



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:25 PM GMT

PDB ID : 3RAJ  
Title : Crystal structure of human CD38 in complex with the Fab fragment of anti-body HB7  
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Deposited on : 2011-03-28  
Resolution : 3.04 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

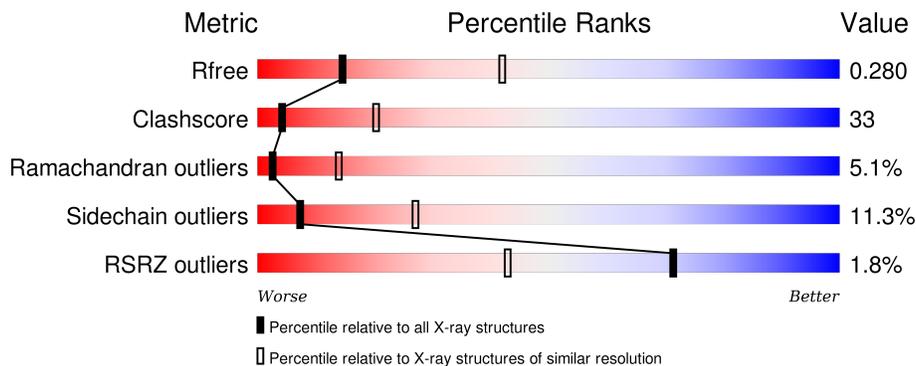
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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	257	 43% 37% 9% 11%
2	H	220	 37% 50% 10% 3%
3	L	211	 44% 48% 7% 2%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5034 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 ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1851	1168	318	351	14	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	GLU	-	EXPRESSION TAG	UNP P28907
A	45	PHE	-	EXPRESSION TAG	UNP P28907
A	49	THR	GLN	ENGINEERED MUTATION	UNP P28907
A	100	ASP	ASN	ENGINEERED MUTATION	UNP P28907
A	164	ASP	ASN	ENGINEERED MUTATION	UNP P28907
A	209	ASP	ASN	ENGINEERED MUTATION	UNP P28907
A	219	ASP	ASN	ENGINEERED MUTATION	UNP P28907

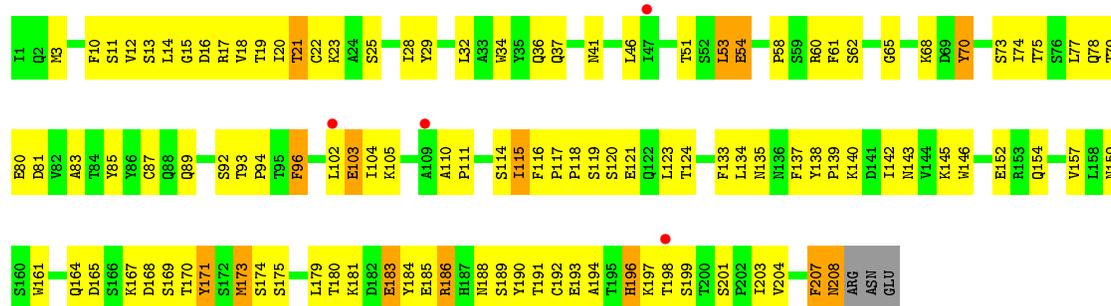
- Molecule 2 is a protein called heavy chain of the Fab fragment of antibody HB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	215	1584	1012	256	309	7	0	0	0

- Molecule 3 is a protein called light chain of the Fab fragment of antibody HB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	208	1599	996	265	332	6	0	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.66Å 271.52Å 136.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 3.04 49.81 – 3.04	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.16-3.04) 90.6 (49.81-3.04)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_378)	Depositor
R, $R_{free}$	0.205 , 0.275 0.202 , 0.280	Depositor DCC
$R_{free}$ test set	1003 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.3	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 88.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19860 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 [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	0.63	0/1896	0.77	1/2570 (0.0%)
2	H	0.46	0/1625	0.66	2/2224 (0.1%)
3	L	0.47	0/1634	0.63	0/2221
All	All	0.53	0/5155	0.69	3/7015 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100	LEU	CA-CB-CG	6.72	130.75	115.30
1	A	192	VAL	CB-CA-C	-5.18	101.56	111.40
2	H	3	VAL	CB-CA-C	-5.04	101.83	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	70	TYR	Peptide

### 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	1851	0	1777	108	0
2	H	1584	0	1518	130	0
3	L	1599	0	1530	100	0
All	All	5034	0	4825	329	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 33.

The worst 5 of 329 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)
2:H:162:ASN:HA	2:H:201:THR:HG23	1.42	1.01
2:H:171:HIS:HB2	3:L:135:ASN:HD21	1.23	1.01
2:H:128:VAL:HG21	2:H:204:VAL:HG21	1.47	0.94
1:A:71:THR:HG22	1:A:78:ARG:H	1.35	0.92
2:H:135:SER:HB2	2:H:220:ARG:HB2	1.53	0.91

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	228/257 (89%)	184 (81%)	30 (13%)	14 (6%)	2	10
2	H	211/220 (96%)	169 (80%)	28 (13%)	14 (7%)	1	8
3	L	206/211 (98%)	163 (79%)	38 (18%)	5 (2%)	7	33
All	All	645/688 (94%)	516 (80%)	96 (15%)	33 (5%)	2	14

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	251	ARG
2	H	10	PRO
2	H	11	SER
2	H	101	ILE

### 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	208/238 (87%)	182 (88%)	26 (12%)	6 23
2	H	174/191 (91%)	157 (90%)	17 (10%)	10 34
3	L	183/187 (98%)	162 (88%)	21 (12%)	7 26
All	All	565/616 (92%)	501 (89%)	64 (11%)	7 27

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	28	PHE
2	H	108	ASP
3	L	191	THR
2	H	64	PHE
2	H	99	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

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	A	230/257 (89%)	-0.09	2 (0%) 85 64	47, 74, 112, 139	0
2	H	215/220 (97%)	-0.02	6 (2%) 56 27	58, 102, 182, 204	0
3	L	208/211 (98%)	0.06	4 (1%) 70 41	70, 112, 150, 160	0
All	All	653/688 (94%)	-0.02	12 (1%) 71 43	47, 94, 159, 204	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	217	ILE	3.9
3	L	102	LEU	2.9
2	H	189	THR	2.9
3	L	109	ALA	2.8
2	H	132	ALA	2.7

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.