



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2017 – 08:17 AM EDT

PDB ID : 5NNL
Title : Inactive dihydroorotase-like domain of Chaetomium thermophilum CAD-like multifunctional protein
Authors : Ramon-Maiques, S.; Moreno-Morcillo, M.; Grande-Garcia, A.
Deposited on : 2017-04-10
Resolution : 2.13 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029077

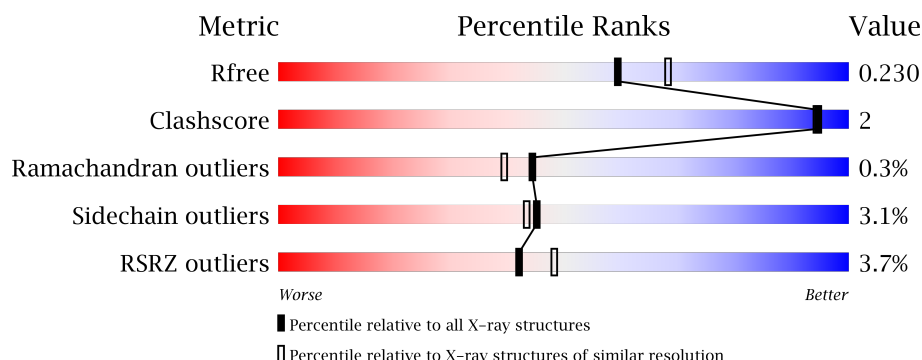
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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	342	<div> <div>4%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	B	342	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10733 atoms, of which 5294 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 Inactive dihydroorotase-like domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	H	N	O	S	0	6	0
			5284	1674	2659	446	496	9			
1	B	342	Total	C	H	N	O	S	0	1	0
			5250	1667	2635	444	495	9			

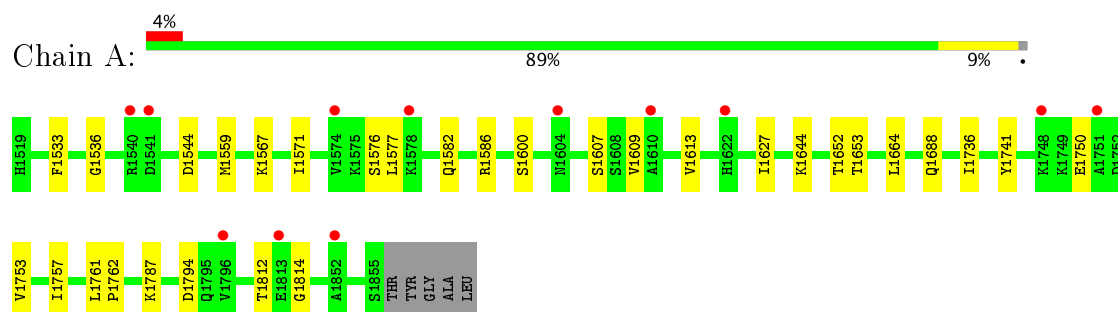
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	112	Total	O	0	0
			112	112		
2	B	87	Total	O	0	0
			87	87		

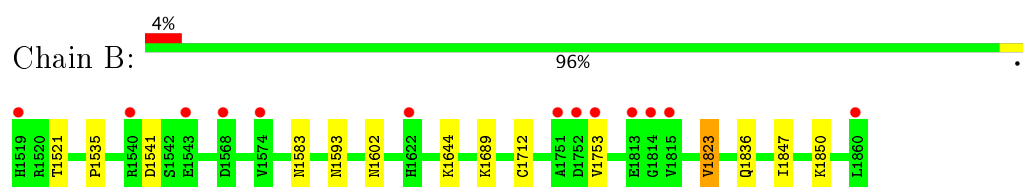
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Inactive dihydroorotase-like domain



- Molecule 1: Inactive dihydroorotase-like domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.77Å 109.18Å 58.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.81 – 2.13 45.81 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.81-2.13) 98.5 (45.81-2.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.199 , 0.232 0.196 , 0.230	Depositor DCC
R_{free} test set	1736 reflections (4.80%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10733	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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	0.27	0/2695	0.46	0/3667
1	B	0.26	0/2671	0.47	2/3640 (0.1%)
All	All	0.27	0/5366	0.46	2/7307 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1823	VAL	CG1-CB-CG2	6.37	121.09	110.90
1	B	1823	VAL	CA-CB-CG1	5.19	118.69	110.90

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	2625	2659	2666	12	0
1	B	2615	2635	2627	5	0
2	A	112	0	0	1	0
2	B	87	0	0	2	0
All	All	5439	5294	5293	16	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 2.

All (16) 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:1613:VAL:O	1:A:1644:LYS:NZ	2.23	0.72
1:B:1535:PRO:HD2	1:B:1753:VAL:HG23	1.82	0.62
1:A:1533:PHE:O	2:A:1901:HOH:O	2.17	0.57
1:A:1609:VAL:HG12	1:A:1609:VAL:O	2.12	0.50
1:B:1593:ASN:ND2	2:B:1905:HOH:O	2.34	0.50
1:A:1571:ILE:HA	1:A:1576:SER:HB3	1.98	0.46
1:A:1536:GLY:N	1:A:1544:ASP:OD2	2.46	0.45
1:B:1583:ASN:O	2:B:1901:HOH:O	2.21	0.45
1:A:1736:ILE:HD13	1:A:1757:ILE:HA	1.99	0.44
1:A:1567:LYS:HD2	1:A:1741:TYR:OH	2.18	0.44
1:A:1787:LYS:NZ	1:A:1794:ASP:OD1	2.42	0.44
1:A:1577:LEU:CD2	1:A:1609:VAL:HG11	2.48	0.43
1:B:1535:PRO:CD	1:B:1753:VAL:HG23	2.49	0.42
1:A:1761:LEU:HB3	1:A:1762:PRO:HD3	2.02	0.42
1:A:1652:THR:OG1	1:A:1653:THR:N	2.54	0.41
1:A:1664:LEU:O	1:B:1689:LYS:HE2	2.21	0.41

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	341/342 (100%)	328 (96%)	12 (4%)	1 (0%)	44	39
1	B	341/342 (100%)	331 (97%)	9 (3%)	1 (0%)	44	39
All	All	682/684 (100%)	659 (97%)	21 (3%)	2 (0%)	44	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1814	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1712	CYS

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	296/294 (101%)	285 (96%)	11 (4%)	39	36
1	B	290/294 (99%)	282 (97%)	8 (3%)	49	48
All	All	586/588 (100%)	567 (97%)	19 (3%)	45	42

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1559	MET
1	A	1582	GLN
1	A	1586	ARG
1	A	1600	SER
1	A	1607	SER
1	A	1627	ILE
1	A	1688	GLN
1	A	1750[A]	GLU
1	A	1750[B]	GLU
1	A	1753	VAL
1	A	1812	THR
1	B	1521	THR
1	B	1541	ASP
1	B	1602	ASN
1	B	1644	LYS
1	B	1823	VAL
1	B	1836	GLN
1	B	1847	ILE
1	B	1850	LYS

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 ⓘ

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	337/342 (98%)	0.44	12 (3%)	43	50	26, 38, 56, 65	0
1	B	342/342 (100%)	0.46	13 (3%)	41	47	27, 42, 63, 73	0
All	All	679/684 (99%)	0.45	25 (3%)	42	48	26, 40, 60, 73	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1751	ALA	5.9
1	B	1622	HIS	4.2
1	B	1751	ALA	3.7
1	B	1814	GLY	3.6
1	B	1568	ASP	3.4
1	B	1540	ARG	3.1
1	B	1815	VAL	3.0
1	A	1604[A]	ASN	2.8
1	B	1753	VAL	2.8
1	A	1622	HIS	2.6
1	B	1519	HIS	2.6
1	A	1578	LYS	2.5
1	A	1852	ALA	2.4
1	A	1541	ASP	2.4
1	B	1543	GLU	2.3
1	A	1796	VAL	2.3
1	B	1752	ASP	2.3
1	A	1540	ARG	2.2
1	B	1813	GLU	2.2
1	B	1860	LEU	2.1
1	A	1574	VAL	2.1
1	B	1574	VAL	2.1
1	A	1610	ALA	2.1
1	A	1813	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1748	LYS	2.0

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.