



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2O3Q
Title : Structural Basis for Formation and Hydrolysis of Calcium Messenger Cyclic ADP-ribose by Human CD38
Authors : Liu, Q.; Kriksunov, I.A.; Graeff, R.; Lee, H.C.; Hao, Q.
Deposited on : 2006-12-01
Resolution : 1.98 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 : 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

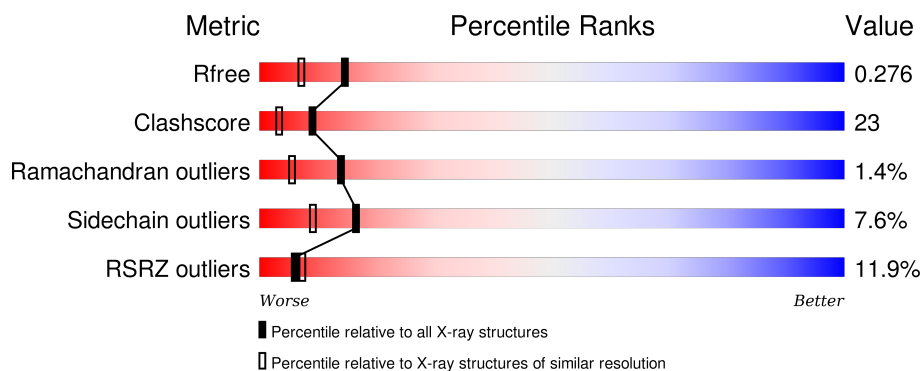
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	262	<div> <div>8%</div> <div>65%</div> <div>28%</div> <div>• •</div> </div>
1	B	262	<div> <div>15%</div> <div>47%</div> <div>39%</div> <div>8%</div> <div>• •</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	CXR	A	301	X	-	-	-
2	CXR	B	301	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4377 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
1	A	252	Total	C	N	O	S	0	0	0
			2008	1266	352	374	16			
1	B	252	Total	C	N	O	S	0	0	0
			2008	1266	352	374	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	CLONING ARTIFACT	UNP P28907
A	40	ARG	-	CLONING ARTIFACT	UNP P28907
A	41	GLU	-	CLONING ARTIFACT	UNP P28907
A	42	ALA	-	CLONING ARTIFACT	UNP P28907
A	43	GLU	-	CLONING ARTIFACT	UNP P28907
A	44	ALA	-	CLONING ARTIFACT	UNP P28907
A	49	THR	GLN	ENGINEERED	UNP P28907
A	100	ASP	ASN	ENGINEERED	UNP P28907
A	164	ASP	ASN	ENGINEERED	UNP P28907
A	209	ASP	ASN	ENGINEERED	UNP P28907
A	219	ASP	ASN	ENGINEERED	UNP P28907
A	226	GLN	GLU	ENGINEERED	UNP P28907
B	39	LYS	-	CLONING ARTIFACT	UNP P28907
B	40	ARG	-	CLONING ARTIFACT	UNP P28907
B	41	GLU	-	CLONING ARTIFACT	UNP P28907
B	42	ALA	-	CLONING ARTIFACT	UNP P28907
B	43	GLU	-	CLONING ARTIFACT	UNP P28907
B	44	ALA	-	CLONING ARTIFACT	UNP P28907
B	49	THR	GLN	ENGINEERED	UNP P28907
B	100	ASP	ASN	ENGINEERED	UNP P28907
B	164	ASP	ASN	ENGINEERED	UNP P28907
B	209	ASP	ASN	ENGINEERED	UNP P28907
B	219	ASP	ASN	ENGINEERED	UNP P28907
B	226	GLN	GLU	ENGINEERED	UNP P28907

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- ORTEP diagram of the molecular structure of 2,6-bis(4-hydroxyphenyl)-4-methylpyrimidin-5(1H)-one (CXR). The structure shows a central pyrimidin-2,6-dione core substituted with two 4-hydroxyphenyl groups and a methyl group. The thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as small spheres of arbitrary radii. The structure is labeled with atom names (C1-C10, N1-N3, O1-O4, H1-H10) and includes a title block with the compound name, formula, and other details.

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	157	Total O 157 157	0	0
3	B	134	Total O 134 134	0	0

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.

Chain A:

8% 65% 28%

LYS ARG GLU ALA GLU ALA R45 W46 R47 Q48 T85 T86 K57 R58 F59 P60 Y70 I73 H74 P75 E76 M77 R78 D81 C82 Q83 S84 V85 W86 F89 K90 I94 P98 Q107 M110 K111 T114 Q115 T116 V117 P118 C119 L123 W124 K129 D130 I131 F135 Q139 R140 D141 M142 F143 T144 L145 F146 D147 L148 L149 L150 D155 W159 E162 F163 D164 T165 S166 K167 G173 P174 D175 W176 R177 K178 S181 N182 N183 S186 V187 F188 W189 K190 R194 R195 F196 A199 V203 V204 D209 R212 S213 Q226 W227 L230 Q236 E239 H244 G245 E248 D249 S250 R251 K260 E263 S264 K268 R269 M270 N274 N277 L278 Y279 D282 L285 Q286 C287 N290 S294 C295 C296 THR SER GLU ILE

Chain B:

15% 47% 39% 8%

Chain B: LYS ARG GLU ALA GLU ALA R45 W46 R47 Q48 T49 K57 R58 F59 P60 E61 R66 Y70 T71 E72 I73 H74 P75 R78 C82 F89 K90 I94 S95 P98 C99 D100 I101 T102 E103 E104 Q107 P108 L109 M110 Q115 K121 I122 L123 L124 R127 I128 L131 Q134 F135 T136 Q137 V138 Q139 R140 D141 M142 F143 T144 F145 E146 D147 T148 L149 L150 G151 Y152 L153 A154 A155 D156 E162 F163 D164 T165 S166 K167 Q171 S172 D175 W176 K177 K178 D179 C180 N183 P184 V185 S186 W189 K190 T191 V192 R195 F196 A197 E198 C201 D202 V203 V204 H205 R206 V207 L208 D209 G210 S211 R212 S213 K214 L215 I216 F216 D217 K218 D219 S220 T221 F222 G223 Q226 V227 H228 N229 L230 Q231 P232 E233 K234 V235 Q236 T237 L238 E239 L243 H244 G245 G246 R247 E248 D249 S250 R251 D252 Q255 D256 P257 T258 T259 K260 E261 L262 E263 S264 T265 T266

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.94Å 53.28Å 65.92Å 105.89° 92.10° 94.81°	Depositor
Resolution (Å)	20.00 – 1.98 28.37 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.98) 81.8 (28.37-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.278 0.211 , 0.276	Depositor DCC
R_{free} test set	1713 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33824 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4377	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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](#)

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

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	1.43	16/2058 (0.8%)	1.25	17/2785 (0.6%)
1	B	1.59	36/2058 (1.7%)	1.21	13/2785 (0.5%)
All	All	1.51	52/4116 (1.3%)	1.23	30/5570 (0.5%)

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
1	B	0	1

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	GLU	C-O	11.62	1.45	1.23
1	B	296	CYS	C-O	11.43	1.45	1.23
1	B	263	GLU	CD-OE1	10.22	1.36	1.25
1	A	173	CYS	CB-SG	-10.14	1.65	1.82
1	B	263	GLU	CD-OE2	8.94	1.35	1.25

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	A	195	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	269	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	251	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	263	GLU	OE1-CD-OE2	7.29	132.05	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	164	ASP	Peptide

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	2008	0	1918	77	0
1	B	2008	0	1919	108	0
2	A	35	0	18	1	0
2	B	35	0	19	5	0
3	A	157	0	0	25	0
3	B	134	0	0	11	0
All	All	4377	0	3874	184	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 23.

The worst 5 of 184 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:B:104:GLU:HG3	3:B:423:HOH:O	1.38	1.20
1:A:78:ARG:HH11	1:A:78:ARG:HG3	1.06	1.16
1:A:176:TRP:HB3	3:A:351:HOH:O	1.53	1.08
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.20	1.08
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.36	1.05

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	250/262 (95%)	226 (90%)	22 (9%)	2 (1%)	24	14
1	B	250/262 (95%)	216 (86%)	29 (12%)	5 (2%)	9	3
All	All	500/524 (95%)	442 (88%)	51 (10%)	7 (1%)	14	5

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	SER
1	B	213	SER
1	B	249	ASP
1	A	294	SER
1	B	164	ASP

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	223/241 (92%)	214 (96%)	9 (4%)	38	31
1	B	223/241 (92%)	198 (89%)	25 (11%)	7	3
All	All	446/482 (92%)	412 (92%)	34 (8%)	16	9

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	LEU

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Mol	Chain	Res	Type
1	B	195	ARG
1	B	268	LYS
1	B	176	TRP
1	A	250	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	GLN
1	B	107	GLN
1	B	236	GLN
1	A	286	GLN
1	B	205	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](#)

2 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	CXR	A	301	-	28,39,39	4.07	14 (50%)	37,62,62	2.11	9 (24%)
2	CXR	B	301	-	28,39,39	3.36	11 (39%)	37,62,62	1.62	8 (21%)

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	CXR	A	301	-	1/1/10/10	0/18/58/58	0/0/5/5
2	CXR	B	301	-	1/1/10/10	0/18/58/58	0/0/5/5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CXR	O3D-C3D	-4.62	1.31	1.43
2	A	301	CXR	C5'-C4'	-4.30	1.37	1.51
2	A	301	CXR	C5D-C4D	-3.01	1.41	1.51
2	A	301	CXR	PB-O1B	-2.72	1.43	1.54
2	B	301	CXR	C2D-C3D	-2.23	1.47	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CXR	PA-O3A-PB	-5.54	117.18	132.73
2	A	301	CXR	C4-C5-N7	-5.16	104.74	109.48
2	A	301	CXR	C4'-O4'-C1'	-3.99	105.33	109.72
2	B	301	CXR	O4'-C1'-N9	-3.41	100.96	108.10
2	B	301	CXR	O2'-C2'-C3'	-3.28	101.16	111.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	CXR	C3'
2	B	301	CXR	C3'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CXR	1	0
2	B	301	CXR	5	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, 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	252/262 (96%)	0.62	20 (7%) 15 18	23, 33, 45, 53	0
1	B	252/262 (96%)	0.88	40 (15%) 3 3	21, 33, 46, 57	0
All	All	504/524 (96%)	0.75	60 (11%) 6 7	21, 33, 46, 57	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	7.4
1	B	294	SER	6.8
1	B	246	GLY	6.6
1	B	249	ASP	6.3
1	A	296	CYS	5.6

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 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, 95th 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(\AA^2)	Q<0.9
2	CXR	B	301	35/35	0.85	0.18	0.43	23,44,59,62	0
2	CXR	A	301	35/35	0.93	0.12	-1.00	21,29,43,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.