



# Full wwPDB X-ray Structure Validation Report

Jun 26, 2014 – 04:50 PM EDT

PDB ID : 4BTO  
Title : Human CD81 Large extracellular loop P31 crystal form  
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Deposited on : 2013-06-18  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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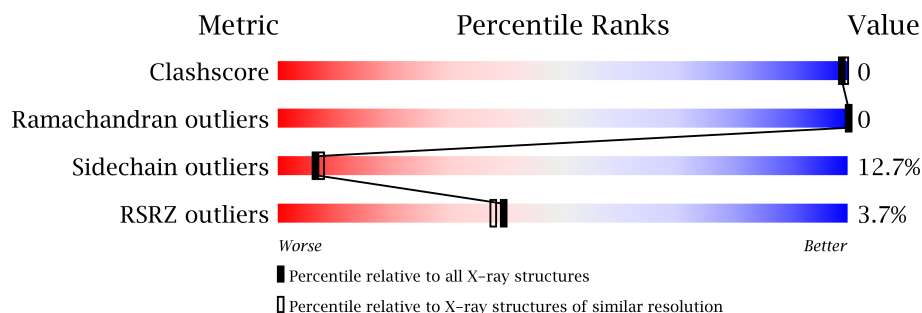
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	98	
1	B	98	
1	C	98	
1	D	98	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EOH	A	1203	-	X
2	EOH	A	1206	-	X
2	EOH	A	1207	-	X
2	EOH	B	1203	-	X
2	EOH	B	1205	-	X
2	EOH	B	1206	-	X
2	EOH	B	1207	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	EOH	C	1204	-	X
2	EOH	C	1205	-	X
2	EOH	D	1203	-	X
2	EOH	D	1204	-	X
2	EOH	D	1205	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5535 atoms, of which 2725 are hydrogens and 0 are deuterium.

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.

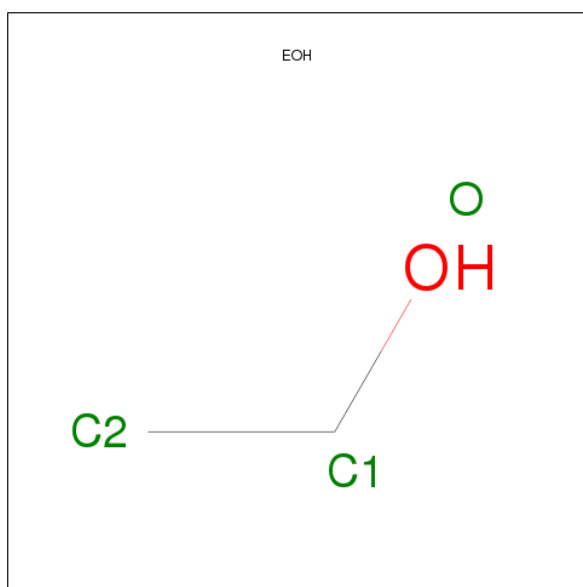
- Molecule 1 is a protein called CD81 ANTIGEN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	89	Total	C	H	N	O	S	0	1	0
			1354	424	668	117	141	4			
1	B	89	Total	C	H	N	O	S	0	1	0
			1354	424	668	117	141	4			
1	C	89	Total	C	H	N	O	S	0	0	0
			1345	421	663	117	140	4			
1	D	89	Total	C	H	N	O	S	0	0	0
			1345	421	663	117	140	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	HIS	-	EXPRESSION TAG	UNP P60033
B	202	HIS	-	EXPRESSION TAG	UNP P60033
C	202	HIS	-	EXPRESSION TAG	UNP P60033
D	202	HIS	-	EXPRESSION TAG	UNP P60033

- Molecule 2 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	2	6	1		
2	A	1	Total	C	H	O	0	0
			9	2	6	1		
2	A	1	Total	C	H	O	0	0
			9	2	6	1		
2	A	1	Total	C	H	O	0	0
			6	2	3	1		
2	A	1	Total	C	H	O	0	0
			9	2	6	1		
2	B	1	Total	C	H	O	0	0
			9	2	6	1		
2	B	1	Total	C	O		0	0
			3	2	1			
2	B	1	Total	C	O		0	0
			3	2	1			
2	B	1	Total	C	O		0	0
			3	2	1			
2	B	1	Total	C	H	O	0	0
			9	2	6	1		
2	C	1	Total	C	H	O	0	0
			9	2	6	1		
2	C	1	Total	C	O		0	0
			3	2	1			
2	C	1	Total	C	O		0	0
			3	2	1			
2	C	1	Total	C	H	O	0	0
			9	2	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C H O 9 2 6 1	0	0
2	D	1	Total C O 3 2 1	0	0
2	D	1	Total C O 3 2 1	0	0
2	D	1	Total C H O 9 2 6 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	6	Total O 6 6	0	0
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	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 errors 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.

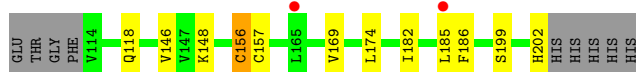
#### • Molecule 1: CD81 ANTIGEN

Chain A: 



#### • Molecule 1: CD81 ANTIGEN

Chain B: 



#### • Molecule 1: CD81 ANTIGEN

Chain C: 



#### • Molecule 1: CD81 ANTIGEN

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.00Å 98.00Å 34.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.94 – 2.40 84.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.94-2.40) 98.2 (84.87-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.196 , 0.236 0.209 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.6	EDS
Estimated twinning fraction	0.479 for -h,-k,l 0.039 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14193 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EOH

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	0.47	0/697	0.63	0/942
1	B	0.47	0/697	0.59	0/942
1	C	0.51	0/690	0.66	0/932
1	D	0.51	0/690	0.64	0/932
All	All	0.49	0/2774	0.63	0/3748

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	686	668	0	0	0
1	B	686	668	0	1	0
1	C	682	663	0	0	0
1	D	682	663	0	0	0
2	A	15	27	3	0	0
2	B	15	12	18	0	0
2	C	12	12	12	0	0
2	D	12	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
3	B	6	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
All	All	2810	2725	45	1	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

All (1) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:156:CYS:SG	1:B:157:CYS:N	2.92	0.43

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	88/98 (90%)	87 (99%)	1 (1%)	0	100	100
1	B	88/98 (90%)	85 (97%)	3 (3%)	0	100	100
1	C	87/98 (89%)	83 (95%)	4 (5%)	0	100	100
1	D	87/98 (89%)	83 (95%)	4 (5%)	0	100	100
All	All	350/392 (89%)	338 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	80/87 (92%)	68 (85%)	12 (15%)	4	5
1	B	80/87 (92%)	69 (86%)	11 (14%)	5	6
1	C	79/87 (91%)	68 (86%)	11 (14%)	5	6
1	D	79/87 (91%)	72 (91%)	7 (9%)	14	21
All	All	318/348 (91%)	277 (87%)	41 (13%)	6	7

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	A	116	LYS
1	A	118	GLN
1	A	146	VAL
1	A	148	LYS
1	A	156	CYS
1	A	163[A]	THR
1	A	163[B]	THR
1	A	169	VAL
1	A	174	LEU
1	A	185	LEU
1	A	202	HIS
1	B	118	GLN
1	B	146	VAL
1	B	148	LYS
1	B	156	CYS
1	B	169	VAL
1	B	174	LEU
1	B	182	ILE
1	B	185	LEU
1	B	186	PHE
1	B	199	SER
1	B	202	HIS
1	C	116	LYS
1	C	118	GLN
1	C	121	LYS
1	C	132	GLN
1	C	144	LYS
1	C	156	CYS
1	C	162	LEU
1	C	173	ASN
1	C	174	LEU
1	C	185	LEU

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Mol	Chain	Res	Type
1	C	202	HIS
1	D	121	LYS
1	D	139	ASP
1	D	146	VAL
1	D	156	CYS
1	D	162	LEU
1	D	173	ASN
1	D	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	132	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	89/98 (90%)	0.27	2 (2%) 59 57	41, 59, 85, 97	0
1	B	89/98 (90%)	0.16	2 (2%) 59 57	41, 58, 84, 96	0
1	C	89/98 (90%)	0.40	5 (5%) 24 22	43, 61, 86, 92	0
1	D	89/98 (90%)	0.43	4 (4%) 32 30	43, 60, 87, 92	0
All	All	356/392 (90%)	0.32	13 (3%) 39 38	41, 60, 87, 97	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	185	LEU	4.8
1	A	186	PHE	4.3
1	D	182	ILE	4.3
1	D	185	LEU	4.0
1	C	182	ILE	4.0
1	D	138	ASP	2.9
1	C	181	ILE	2.7
1	C	186	PHE	2.5
1	D	186	PHE	2.2
1	B	165	LEU	2.1
1	A	202	HIS	2.1
1	C	140	ALA	2.1
1	B	185	LEU	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EOH	B	1203	3/3	0.26	5.42	85,86,87,87	0
2	EOH	A	1207	3/3	0.50	4.02	66,67,70,70	0
2	EOH	C	1205	3/3	0.25	3.86	69,69,69,70	0
2	EOH	B	1206	3/3	0.34	3.85	63,63,63,65	0
2	EOH	B	1205	3/3	0.20	3.49	73,73,75,76	0
2	EOH	A	1203	3/3	0.24	3.12	89,89,90,90	0
2	EOH	D	1205	3/3	0.23	3.04	72,72,73,75	0
2	EOH	A	1206	3/3	0.26	2.90	62,62,63,63	0
2	EOH	B	1207	3/3	0.31	2.44	59,60,64,64	0
2	EOH	C	1204	3/3	0.20	2.19	66,66,67,68	0
2	EOH	D	1203	3/3	0.24	2.00	71,73,74,74	0
2	EOH	D	1204	3/3	0.21	2.00	70,70,71,71	0
2	EOH	A	1204	3/3	0.21	1.80	58,59,63,63	0
2	EOH	C	1203	3/3	0.22	1.67	69,70,72,72	0
2	EOH	B	1204	3/3	0.21	1.15	56,56,58,62	0
2	EOH	D	1206	3/3	0.18	-0.42	72,72,73,73	0
2	EOH	A	1205	3/3	0.15	-0.65	76,76,78,78	0
2	EOH	C	1206	3/3	0.17	-1.95	72,73,78,78	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.