wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:54 PM GMT

PDB ID : 1MND
Title : TRUNCATED HEAD OF MYOSIN FROM DICTYOSTELIUM DISCOIDEUM COMPLEXED WITH MGADP-ALF4
Authors : Smith, C.A.; Rayment, I.
Deposited on : 1995-04-15
Resolution : 2.60 Å(reported)

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) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Clashscore		74
Ramachandran outliers		3.0%
Sidechain outliers		27.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
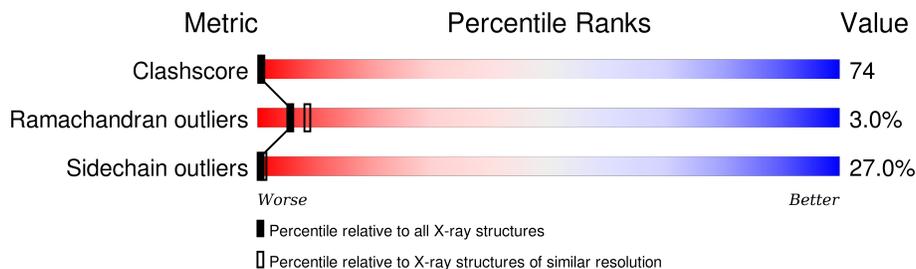
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	762	17% 45% 19% • 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5141 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	641	5005	3181	856	953	15	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASP	LYS	CONFLICT	UNP P08799
A	312	CYS	TYR	CONFLICT	UNP P08799
A	321	GLU	SER	CONFLICT	UNP P08799
A	322	ASP	GLU	CONFLICT	UNP P08799
A	443	SER	GLN	CONFLICT	UNP P08799
A	446	ALA	LYS	CONFLICT	UNP P08799
A	489	VAL	LEU	CONFLICT	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).
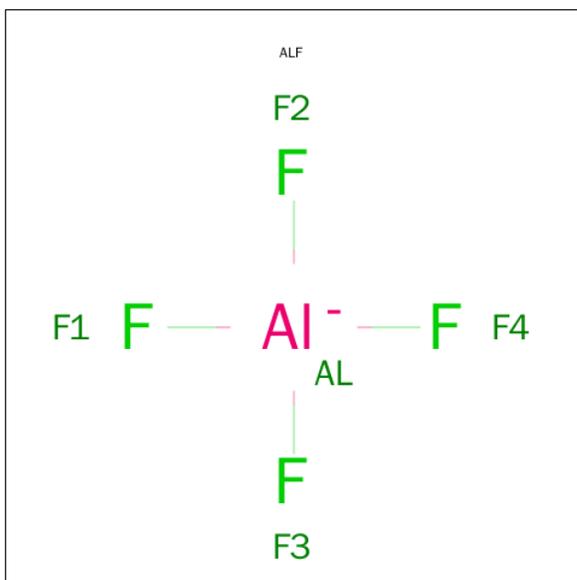
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	Al 1	F 4	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
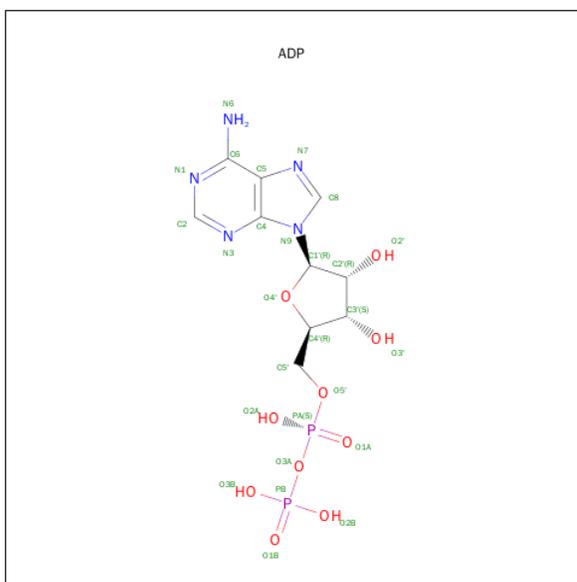
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total 103	O 103	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.

Note EDS was not executed.

• Molecule 1: MYOSIN
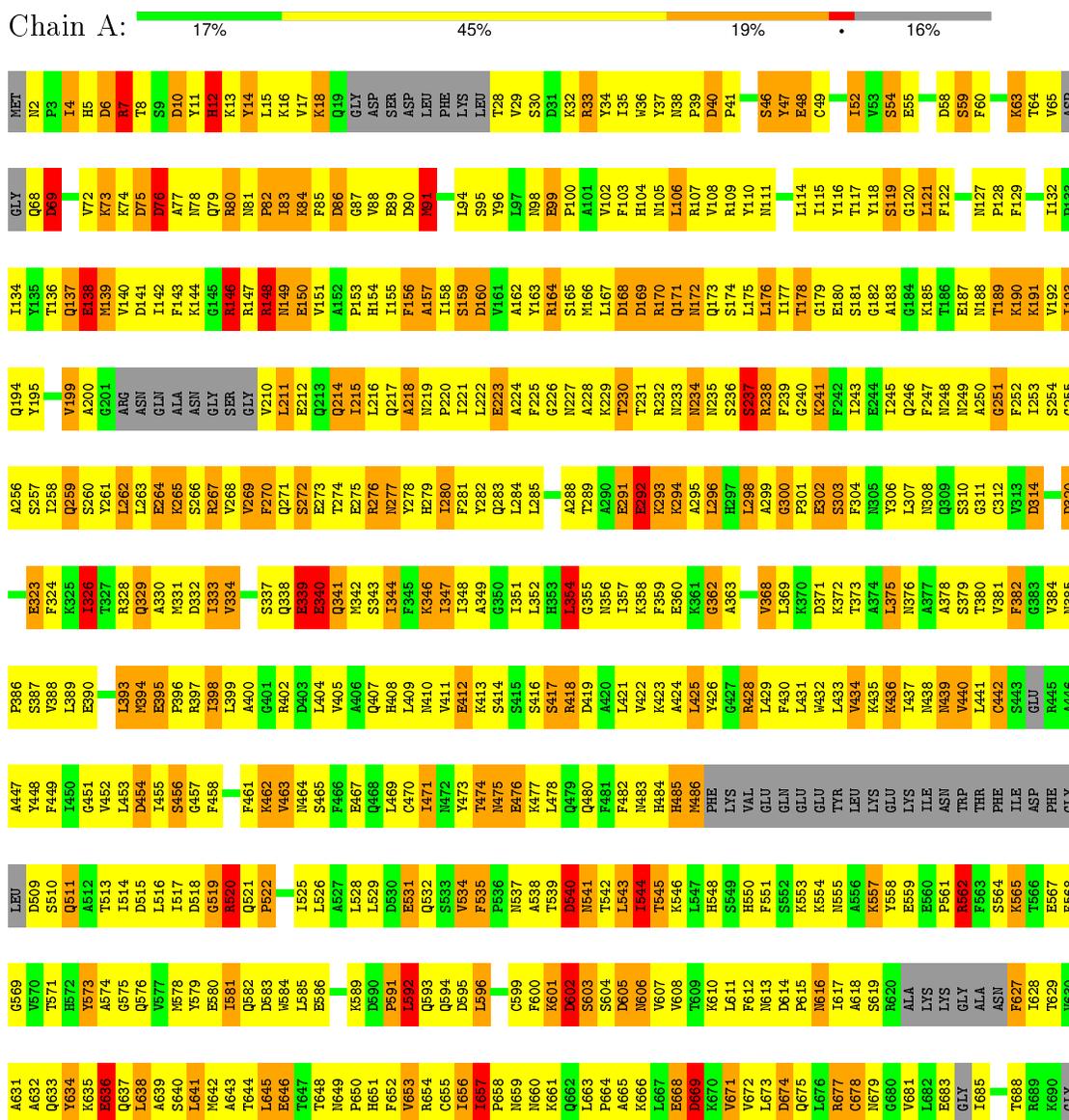
PHE PRO ASN ARG ILE ILE TYR ALA ASP PHE VAL LYS ARG TYR LEU LEU ALA PRO ASN VAL PRO ARG ASP ALA GLU ASP SER GLN LYS ALA THR ASP ALA VAL LEU LYS HIS LEU ASN ILE ASP PRO GLU GLN TYR ARG PHE GLY ILE THR LYS ILE PHE PHE ARG ALA GLY GLN LEU

ALA ARG ILE GLU GLU ALA ARG GLU LEU PRO ASN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.90Å 149.00Å 153.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5141	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

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: ALF, MG, ADP

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	1.00	19/5096 (0.4%)	1.43	64/6889 (0.9%)

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	A	3	5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	MET	CA-C	-8.48	1.30	1.52
1	A	646	GLU	CD-OE2	6.95	1.33	1.25
1	A	412	GLU	CD-OE2	6.48	1.32	1.25
1	A	390	GLU	CD-OE2	6.32	1.32	1.25
1	A	323	GLU	CD-OE2	6.25	1.32	1.25

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	442	CYS	CA-CB-SG	17.81	146.06	114.00
1	A	677	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	14	TYR	CB-CG-CD2	-8.44	115.94	121.00
1	A	69	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	A	238	ARG	NE-CZ-NH2	8.07	124.34	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	169	ASP	CA
1	A	534	VAL	CA
1	A	613	ASN	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	ILE	Mainchain
1	A	354	LEU	Mainchain
1	A	540	ASP	Mainchain
1	A	544	ILE	Mainchain
1	A	596	LEU	Mainchain

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	5005	0	4841	730	0
2	A	1	0	0	0	0
3	A	5	0	0	1	0
4	A	27	0	12	5	0
5	A	103	0	0	21	0
All	All	5141	0	4853	731	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 74.

The worst 5 of 731 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:614:ASP:HB3	1:A:617:ILE:CB	1.72	1.19
1:A:279:HIS:CE1	5:A:1002:HOH:O	1.98	1.16
1:A:285:LEU:HD21	1:A:298:LEU:HG	1.26	1.15
1:A:561:PRO:HG3	1:A:567:GLU:O	1.47	1.13
1:A:268:VAL:HA	1:A:277:ASN:HD21	1.14	1.12

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	625/762 (82%)	510 (82%)	96 (15%)	19 (3%)	5	8

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
1	A	669	ASP
1	A	86	ASP
1	A	300	GLY
1	A	362	GLY

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	530/665 (80%)	387 (73%)	143 (27%)	0	1

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	LYS
1	A	346	LYS
1	A	627	PHE
1	A	296	LEU
1	A	326	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	HIS
1	A	329	GLN
1	A	606	ASN
1	A	283	GLN
1	A	305	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#|Z| > 2$
4	ADP	A	998	3,2	22,29,29	0.86	1 (4%)	27,45,45	1.09	2 (7%)
3	ALF	A	999	2,5,4	0,4,4	0.00	-	0,6,6	0.00	-

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
4	ADP	A	998	3,2	-	0/12/32/32	0/3/3/3
3	ALF	A	999	2,5,4	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	998	ADP	O4'-C1'	-2.15	1.38	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	998	ADP	O3'-C3'-C2'	2.42	119.71	111.83
4	A	998	ADP	O3A-PA-O5'	2.85	110.51	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	998	ADP	5	0
3	A	999	ALF	1	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)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.