



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:30 PM UTC

PDB ID : 9C68 / pdb_00009c68
Title : The CRISPR associated CARF-adenosine deaminase Cad1-CARF in the cA6 bound form
Authors : Majumder, P.; Patel, D.J.
Deposited on : 2024-06-07
Resolution : 1.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

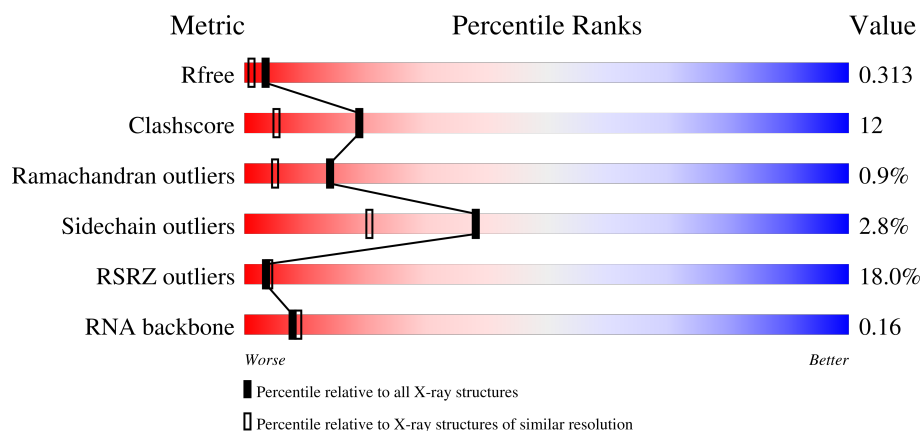
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)
RNA backbone	3983	1006 (2.22-1.42)

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 ≥ 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	A	185	18% 66% 20% • 13%
1	B	185	13% 69% 21% 10%
2	C	6	33% 17% 17% 50% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2809 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 Adenosine deaminase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1288	830	213	236	9			
1	B	167	Total	C	N	O	S	0	0	0
			1340	865	224	242	9			

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	6	0
			132	60	30	36	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	22	Total	O	0	0
			22	22		
3	C	8	Total	O	0	0
			8	8		

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.92Å 85.92Å 188.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.96 – 1.82 42.96 – 1.82	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.96-1.82) 100.0 (42.96-1.82)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.82Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.268 , 0.312 0.270 , 0.313	Depositor DCC
R_{free} test set	1902 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2809	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.333 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	A	0.46	0/1324	0.82	2/1794 (0.1%)
1	B	0.40	0/1378	0.66	0/1867
2	C	0.47	0/149	1.14	1/230 (0.4%)
All	All	0.43	0/2851	0.77	3/3891 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ILE	CA-C-N	-5.74	111.10	121.14
1	A	134	ILE	C-N-CA	-5.74	111.10	121.14
2	C	5[A]	A	P-O3'-C3'	-5.56	111.86	120.20

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	A	1288	0	1232	29	1
1	B	1340	0	1301	30	0
2	C	132	0	67	10	0
3	A	19	0	0	2	0
3	B	22	0	0	4	0
3	C	8	0	0	1	0
All	All	2809	0	2600	63	1

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 12.

All (63) 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:114:ALA:HB1	3:B:209:HOH:O	1.84	0.77
1:B:71:GLU:O	1:B:75:GLU:HG3	1.90	0.70
1:A:117:PHE:O	1:A:160:LEU:HD11	1.92	0.70
1:A:69:LEU:H	1:A:74:PHE:HD2	1.38	0.69
1:B:154:GLU:HG3	3:B:209:HOH:O	1.93	0.67
1:A:157:TRP:C	3:A:201:HOH:O	2.38	0.67
1:B:62:CYS:HB3	3:B:203:HOH:O	1.97	0.65
1:B:28:GLU:N	1:B:28:GLU:OE2	2.30	0.65
1:A:83:GLN:O	1:A:87:THR:HG23	1.97	0.64
1:B:72:ARG:HD3	1:B:72:ARG:C	2.24	0.62
1:B:57:PHE:CZ	1:B:59:ILE:HD11	2.36	0.60
1:B:119:ALA:HB3	3:B:209:HOH:O	2.01	0.59
1:A:56:ARG:HA	1:A:56:ARG:HH11	1.68	0.59
1:A:158:ALA:HB1	1:A:161:ARG:HH11	1.68	0.57
1:A:140:ALA:HB1	1:A:145:GLN:HB2	1.85	0.57
2:C:1[A]:A:P	2:C:6[A]:A:O3'	2.64	0.56
1:B:143:LYS:HB2	1:B:145:GLN:HG3	1.88	0.55
1:A:73:ASP:N	1:A:78:GLN:H	2.05	0.54
1:A:128:ASP:OD2	1:A:145:GLN:NE2	2.40	0.54
1:B:3:ARG:NH2	1:B:25:GLU:OE1	2.41	0.54
1:A:127:ALA:C	2:C:3[A]:A:H2	2.16	0.53
1:A:160:LEU:HD13	3:A:201:HOH:O	2.09	0.53
1:B:111:GLN:O	1:B:115:THR:HG23	2.09	0.52
1:B:133:ASN:OD1	1:B:135:GLU:N	2.41	0.52
1:B:126:LEU:HD11	2:C:6[A]:A:H5''	1.92	0.51
1:A:102:GLY:HA3	1:A:106:MET:HG3	1.92	0.51
1:B:36:ASP:HB3	1:B:61:LYS:HD2	1.94	0.50
2:C:3[A]:A:H8	3:C:102:HOH:O	1.94	0.50
2:C:2[A]:A:H2'	2:C:2[A]:A:N3	2.26	0.49
1:A:70:ASN:O	1:A:74:PHE:HA	2.12	0.49
1:A:34:THR:HG23	1:A:35:THR:O	2.12	0.49
1:A:65:LEU:HD21	1:A:74:PHE:HB3	1.95	0.47
1:B:138:PHE:HD1	1:B:141:LEU:HD11	1.80	0.47
1:A:74:PHE:CD1	1:A:74:PHE:O	2.69	0.46
1:B:126:LEU:CD1	2:C:6[A]:A:H5''	2.46	0.46
1:B:138:PHE:O	1:B:141:LEU:HD12	2.16	0.45
2:C:5[A]:A:H2'	2:C:5[A]:A:N3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:HA	1:B:61:LYS:HD2	1.99	0.45
1:A:157:TRP:HB3	1:A:158:ALA:H	1.57	0.44
1:A:3:ARG:HH21	1:A:23:VAL:HG21	1.81	0.44
1:A:65:LEU:CD2	1:A:74:PHE:HB3	2.47	0.44
1:A:16:VAL:HB	1:A:17:PRO:HD3	1.99	0.44
1:A:163:LEU:HD23	1:A:163:LEU:H	1.83	0.44
1:B:137:MET:O	1:B:141:LEU:HG	2.18	0.44
1:A:23:VAL:HG23	1:A:26:GLY:H	1.82	0.43
1:A:162:ARG:HD2	1:A:163:LEU:N	2.34	0.43
1:A:158:ALA:HB1	1:A:161:ARG:NH1	2.32	0.43
1:B:3:ARG:HB2	1:B:28:GLU:OE2	2.19	0.43
1:B:16:VAL:HB	1:B:17:PRO:HD3	2.01	0.43
2:C:6[A]:A:N3	2:C:6[A]:A:H2'	2.34	0.43
1:B:82:TRP:CZ2	1:B:112:LYS:HG2	2.54	0.43
1:A:56:ARG:HA	1:A:56:ARG:HD2	1.64	0.42
1:B:34:THR:HG23	1:B:35:THR:O	2.19	0.42
1:B:163:LEU:O	1:B:166:ILE:HG12	2.20	0.42
1:B:127:ALA:C	2:C:6[A]:A:H2	2.27	0.42
1:A:162:ARG:HD2	1:A:163:LEU:HG	2.03	0.41
1:B:57:PHE:HZ	1:B:59:ILE:HD11	1.84	0.41
1:A:14:MET:HE3	1:A:14:MET:HB3	1.82	0.41
1:A:104:LYS:HD2	1:B:107:SER:OG	2.21	0.41
1:B:126:LEU:HG	2:C:6[A]:A:H5''	2.03	0.41
1:B:138:PHE:HA	1:B:141:LEU:HD11	2.01	0.41
1:A:69:LEU:N	1:A:74:PHE:HD2	2.12	0.40
1:B:145:GLN:C	1:B:146:ILE:HD13	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLU:OE2	1:A:142:GLN:NE2[8_555]	1.99	0.21

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	157/185 (85%)	149 (95%)	6 (4%)	2 (1%)	9	2
1	B	165/185 (89%)	162 (98%)	2 (1%)	1 (1%)	21	11
All	All	322/370 (87%)	311 (97%)	8 (2%)	3 (1%)	14	5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	68	ILE
1	B	93	GLU

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	140/163 (86%)	135 (96%)	5 (4%)	31	13
1	B	146/163 (90%)	143 (98%)	3 (2%)	47	32
All	All	286/326 (88%)	278 (97%)	8 (3%)	38	21

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	6	LEU
1	A	87	THR
1	A	91	ASP
1	A	163	LEU
1	B	23	VAL
1	B	97	VAL
1	B	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	145	GLN
1	B	46	ASN
1	B	78	GLN
1	B	120	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	5/6 (83%)	4 (80%)	1 (20%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2[A]	A
2	C	3[A]	A
2	C	5[A]	A
2	C	6[A]	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	2[A]	A

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 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

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	161/185 (87%)	1.41	34 (21%) 2 2	30, 41, 58, 69	0
1	B	167/185 (90%)	1.18	24 (14%) 6 6	33, 42, 61, 70	0
2	C	6/6 (100%)	0.94	2 (33%) 1 1	36, 37, 41, 44	0
All	All	334/376 (88%)	1.28	60 (17%) 3 4	30, 41, 59, 70	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	9.1
1	A	74	PHE	6.5
1	A	158	ALA	6.3
1	A	75	GLU	5.9
1	A	162	ARG	5.7
1	A	73	ASP	5.2
1	B	141	LEU	4.7
1	B	2	SER	4.7
1	A	70	ASN	4.6
1	A	76	PHE	4.5
1	A	2	SER	4.2
1	B	146	ILE	3.8
1	A	63	HIS	3.5
1	B	56	ARG	3.3
1	A	54	ASN	3.2
1	B	40	PHE	3.1
1	B	92	ASN	3.1
1	A	67	ASP	3.1
1	A	44	VAL	3.1
1	B	168	PRO	3.1
1	A	146	ILE	2.9
1	A	64	GLY	2.9
1	B	133	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	142	GLN	2.8
1	A	142	GLN	2.8
1	A	68	ILE	2.8
1	B	63	HIS	2.8
1	A	83	GLN	2.7
1	B	69	LEU	2.7
1	A	139	ASP	2.7
1	A	161	ARG	2.7
1	B	159	ALA	2.7
1	A	157	TRP	2.7
1	A	55	VAL	2.7
1	A	23	VAL	2.6
1	B	38	GLU	2.6
2	C	6[A]	A	2.5
1	A	159	ALA	2.5
1	B	23	VAL	2.5
1	B	50	HIS	2.5
1	A	135	GLU	2.5
1	B	129	ASN	2.5
1	A	3	ARG	2.5
1	A	56	ARG	2.5
1	A	71	GLU	2.4
1	A	50	HIS	2.4
1	A	82	TRP	2.3
1	B	134	ILE	2.2
1	A	145	GLN	2.2
1	A	92	ASN	2.2
1	A	93	GLU	2.2
1	A	134	ILE	2.2
1	B	139	ASP	2.1
2	C	3[A]	A	2.1
1	B	25	GLU	2.1
1	B	41	ASN	2.0
1	B	152	GLY	2.0
1	B	3	ARG	2.0
1	B	55	VAL	2.0
1	B	125	VAL	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 [i](#)

There are no oligosaccharides 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.