



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:57 pm BST

PDB ID : 3I5I
Title : The crystal structure of squid myosin S1 in the presence of SO₄²⁻
Authors : Yang, Y.; Gourinath, S.; Kovacs, M.; Nyitray, L.; Reutzel, R.; Himmel, D.M.;
O'Neill-Hennessey, E.; Reshetnikova, L.; Szent-Gyorgyi, A.G.; Brown, J.H.;
Cohen, C.
Deposited on : 2009-07-05
Resolution : 3.30 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

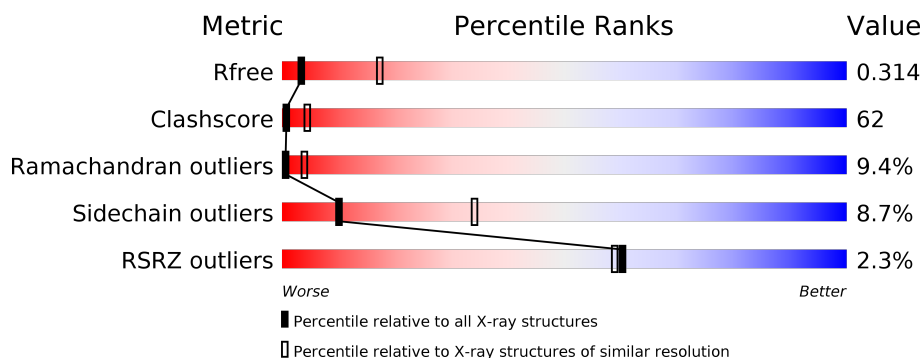
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 $\leq 5\%$. 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	839	<div> <div>2%</div> <div> <div>32%</div> <div>54%</div> <div>9%</div> <div>• •</div> </div> </div>
2	B	153	<div> <div>6%</div> <div> <div>14%</div> <div>52%</div> <div>25%</div> <div>• 5%</div> </div> </div>
3	C	159	<div> <div>%</div> <div> <div>42%</div> <div>43%</div> <div>13%</div> <div>• •</div> </div> </div>

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
4	SO4	A	1001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8904 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 isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	808	Total	C	N	O	S	0	0	0
			6493	4150	1111	1193	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	LYS	GLU	CONFLICT	UNP O44934
A	744	ALA	VAL	CONFLICT	UNP O44934

- Molecule 2 is a protein called Myosin regulatory light chain LC-2, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1166	733	191	233	9			

- Molecule 3 is a protein called Myosin catalytic light chain LC-1, mantle muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1239	773	203	253	10			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



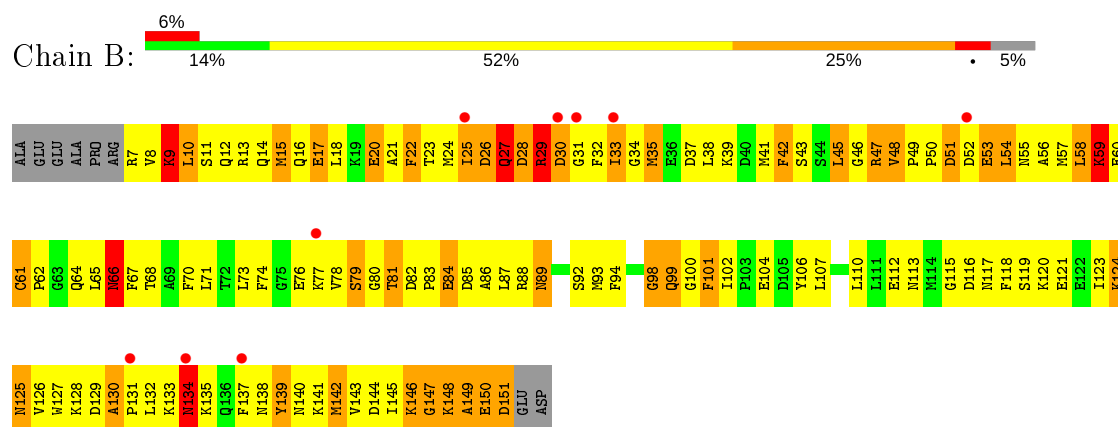
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

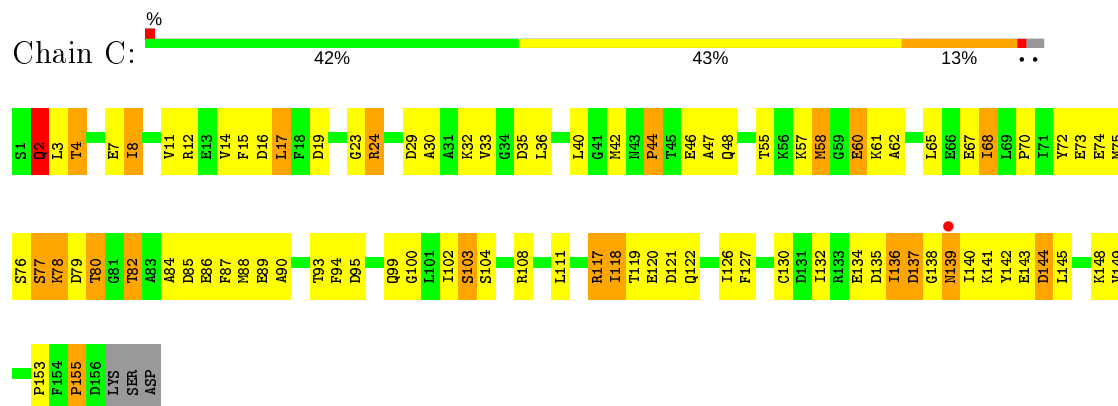
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		



- Molecule 2: Myosin regulatory light chain LC-2, mantle muscle



- Molecule 3: Myosin catalytic light chain LC-1, mantle muscle



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.19Å 100.15Å 80.19Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.30 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-3.30) 97.2 (49.30-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.330 0.251 , 0.314	Depositor DCC
R_{free} test set	2180 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4

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	0.52	0/6631	0.87	12/8938 (0.1%)
2	B	0.56	0/1186	1.17	11/1588 (0.7%)
3	C	0.59	0/1258	1.01	5/1687 (0.3%)
All	All	0.53	0/9075	0.93	28/12213 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	28	ASP	N-CA-C	12.34	144.32	111.00
3	C	2	GLN	N-CA-C	10.93	140.51	111.00
2	B	27	GLN	N-CA-C	-10.82	81.79	111.00
3	C	138	GLY	N-CA-C	-10.50	86.84	113.10
2	B	100	GLY	N-CA-C	-9.60	89.09	113.10

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	6493	0	6496	787	0
2	B	1166	0	1125	238	1
3	C	1239	0	1190	136	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	4	0
5	C	1	0	0	0	0
All	All	8904	0	8811	1104	1

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 62.

The worst 5 of 1104 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:141:ARG:NH2	1:A:199:SER:HB3	1.54	1.20
1:A:191:GLN:HG2	1:A:221:GLU:HG2	1.19	1.18
2:B:26:ASP:OD1	2:B:28:ASP:HB2	1.47	1.15
1:A:293:LEU:HD23	1:A:333:MET:HE1	1.26	1.15
1:A:259:GLN:H	1:A:261:LYS:HE2	1.13	1.12

All (1) 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)
2:B:16:GLN:OE1	2:B:68:THR:OG1[2_556]	2.10	0.10

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	802/839 (96%)	625 (78%)	109 (14%)	68 (8%)	1 5
2	B	143/153 (94%)	89 (62%)	26 (18%)	28 (20%)	0 0
3	C	154/159 (97%)	130 (84%)	17 (11%)	7 (4%)	2 15
All	All	1099/1151 (96%)	844 (77%)	152 (14%)	103 (9%)	0 4

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	8	PRO
1	A	52	LYS
1	A	61	ASP
1	A	62	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	704/731 (96%)	653 (93%)	51 (7%)	14	41
2	B	128/134 (96%)	107 (84%)	21 (16%)	2	10
3	C	134/137 (98%)	122 (91%)	12 (9%)	9	32
All	All	966/1002 (96%)	882 (91%)	84 (9%)	10	34

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	620	VAL
1	A	765	LYS
3	C	78	LYS
1	A	622	MET
1	A	664	SER

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	494	HIS
1	A	607	ASN
2	B	89	ASN
1	A	600	ASN
1	A	605	ASN

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](#)

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	$\# Z > 2$
4	SO4	A	1001	-	4,4,4	0.20	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	SO4	4	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](#)

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	808/839 (96%)	-0.03	16 (1%) 65 64	13, 64, 137, 163	0
2	B	145/153 (94%)	0.51	9 (6%) 20 20	34, 100, 146, 163	0
3	C	156/159 (98%)	-0.12	1 (0%) 89 90	13, 47, 106, 152	0
All	All	1109/1151 (96%)	0.03	26 (2%) 60 59	13, 66, 140, 163	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	30	ASP	6.2
2	B	77	LYS	4.8
1	A	202	GLY	4.6
3	C	139	ASN	4.1
1	A	643	ALA	3.8

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](#)

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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	C	2001	1/1	0.79	0.14	58,58,58,58	0
4	SO4	A	1001	5/5	0.93	0.41	58,58,58,58	5

6.5 Other polymers [i](#)

There are no such residues in this entry.