



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:10 AM GMT

PDB ID : 3U4I
Title : CD38 structure-based inhibitor design using the N1-cyclic inosine 5'-diphosphate ribose template
Authors : Liu, Q.; Hao, Q.; Lee, H.C.; Graeff, R.
Deposited on : 2011-10-08
Resolution : 2.12 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

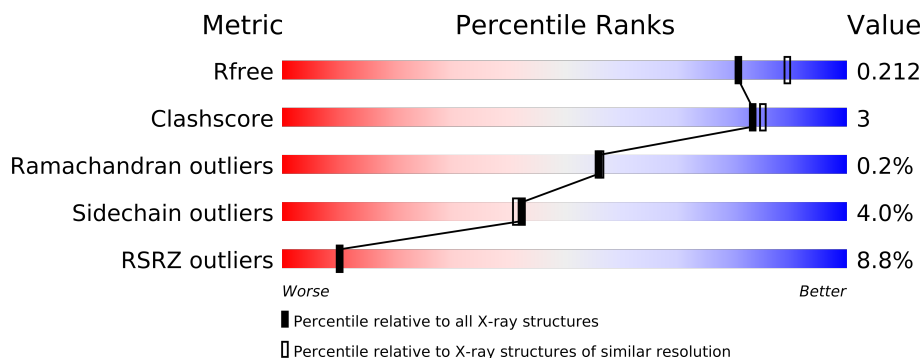
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.12 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}	66092	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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. 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	262	
1	B	262	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4161 atoms, of which 0 are hydrogen 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.

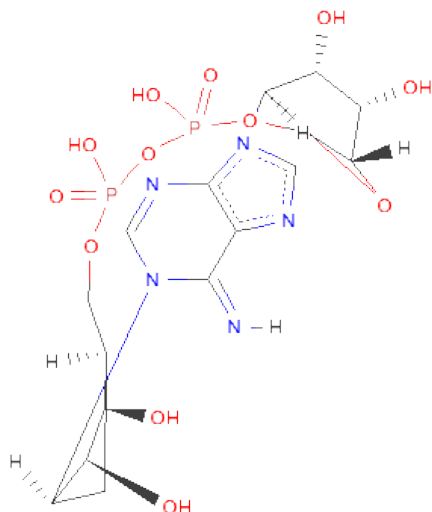
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			2014	1271	350	377	16			
1	B	240	Total	C	N	O	S	0	0	0
			1964	1244	342	363	15			

There are 22 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is CYCLIC ADENOSINE 5'-DIPHOSPHOCARBOCYCLICRIBOSE (three-letter code: CVR) (formula: C₁₆H₂₃N₅O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	16	5	12	2		

- Molecule 3 is water.

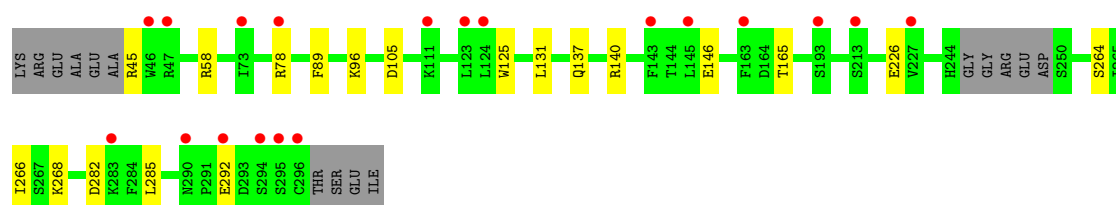
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	74	Total O 74 74	0	0
3	B	74	Total O 74 74	0	0

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.

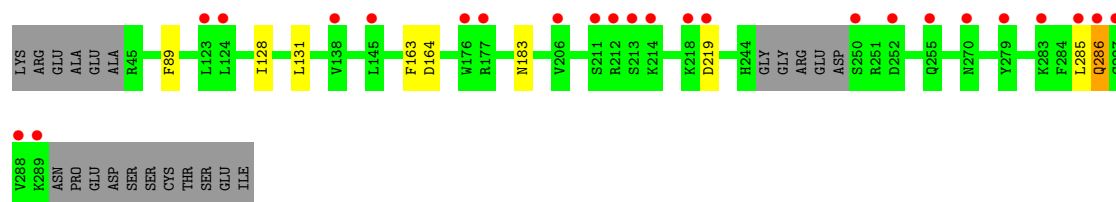
• Molecule 1: ADP-ribosyl cyclase 1

Chain A: 



• Molecule 1: ADP-ribosyl cyclase 1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.22Å 54.00Å 66.55Å 105.20° 91.08° 94.68°	Depositor
Resolution (Å)	23.43 – 2.12 28.56 – 2.12	Depositor EDS
% Data completeness (in resolution range)	95.8 (23.43-2.12) 95.8 (28.56-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.289)	Depositor
R, R_{free}	0.179 , 0.217 0.174 , 0.212	Depositor DCC
R_{free} test set	1550 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30775 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4161	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: CVR

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	0.37	0/2064	0.48	0/2796
1	B	0.37	0/2013	0.48	0/2726
All	All	0.37	0/4077	0.48	0/5522

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	2014	0	0	7	0
1	B	1964	0	0	3	0
2	A	35	0	19	7	0
3	A	74	0	0	1	0
3	B	74	0	0	0	0
All	All	4161	0	19	12	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 3.

All (12) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:264:SER:OG	1:B:163:PHE:CZ	2.57	0.57
2:A:401:CVR:N6	2:A:401:CVR:H2D	2.20	0.56
1:A:146:GLU:OE2	2:A:401:CVR:N6	2.41	0.54
1:A:226:GLU:OE1	2:A:401:CVR:H4D	2.09	0.51
2:A:401:CVR:N7	3:A:574:HOH:O	2.34	0.51
2:A:401:CVR:N3	2:A:401:CVR:H2'	2.28	0.48
2:A:401:CVR:H2	2:A:401:CVR:H4XA	1.31	0.45
1:A:96:LYS:NZ	1:A:105:ASP:OD1	2.49	0.45
1:A:268:LYS:CD	1:B:163:PHE:CE1	3.03	0.41
1:A:125:TRP:N	2:A:401:CVR:HO3D	2.17	0.41
1:A:282:ASP:N	1:A:282:ASP:OD1	2.53	0.41
1:B:286:GLN:NE2	1:B:286:GLN:CA	2.85	0.40

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	243/262 (93%)	233 (96%)	10 (4%)	0	100	100
1	B	236/262 (90%)	227 (96%)	8 (3%)	1 (0%)	43	39
All	All	479/524 (91%)	460 (96%)	18 (4%)	1 (0%)	56	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	ILE

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	230/241 (95%)	219 (95%)	11 (5%)	35	32
1	B	223/241 (92%)	216 (97%)	7 (3%)	52	54
All	All	453/482 (94%)	435 (96%)	18 (4%)	42	41

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	58	ARG
1	A	78	ARG
1	A	89	PHE
1	A	131	LEU
1	A	137	GLN
1	A	140	ARG
1	A	165	THR
1	A	266	ILE
1	A	285	LEU
1	A	292	GLU
1	B	89	PHE
1	B	131	LEU
1	B	164	ASP
1	B	183	ASN
1	B	219	ASP
1	B	285	LEU
1	B	286	GLN

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	CVR	A	401	-	39,39,39	2.28	12 (30%)	60,62,62	1.91	13 (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	CVR	A	401	-	-	0/23/58/58	0/0/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CVR	C3'-C2'	-7.66	1.32	1.53
2	A	401	CVR	C4X-C1D	-5.26	1.33	1.54
2	A	401	CVR	O2'-C2'	-4.19	1.32	1.43
2	A	401	CVR	O3'-C3'	-3.92	1.33	1.43
2	A	401	CVR	C6-C5	3.51	1.48	1.39
2	A	401	CVR	C5-C4	3.46	1.48	1.40
2	A	401	CVR	C1D-N1	-3.20	1.39	1.50
2	A	401	CVR	C2-N3	2.80	1.35	1.30
2	A	401	CVR	C6-N1	2.59	1.41	1.38
2	A	401	CVR	C2'-C1'	-2.50	1.49	1.53
2	A	401	CVR	C6-N6	2.07	1.35	1.28
2	A	401	CVR	C4-N9	-2.06	1.34	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	CVR	C2D-C1D-N1	5.94	123.83	112.93
2	A	401	CVR	N3-C4-N9	5.52	135.41	125.43
2	A	401	CVR	C3'-C2'-C1'	4.78	108.39	100.91
2	A	401	CVR	O4'-C1'-N9	3.70	111.88	108.44
2	A	401	CVR	C4-C5-N7	-3.60	106.44	109.52
2	A	401	CVR	C5-C4-N3	-3.45	118.18	125.70
2	A	401	CVR	C2'-C3'-C4'	3.43	109.48	102.65
2	A	401	CVR	C2-N3-C4	2.95	121.27	116.23
2	A	401	CVR	C6-N1-C1D	2.71	124.05	121.06
2	A	401	CVR	PB-O3A-PA	-2.47	124.43	131.68
2	A	401	CVR	C4D-C4X-C1D	2.44	111.49	102.12
2	A	401	CVR	O4'-C1'-C2'	-2.40	103.09	106.77
2	A	401	CVR	C4X-C1D-C2D	2.10	107.04	104.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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 ⓘ

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, 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	247/262 (94%)	0.29	19 (7%) 13 14	22, 44, 81, 123	0
1	B	240/262 (91%)	0.49	24 (10%) 8 8	20, 52, 105, 126	0
All	All	487/524 (92%)	0.39	43 (8%) 10 10	20, 47, 98, 126	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	ARG	7.9
1	B	213	SER	6.0
1	A	46	TRP	4.6
1	B	287	CYS	4.5
1	B	250	SER	4.2
1	A	292	GLU	4.1
1	B	289	LYS	3.9
1	B	214	LYS	3.6
1	B	288	VAL	3.6
1	B	219	ASP	3.4
1	B	270	ASN	3.4
1	B	212	ARG	3.2
1	A	78	ARG	3.2
1	B	124	LEU	3.1
1	A	294	SER	3.1
1	B	285	LEU	3.1
1	B	211	SER	3.0
1	A	124	LEU	2.8
1	B	252	ASP	2.8
1	A	145	LEU	2.8
1	B	145	LEU	2.8
1	B	279	TYR	2.8
1	B	286	GLN	2.8
1	B	176	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	138	VAL	2.7
1	B	218	LYS	2.6
1	A	123	LEU	2.6
1	A	295	SER	2.6
1	A	111	LYS	2.5
1	A	213	SER	2.4
1	A	73	ILE	2.3
1	A	296	CYS	2.2
1	A	143	PHE	2.2
1	A	290	ASN	2.2
1	B	177	ARG	2.2
1	A	283	LYS	2.2
1	A	227	VAL	2.1
1	B	255	GLN	2.1
1	B	283	LYS	2.1
1	A	163	PHE	2.1
1	B	206	VAL	2.1
1	B	123	LEU	2.1
1	A	193	SER	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CVR	A	401	35/35	0.17	-0.05	39,66,86,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.