0	13	0	0
3	A	12	0	26	10	0
4	A	48	0	76	10	0
5	A	38	0	0	2	0
All	All	3126	0	2973	87	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 15.

The worst 5 of 87 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:148:LEU:HD21	3:A:1104:D12:H62	1.52	0.88
1:A:69:LEU:HG	4:A:1105:MK0:HACB	1.61	0.83
1:A:73:TYR:HB2	4:A:1105:MK0:HACA	1.60	0.83
1:A:28:GLY:HA3	4:A:1105:MK0:HAOA	1.67	0.75
3:A:1104:D12:H122	4:A:1105:MK0:O6	1.87	0.75

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	370/397 (93%)	349 (94%)	19 (5%)	2 (0%)	34 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1102	GLY
1	A	92	TYR

### 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	327/339 (96%)	304 (93%)	23 (7%)	19 34

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	156	THR
1	A	251	ASP
1	A	146	HIS
1	A	162	LEU

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

Mol	Chain	Res	Type
1	A	161	ASN
1	A	241	GLN
1	A	204	GLN
1	A	105	HIS
1	A	232	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](#)

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	NAG	A	1	1	14,14,15	0.68	0	15,19,21	2.29	3 (20%)
3	D12	A	1104	-	11,11,11	0.30	0	10,10,10	0.39	0
4	MK0	A	1105	-	47,48,48	0.54	1 (2%)	59,61,61	1.48	11 (18%)

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	NAG	A	1	1	-	0/6/23/26	0/1/1/1
3	D12	A	1104	-	-	0/9/9/9	0/0/0/0
4	MK0	A	1105	-	-	0/46/66/66	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1105	MK0	PBV-O1	2.16	1.66	1.60

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1105	MK0	CAV-CBH-CBP	-3.17	104.96	115.49
4	A	1105	MK0	PBV-OBI-CAX	-2.44	107.54	121.50
4	A	1105	MK0	CAT-CBD-CBO	-2.24	108.06	115.49
4	A	1105	MK0	O1-C1-C2	2.05	112.21	108.39
2	A	1	NAG	O7-C7-N2	2.11	126.17	121.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1104	D12	10	0
4	A	1105	MK0	10	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](#)

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<sup>th</sup> 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>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	376/397 (94%)	0.44	30 (7%) 15 16	33, 53, 87, 114	46 (12%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	CYS	15.6
1	A	90	SER	9.6
1	A	182	VAL	7.7
1	A	136	GLY	6.9
1	A	183	HIS	6.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MK0	A	1105	48/48	0.66	0.42	6.54	42,67,114,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1	14/15	0.35	0.49	4.72	101,111,114,115	0
3	D12	A	1104	12/12	0.70	0.37	1.72	66,72,80,84	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.