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wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:45 am BST

PDB ID	:	2Y9E
Title	:	Structural basis for the allosteric interference of myosin function by mutants G680A and G680V of Dictyostelium myosin-2
Authors	:	Preller, M.; Bauer, S.; Adamek, N.; Fujita-Becker, S.; Fedorov, R.; Geeves, M.A.; Manstein, D.J.
Deposited on	:	2011-02-14
Resolution	:	3.40 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
https://www.wwpdb.org/validation/2017/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:

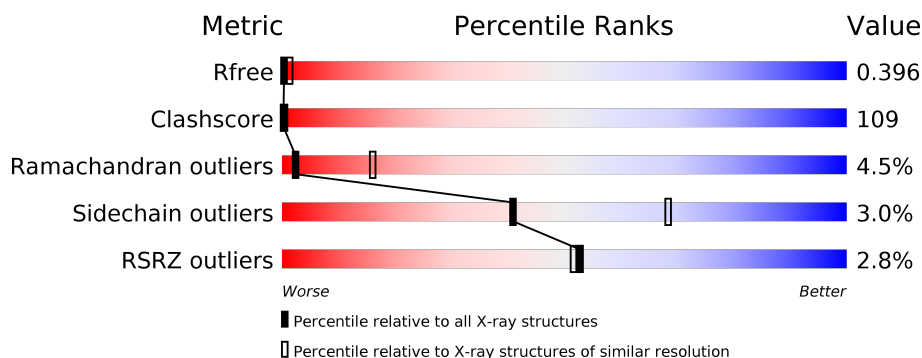|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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
Rfree		0.396
Clashscore		109
Ramachandran outliers		4.5%
Sidechain outliers		3.0%
RSRZ outliers		2.8%

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))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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 <=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	X	758	3% 19% 67% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6348 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	758	Total 6092	C 3870	N 1053	O 1153	S 16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	680	VAL	GLY	engineered mutation	UNP P08799

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	256	Total 256	O 256	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 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: MYOSIN-2

Chain X:

I697 Y698 A699 D700 F701 V702 K703 R704 Y705 Y706 L707 L708 A709 P710 N711 V712 P713 R714 D715 A716 E717 D718 S719 Q720 K721 A722 T723 D724 A725 V726 L727 K728 H729 L730 N731 I732 D733 P734 E735 Q736 Y737 G740 I741 T742 K743 I744 F745 F746 R747 A748 G749 Q750 L751 A752 R753 I754 E755 E756 A757

R758 E759
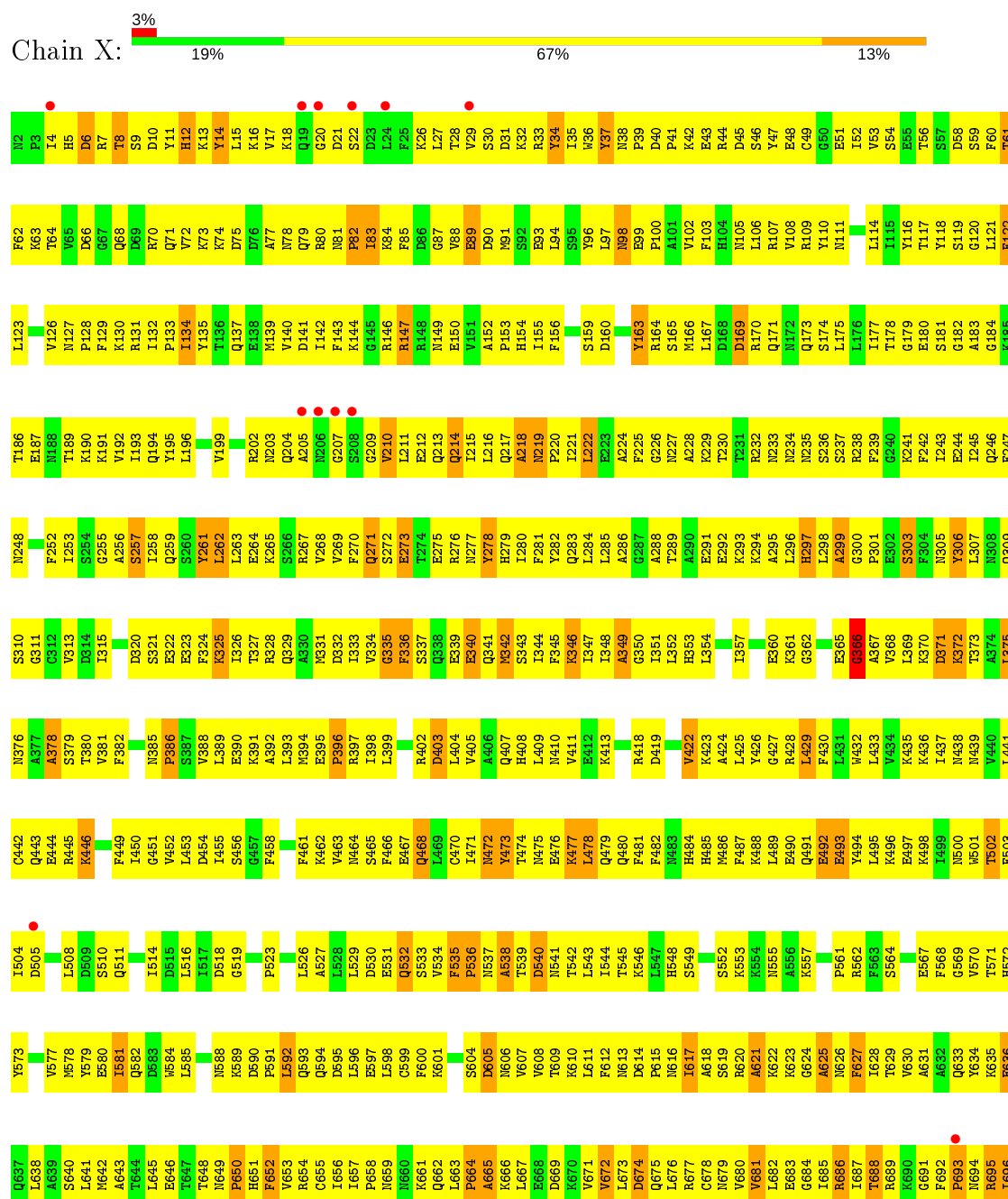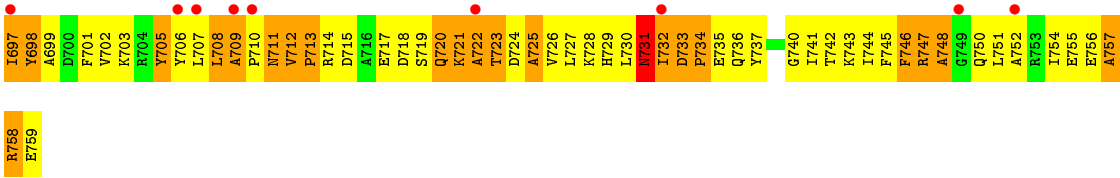
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.00Å 105.80Å 180.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.40 19.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-3.40) 99.7 (19.96-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.36Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.282 , 0.372 0.292 , 0.396	Depositor DCC
R_{free} test set	760 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å²)	40.2	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.23 , 68.5	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	6348	wwPDB-VP
Average B, all atoms (Å²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	X	0.50	0/6212	1.09	76/8382 (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	X	0	2

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	532	GLN	N-CA-CB	-11.79	89.38	110.60
1	X	581	ILE	CB-CA-C	-11.27	89.07	111.60
1	X	403	ASP	N-CA-CB	-10.86	91.05	110.60
1	X	502	THR	N-CA-C	-10.20	83.47	111.00
1	X	581	ILE	N-CA-C	8.98	135.24	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	169	ASP	Peptide
1	X	696	ILE	Peptide

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	X	6092	0	6051	1324	4
2	X	256	0	0	84	0
All	All	6348	0	6051	1324	4

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 109.

The worst 5 of 1324 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:X:242:PHE:CE2	1:X:244:GLU:HG3	1.39	1.54
1:X:163:TYR:CE1	1:X:167:LEU:HD11	1.44	1.49
1:X:242:PHE:CE2	1:X:244:GLU:CG	1.97	1.46
1:X:247:PHE:CD1	1:X:253:ILE:HA	1.48	1.46
1:X:242:PHE:CE2	1:X:244:GLU:CB	2.00	1.44

All (4) 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:X:22:SER:OG	1:X:541:ASN:ND2[3_655]	2.04	0.16
1:X:403:ASP:OD1	1:X:405:VAL:CA[2_556]	2.04	0.16
1:X:445:ARG:NH1	1:X:582:GLN:OE1[1_455]	2.10	0.10
1:X:29:VAL:CG2	1:X:537:ASN:OD1[3_655]	2.18	0.02

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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	756/758 (100%)	579 (77%)	143 (19%)	34 (4%)	2	16

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	6	ASP
1	X	8	THR
1	X	32	LYS
1	X	210	VAL
1	X	540	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	X	663/663 (100%)	643 (97%)	20 (3%)	41	68

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	261	TYR
1	X	273	GLU
1	X	636	GLU
1	X	147	ARG
1	X	232	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	376	ASN
1	X	475	ASN
1	X	694	ASN
1	X	408	HIS

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Mol	Chain	Res	Type
1	X	438	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 ⓘ

There are no ligands in this entry.

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 (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	X	758/758 (100%)	-0.11	21 (2%)	53	51	0, 7, 48, 80	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	206	ASN	5.5
1	X	24	LEU	4.3
1	X	207	GLY	3.9
1	X	722	ALA	3.7
1	X	732	ILE	3.7

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.