



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:45 pm GMT

PDB ID : 1L2O
Title : SCALLOP MYOSIN S1-ADP-p-PDM IN THE ACTIN-DETACHED CON-
FORMATION
Authors : Himmel, M.; Gourinath, S.; Reshetnikova, L.; Shen, Y.; Szent-Gyorgyi, G.;
Cohen, C.
Deposited on : 2002-02-22
Resolution : 2.80 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

<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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

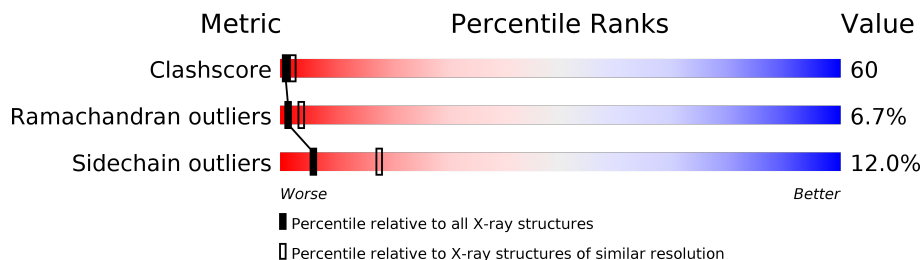
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	835	
2	B	156	
3	C	156	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PDM	A	900	X	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8339 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 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	777	Total	C	N	O	S	0	0	0
			6011	3825	1035	1116	35			

- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1072	678	169	218	7			

- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1174	744	183	240	7			

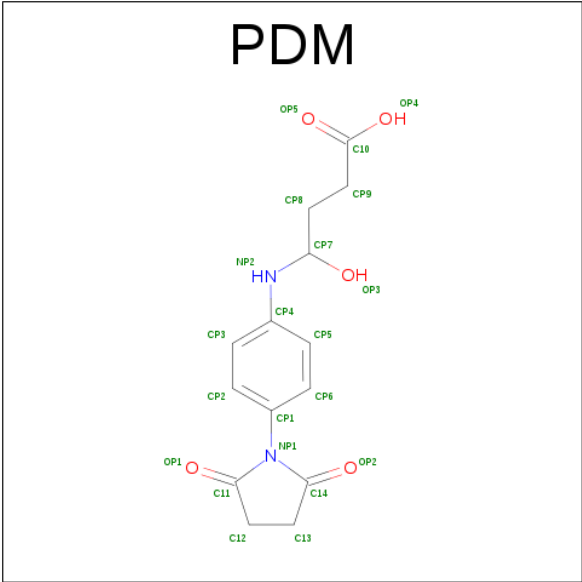
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

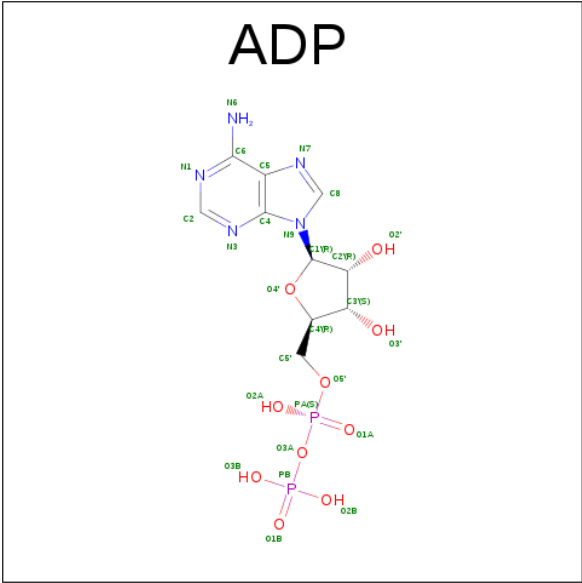
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 4-[4-(2,5-DIOXO-PYRROLIDIN-1-YL)-PHENYLAMINO]-4-HYDROXY-BU TYRIC ACID (three-letter code: PDM) (formula: C₁₄H₁₆N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			21	14	2	5		

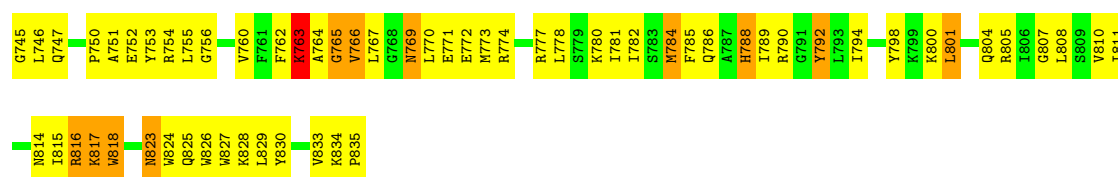
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is water.

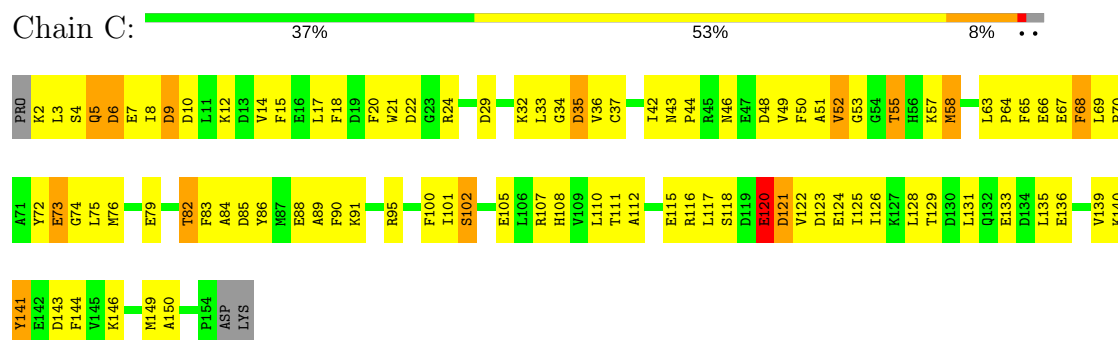
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	25	Total 25	O 25	0	0
8	B	2	Total 2	O 2	0	0
8	C	4	Total 4	O 4	0	0



• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.80 Å 57.00 Å 150.50 Å 95.60° 96.30° 101.50°	Depositor
Resolution (Å)	54.16 – 2.80	Depositor
% Data completeness (in resolution range)	72.0 (54.16-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.280 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8339	wwPDB-VP
Average B, all atoms (Å ²)	89.0	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: MG, PDM, CA, 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	0.51	0/6126	0.89	25/8280 (0.3%)
2	B	0.52	0/1089	0.88	4/1464 (0.3%)
3	C	0.49	0/1198	0.72	0/1619
All	All	0.51	0/8413	0.87	29/11363 (0.3%)

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	151	SER	N-CA-C	8.57	134.13	111.00
1	A	407	THR	N-CA-C	-7.83	89.86	111.00
2	B	150	GLY	N-CA-C	7.39	131.57	113.10
1	A	510	ILE	CB-CA-C	-7.33	96.95	111.60
1	A	695	GLY	O-C-N	7.20	134.22	122.70

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	6011	0	5802	750	0
2	B	1072	0	997	155	0
3	C	1174	0	1061	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	21	0	10	15	0
7	A	27	0	12	3	0
8	A	25	0	0	19	0
8	B	2	0	0	0	0
8	C	4	0	0	2	0
All	All	8339	0	7882	974	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 60.

The worst 5 of 974 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:705:LYS:CG	6:A:900:PDM:H122	1.28	1.60
1:A:134:ASP:OD1	1:A:195:LYS:HE3	1.16	1.27
1:A:705:LYS:CD	6:A:900:PDM:H122	1.59	1.23
1:A:705:LYS:HG2	6:A:900:PDM:C12	1.67	1.22
1:A:46:ALA:HA	1:A:61:VAL:HG23	1.22	1.18

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	759/835 (91%)	552 (73%)	150 (20%)	57 (8%)	1 2
2	B	140/156 (90%)	105 (75%)	27 (19%)	8 (6%)	2 5
3	C	151/156 (97%)	119 (79%)	27 (18%)	5 (3%)	4 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1050/1147 (92%)	776 (74%)	204 (19%)	70 (7%)	1 4

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	MET
1	A	834	LYS
2	B	136	GLY
3	C	102	SER

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	621/728 (85%)	547 (88%)	74 (12%)	6 18
2	B	109/133 (82%)	96 (88%)	13 (12%)	6 18
3	C	119/132 (90%)	104 (87%)	15 (13%)	5 16
All	All	849/993 (86%)	747 (88%)	102 (12%)	6 18

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	553	GLN
1	A	645	ILE
3	C	58	MET
1	A	554	ASN
1	A	592	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	453	ASN
1	A	553	GLN

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Mol	Chain	Res	Type
2	B	68	ASN
1	A	486	GLN
1	A	489	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 5 ligands modelled in this entry, 3 are 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
6	PDM	A	900	1	18,22,22	3.24	8 (44%)	25,30,30	1.62	3 (12%)
7	ADP	A	999	5	25,29,29	1.55	5 (20%)	24,45,45	1.06	3 (12%)

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
6	PDM	A	900	1	1/1/5/6	0/11/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	A	999	5	-	0/12/32/32	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	900	PDM	CP7-NP2	-7.50	1.34	1.43
6	A	900	PDM	OP3-CP7	-5.85	1.24	1.40
6	A	900	PDM	C13-C12	-4.19	1.41	1.52
6	A	900	PDM	C14-NP1	-3.84	1.35	1.40
6	A	900	PDM	C11-NP1	-3.83	1.35	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	999	ADP	O3A-PB-O1B	-2.44	96.45	111.44
7	A	999	ADP	C4'-O4'-C1'	2.21	112.12	109.77
7	A	999	ADP	C4-C5-N7	2.61	111.94	109.41
6	A	900	PDM	OP3-CP7-CP8	3.04	115.86	109.25
6	A	900	PDM	CP8-CP7-NP2	3.16	114.53	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	900	PDM	CP7

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	900	PDM	15	0
7	A	999	ADP	3	0

5.7 Other polymers [i](#)

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.