



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 09:08 AM EDT

PDB ID : 3O2D  
Title : Crystal structure of HIV-1 primary receptor CD4 in complex with a potent antiviral antibody  
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Deposited on : 2010-07-22  
Resolution : 2.19 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

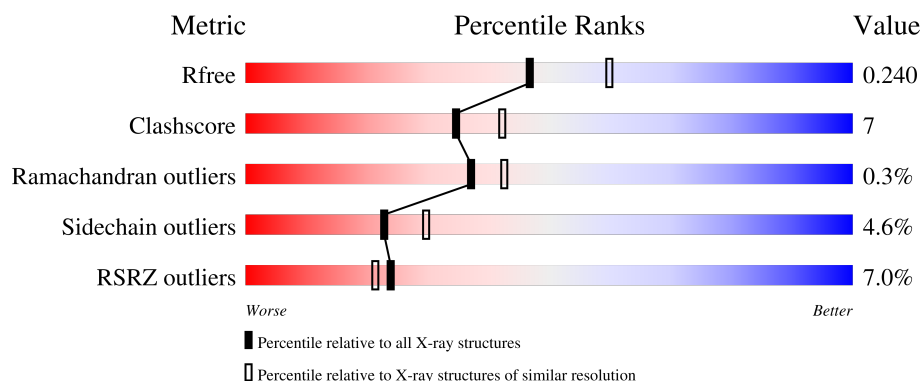
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\leq 5\%$ . 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	L	219	<div> <div>0%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
2	H	225	<div> <div>3%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
3	A	188	<div> <div>18%</div> <div>74%</div> <div>17%</div> <div>5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4966 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 ibalizumab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1684	1056	281	341	6			

- Molecule 2 is a protein called ibalizumab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1684	1061	276	340	7			

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	178	Total	C	N	O	S	0	0	0
			1383	865	242	272	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	-	expression tag	UNP P01730
A	184	HIS	-	expression tag	UNP P01730
A	185	HIS	-	expression tag	UNP P01730
A	186	HIS	-	expression tag	UNP P01730
A	187	HIS	-	expression tag	UNP P01730
A	188	HIS	-	expression tag	UNP P01730

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	104	Total	O	0	0
			104	104		
4	H	80	Total	O	0	0
			80	80		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.16Å 66.27Å 266.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.19 48.60 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.7 (48.60-2.19) 93.7 (48.60-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.192 , 0.224 0.209 , 0.240	Depositor DCC
$R_{free}$ test set	2295 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	L	0.81	0/1720	0.84	4/2334 (0.2%)
2	H	0.73	0/1727	0.74	1/2356 (0.0%)
3	A	0.60	0/1402	0.71	0/1891
All	All	0.72	0/4849	0.77	5/6581 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	178	LEU	CA-CB-CG	7.36	132.23	115.30
1	L	61	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	L	54	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	L	21	MET	CG-SD-CE	-5.23	91.83	100.20
1	L	54	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	L	1684	0	1634	31	0
2	H	1684	0	1625	25	0
3	A	1383	0	1414	17	0
4	A	31	0	0	2	0
4	H	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	104	0	0	1	0
All	All	4966	0	4673	70	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 7.

The worst 5 of 70 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:L:13:VAL:HG21	1:L:19:VAL:HG22	1.56	0.88
3:A:104:SER:HA	4:A:213:HOH:O	1.75	0.85
2:H:11:VAL:HG22	2:H:147:PRO:HG3	1.65	0.79
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.68	0.76
1:L:197:HIS:CD2	1:L:199:GLY:H	2.07	0.71

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	L	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
2	H	220/225 (98%)	212 (96%)	8 (4%)	0	100	100
3	A	176/188 (94%)	160 (91%)	14 (8%)	2 (1%)	12	10
All	All	610/632 (96%)	580 (95%)	28 (5%)	2 (0%)	37	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	88	ASP
3	A	105	ASP



### 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	L	192/194 (99%)	191 (100%)	1 (0%)	86	93
2	H	190/192 (99%)	183 (96%)	7 (4%)	29	39
3	A	161/170 (95%)	144 (89%)	17 (11%)	5	5
All	All	543/556 (98%)	518 (95%)	25 (5%)	23	30

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	73	ASN
3	A	90	LYS
3	A	174	ILE
3	A	88	ASP
3	A	104	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	73	ASN
3	A	110	GLN
3	A	139	GLN
3	A	137	ASN
2	H	155	ASN

### 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 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 [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	L	216/219 (98%)	-0.11	3 (1%) 73 70	20, 35, 48, 56	0
2	H	222/225 (98%)	0.11	7 (3%) 50 47	24, 38, 61, 85	0
3	A	178/188 (94%)	1.17	33 (18%) 4 3	29, 66, 101, 115	1 (0%)
All	All	616/632 (97%)	0.34	43 (6%) 24 21	20, 40, 85, 115	1 (0%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	43	PHE	12.3
3	A	24	ILE	6.0
3	A	104	SER	4.8
3	A	178	ALA	4.7
2	H	132	SER	4.6

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.