



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:42 PM GMT

PDB ID : 1D1B
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH O,P-DINITROPHENYL AMINOPROPYLDIPHOS
PHATEBERYLLIUM TRIFLUORIDE.
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on : 1999-09-15
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary 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>

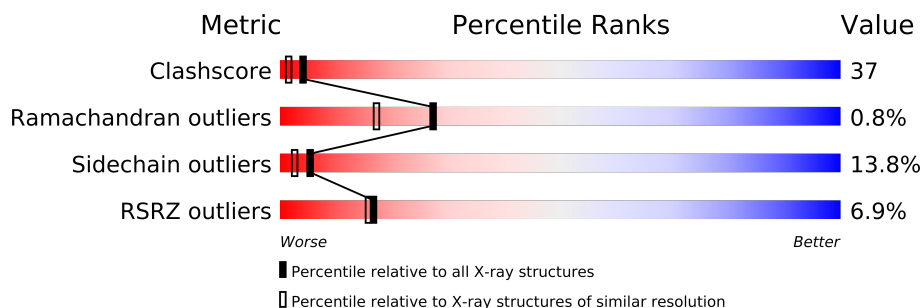
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	761	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6374 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	0	0	0
			5803	3689	997	1101	16			

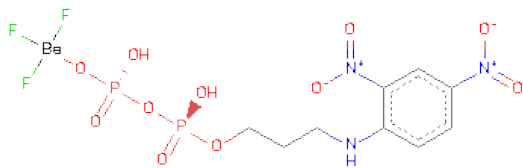
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	SEE REMARK 999	UNP P08799
A	760	PRO	GLN	ENGINEERED	UNP P08799
A	761	ASN	ARG	ENGINEERED	UNP P08799

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

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

- Molecule 3 is O,P-DINITROPHENYL AMINOPROPYLDIPHOSPHATEBERYLLIUM TRIFLUORIDE (three-letter code: DAQ) (formula: C₉H₁₂BeF₃N₃O₁₁P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	29	1	9	3	3	11	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	541	Total	O	0	0
			541	541		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.88Å 180.46Å 54.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 28.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (25.00-2.00) 97.1 (28.84-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.00Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.204 , (Not available) 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 111.6	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 67444 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: MG, DAQ

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	1.84	43/5914 (0.7%)	1.70	97/7992 (1.2%)

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	0	1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ASP	CG-OD2	80.26	3.10	1.25
1	A	40	ASP	CB-CG	53.89	2.65	1.51
1	A	40	ASP	CG-OD1	50.48	2.41	1.25
1	A	657	ILE	CG1-CD1	21.70	3.00	1.50
1	A	99	GLU	CD-OE2	8.03	1.34	1.25

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ASP	CB-CG-OD1	-51.79	71.69	118.30
1	A	40	ASP	CB-CG-OD2	-21.04	99.37	118.30
1	A	657	ILE	CB-CG1-CD1	-19.29	59.90	113.90
1	A	238	ARG	NE-CZ-NH1	14.89	127.74	120.30
1	A	238	ARG	NE-CZ-NH2	-14.51	113.05	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ASP	Sidechain

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	5803	0	5638	421	0
2	A	1	0	0	0	0
3	A	29	0	10	5	0
4	A	541	0	0	30	0
All	All	6374	0	5648	422	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 37.

The worst 5 of 422 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:THR:HB	1:A:292:GLU:OE2	1.38	1.19
1:A:532:GLN:OE1	1:A:542:THR:HG22	1.38	1.19
1:A:289:THR:HG22	1:A:291:GLU:H	1.05	1.14
1:A:62:PHE:HE2	1:A:72:VAL:CG2	1.61	1.12
1:A:686:ARG:HB2	1:A:686:ARG:HH11	0.95	1.10

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	726/761 (95%)	679 (94%)	41 (6%)	6 (1%)	27 17

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	ARG
1	A	719	SER
1	A	7	ARG
1	A	362	GLY
1	A	32	LYS

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	615/665 (92%)	530 (86%)	85 (14%)	5 2

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	MET
1	A	436	LYS
1	A	738	ARG
1	A	368	VAL
1	A	379	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	A	338	GLN
1	A	594	GLN
1	A	309	GLN
1	A	491	GLN

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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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$
3	DAQ	A	999	2	28,29,29	1.88	5 (17%)	36,43,43	1.71	6 (16%)

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
3	DAQ	A	999	2	-	0/23/29/29	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	DAQ	PB-OB3	6.06	1.64	1.51
3	A	999	DAQ	C2-N2	4.78	1.53	1.46
3	A	999	DAQ	F3-BE	-2.90	1.49	1.55
3	A	999	DAQ	F2-BE	-2.21	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	DAQ	C1-NA3	2.17	1.44	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	DAQ	C3-C4-N4	4.98	122.65	118.71
3	A	999	DAQ	C3-C2-N2	4.64	120.48	115.82
3	A	999	DAQ	C3-C2-C1	-3.01	118.94	121.69
3	A	999	DAQ	O2B-N2-O2A	-3.00	115.28	121.35
3	A	999	DAQ	O2B-N2-C2	2.13	123.81	117.25

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	736/761 (96%)	0.10	51 (6%) 17 16	11, 36, 88, 100	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	8.5
1	A	24	LEU	7.0
1	A	53	VAL	5.6
1	A	65	VAL	5.5
1	A	27	LEU	5.0

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
3	DAQ	A	999	29/29	0.11	1.39	3,23,100,100	12

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	998	1/1	0.07	-0.51	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.