



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2016 – 10:55 PM EDT

PDB ID : 5BNF
Title : Apo structure of porcine CD38
Authors : Ting, K.Y.; Leung, C.P.F.; Graeff, R.M.; Lee, H.C.; Hao, Q.; Kotaka, M.
Deposited on : 2015-05-26
Resolution : 2.30 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

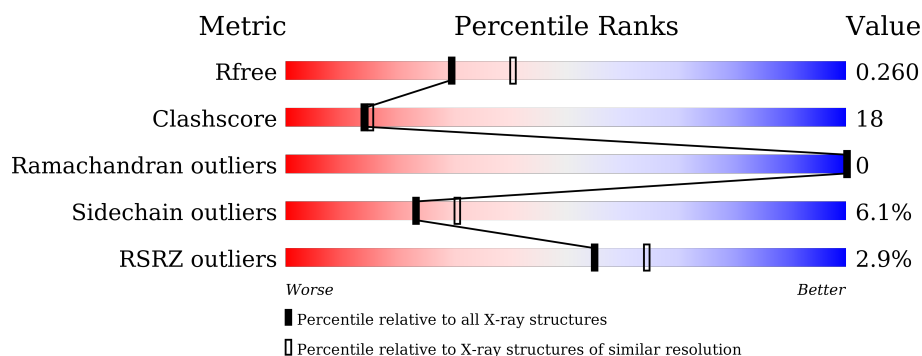
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 ≥ 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	232	
1	B	232	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3827 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1770	1114	310	334	12			
1	B	232	Total	C	N	O	S	0	0	0
			1854	1167	325	350	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		
2	B	122	Total	O	0	0
			122	122		

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 ($\text{RSRZ} > 2$). 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.

Chain A:

4% 56% 36%

THR LYS THR GLN G146 G146 F148 F148 T149 T149 E151 E151 M152 M152 T153 T153 L154 L154 L155 L155 G156 G156 Y157 Y157 I158 I158 A159 A159 D160 D160 D161 D161 L162 L162 S163 S163 K167 K167 E172 E172 I173 I173 N174 N174 L175 L175 S177 S177 C178 C178 D180 D180 M183 M183 C184 C184 S190 S190 N194 N194 L195 L195 L196 L196 S197 S197 K198 K198 E202 E202 M207 M207 V208 V208 Q209 Q209 V210 V210 F211 F211 L212 L212 S215 S215 A219 A219

W54 W54 N55 N55 S59 S59 L68 L68 R69 R69 Y72 Y72 W73 W73 Y74 Y74 W75 W75 W77 W77 W78 W78 Q79 Q79 R80 R80 E81 E81 L82 L82 G83 G83 D84 D84 R85 R85 D86 D86 C87 C87 Q88 Q88 R89 R89 I90 I90 K91 K91 K92 K92 A93 A93 F94 F94 S100 S100 E108 E108 L113 L113 L114 L114 M115 M115 Q120 Q120 T121 T121 V122 V122 P123 P123 C124 C124 D125 D125 K126 K126 F129 F129 W130 W130 S131 S131 K132 K132 T133 T133 R134 R134 K134 K134 E135 E135 LEU LEU HIS HIS GLN GLN THR THR

Chain B:

74% 24%

W54 N55 V61 D62 F63 Q64 Y74 V78 Q79 E81 D84 K92 A93 F94 T95 I99 M115 C124 D125 V128 F129 E135 L136 A137 H138 Q139 T140 T141 Q144 L147 F148 T149 L150 F151 M152 T153 L154 L155 S177 G178 P179 D180 N183 L196

S197 K198 E202 M207 Q208 Q209 L212 N213 I216 A219 F220 D221 K222 T223 L242 K243 A244 W245 R255 D256 T257 M264 Q267 L270 Q280 E281 Y282 Y283 R284 P285

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.54Å 103.86Å 63.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 24.53 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.30) 99.8 (24.53-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.261 0.207 , 0.260	Depositor DCC
R_{free} test set	1080 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3827	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.33	0/1805	0.60	0/2433
1	B	0.35	0/1893	0.59	0/2554
All	All	0.34	0/3698	0.60	0/4987

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	1770	0	1736	83	0
1	B	1854	0	1819	48	0
2	A	81	0	0	4	0
2	B	122	0	0	3	0
All	All	3827	0	3555	131	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 18.

The worst 5 of 131 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:226:PHE:O	1:A:231:VAL:HG23	1.65	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:HB2	1:A:126:LYS:HG3	1.49	0.93
1:B:149:THR:H	1:B:152:ASN:HD22	0.97	0.93
1:B:242:LEU:HD23	1:B:270:LEU:HD11	1.53	0.90
1:A:184:CYS:HB2	2:A:301:HOH:O	1.72	0.88

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	218/232 (94%)	206 (94%)	12 (6%)	0	100	100
1	B	230/232 (99%)	223 (97%)	7 (3%)	0	100	100
All	All	448/464 (97%)	429 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	200/209 (96%)	186 (93%)	14 (7%)	19	23
1	B	209/209 (100%)	198 (95%)	11 (5%)	28	37
All	All	409/418 (98%)	384 (94%)	25 (6%)	23	30

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

Mol	Chain	Res	Type
1	A	252	LYS
1	A	284	ARG
1	B	255	ARG
1	A	282	ASN
1	B	64	GLN

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

Mol	Chain	Res	Type
1	B	79	GLN
1	B	88	GLN
1	B	209	GLN
1	B	55	ASN
1	B	248	HIS

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	222/232 (95%)	0.05	10 (4%) 37 46	19, 41, 89, 116	0
1	B	232/232 (100%)	-0.31	3 (1%) 79 84	15, 32, 70, 94	0
All	All	454/464 (97%)	-0.13	13 (2%) 55 64	15, 36, 80, 116	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	LYS	5.9
1	A	133	THR	5.0
1	A	251	GLY	3.6
1	A	284	ARG	3.4
1	A	252	LYS	3.2

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 [i](#)

There are no such residues in this entry.