wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 08:04 PM EST

PDB ID	:	1I84
Title	:	CRYO-EM STRUCTURE OF THE HEAVY MEROMYOSIN SUBFRAGMENT OF CHICKEN GIZZARD SMOOTH MUSCLE MYOSIN WITH REGULATORY LIGHT CHAIN IN THE DEPHOSPHORYLATED STATE. ONLY C ALPHAS PROVIDED FOR REGULATORY LIGHT CHAIN. ONLY BACKBONE ATOMS PROVIDED FOR S2 FRAGMENT.
Authors	:	Wendt, T.; Taylor, D.; Trybus, K.M.; Taylor, K.
Deposited on	:	2001-03-12
Resolution	:	20.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

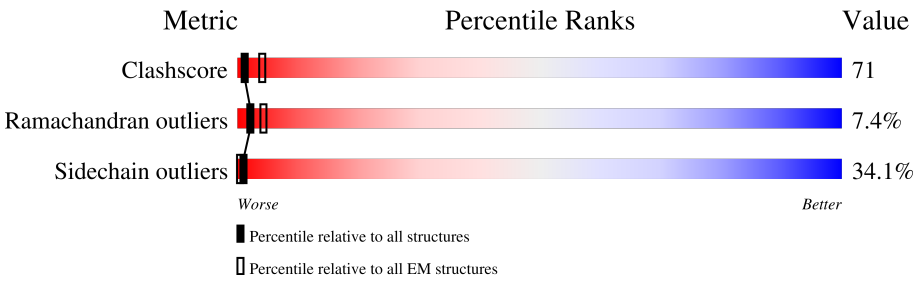
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 20.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	S	1184	21% 36% 18% • 23%
1	V	1184	22% 36% 18% • 23%
2	T	150	17% 54% 27% ••
2	W	150	18% 52% 28% ••
3	U	166	82% • 17%
3	Z	166	82% • 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16580 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SMOOTH MUSCLE MYOSIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	S	909	6992	4423	1226	1311	32	0	0
1	V	909	6992	4423	1226	1311	32	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	ALA	SER	SEE REMARK 999	? P10587
S	820	GLU	THR	SEE REMARK 999	? P10587
S	821	SER	ALA	SEE REMARK 999	? P10587
S	822	ILE	MET	SEE REMARK 999	? P10587
S	823	PHE	LYS	SEE REMARK 999	? P10587
S	824	CYS	VAL	SEE REMARK 999	? P10587
S	827	TYR	ARG	SEE REMARK 999	? P10587
S	829	VAL	CYS	SEE REMARK 999	? P10587
S	830	ARG	ALA	SEE REMARK 999	? P10587
S	831	SER	ALA	SEE REMARK 999	? P10587
S	832	PHE	TYR	SEE REMARK 999	? P10587
S	833	MET	LEU	SEE REMARK 999	? P10587
S	834	ASN	LYS	SEE REMARK 999	? P10587
S	835	VAL	LEU	SEE REMARK 999	? P10587
S	836	MLY	ARG	SEE REMARK 999	? P10587
S	837	HIS	ASN	SEE REMARK 999	? P10587
S	839	PRO	GLN	SEE REMARK 999	? P10587
S	841	MET	TRP	SEE REMARK 999	? P10587
S	842	MLY	ARG	SEE REMARK 999	? P10587
S	845	PHE	THR	SEE REMARK 999	? P10587
S	846	MLY	LYS	SEE REMARK 999	? P10587
S	847	ILE	VAL	SEE REMARK 999	? P10587
S	848	MLY	LYS	SEE REMARK 999	? P10587
S	852	LYS	GLN	SEE REMARK 999	? P10587
S	1176	GLY	-	expression tag	? P10587
S	1177	SER	-	expression tag	? P10587

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	1178	ASP	-	expression tag	? P10587
S	1179	TYR	-	expression tag	? P10587
S	1180	LYS	-	expression tag	? P10587
S	1181	ASP	-	expression tag	? P10587
S	1182	ASP	-	expression tag	? P10587
S	1183	ASP	-	expression tag	? P10587
S	1184	ASP	-	expression tag	? P10587
S	1185	LYS	-	expression tag	? P10587
V	2	ALA	SER	SEE REMARK 999	? P10587
V	820	GLU	THR	SEE REMARK 999	? P10587
V	821	SER	ALA	SEE REMARK 999	? P10587
V	822	ILE	MET	SEE REMARK 999	? P10587
V	823	PHE	LYS	SEE REMARK 999	? P10587
V	824	CYS	VAL	SEE REMARK 999	? P10587
V	827	TYR	ARG	SEE REMARK 999	? P10587
V	829	VAL	CYS	SEE REMARK 999	? P10587
V	830	ARG	ALA	SEE REMARK 999	? P10587
V	831	SER	ALA	SEE REMARK 999	? P10587
V	832	PHE	TYR	SEE REMARK 999	? P10587
V	833	MET	LEU	SEE REMARK 999	? P10587
V	834	ASN	LYS	SEE REMARK 999	? P10587
V	835	VAL	LEU	SEE REMARK 999	? P10587
V	836	MLY	ARG	SEE REMARK 999	? P10587
V	837	HIS	ASN	SEE REMARK 999	? P10587
V	839	PRO	GLN	SEE REMARK 999	? P10587
V	841	MET	TRP	SEE REMARK 999	? P10587
V	842	MLY	ARG	SEE REMARK 999	? P10587
V	845	PHE	THR	SEE REMARK 999	? P10587
V	846	MLY	LYS	SEE REMARK 999	? P10587
V	847	ILE	VAL	SEE REMARK 999	? P10587
V	848	MLY	LYS	SEE REMARK 999	? P10587
V	852	LYS	GLN	SEE REMARK 999	? P10587
V	1176	GLY	-	expression tag	? P10587
V	1177	SER	-	expression tag	? P10587
V	1178	ASP	-	expression tag	? P10587
V	1179	TYR	-	expression tag	? P10587
V	1180	LYS	-	expression tag	? P10587
V	1181	ASP	-	expression tag	? P10587
V	1182	ASP	-	expression tag	? P10587
V	1183	ASP	-	expression tag	? P10587
V	1184	ASP	-	expression tag	? P10587
V	1185	LYS	-	expression tag	? P10587

- Molecule 2 is a protein called SMOOTH MUSCLE MYOSIN ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T	148	1160	722	193	234	11	0	0
2	W	148	1160	722	193	234	11	0	0

- Molecule 3 is a protein called SMOOTH MUSCLE MYOSIN REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	U	138	138	138	0	138
3	Z	138	138	138	0	138

There are 18 discrepancies between the modelled and reference sequences:

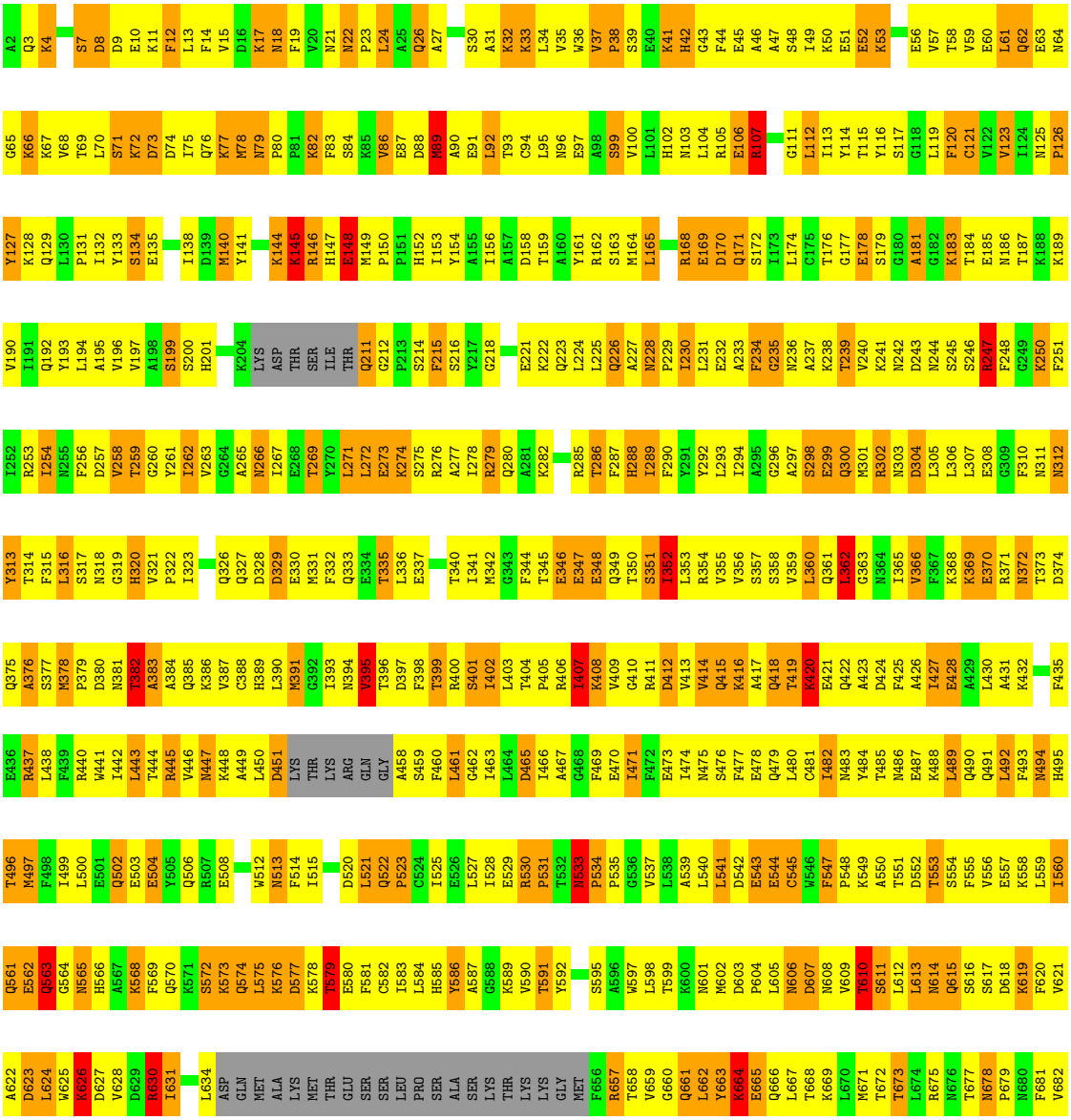
Chain	Residue	Modelled	Actual	Comment	Reference
Z	21	GLU	GLN	SEE REMARK 999	UNP P02609
Z	23	GLU	GLN	SEE REMARK 999	UNP P02609
Z	25	GLU	GLN	SEE REMARK 999	UNP P02609
Z	26	ASP	GLU	SEE REMARK 999	UNP P02609
Z	38	ALA	ARG	SEE REMARK 999	UNP P02609
Z	124	GLY	GLN	SEE REMARK 999	UNP P02609
Z	125	GLY	CYS	SEE REMARK 999	UNP P02609
Z	126	GLY	ASP	SEE REMARK 999	UNP P02609
Z	163	ALA	LYS	SEE REMARK 999	UNP P02609
U	21	GLU	GLN	SEE REMARK 999	UNP P02609
U	23	GLU	GLN	SEE REMARK 999	UNP P02609
U	25	GLU	GLN	SEE REMARK 999	UNP P02609
U	26	ASP	GLU	SEE REMARK 999	UNP P02609
U	38	ALA	ARG	SEE REMARK 999	UNP P02609
U	124	GLY	GLN	SEE REMARK 999	UNP P02609
U	125	GLY	CYS	SEE REMARK 999	UNP P02609
U	126	GLY	ASP	SEE REMARK 999	UNP P02609
U	163	ALA	LYS	SEE REMARK 999	UNP P02609

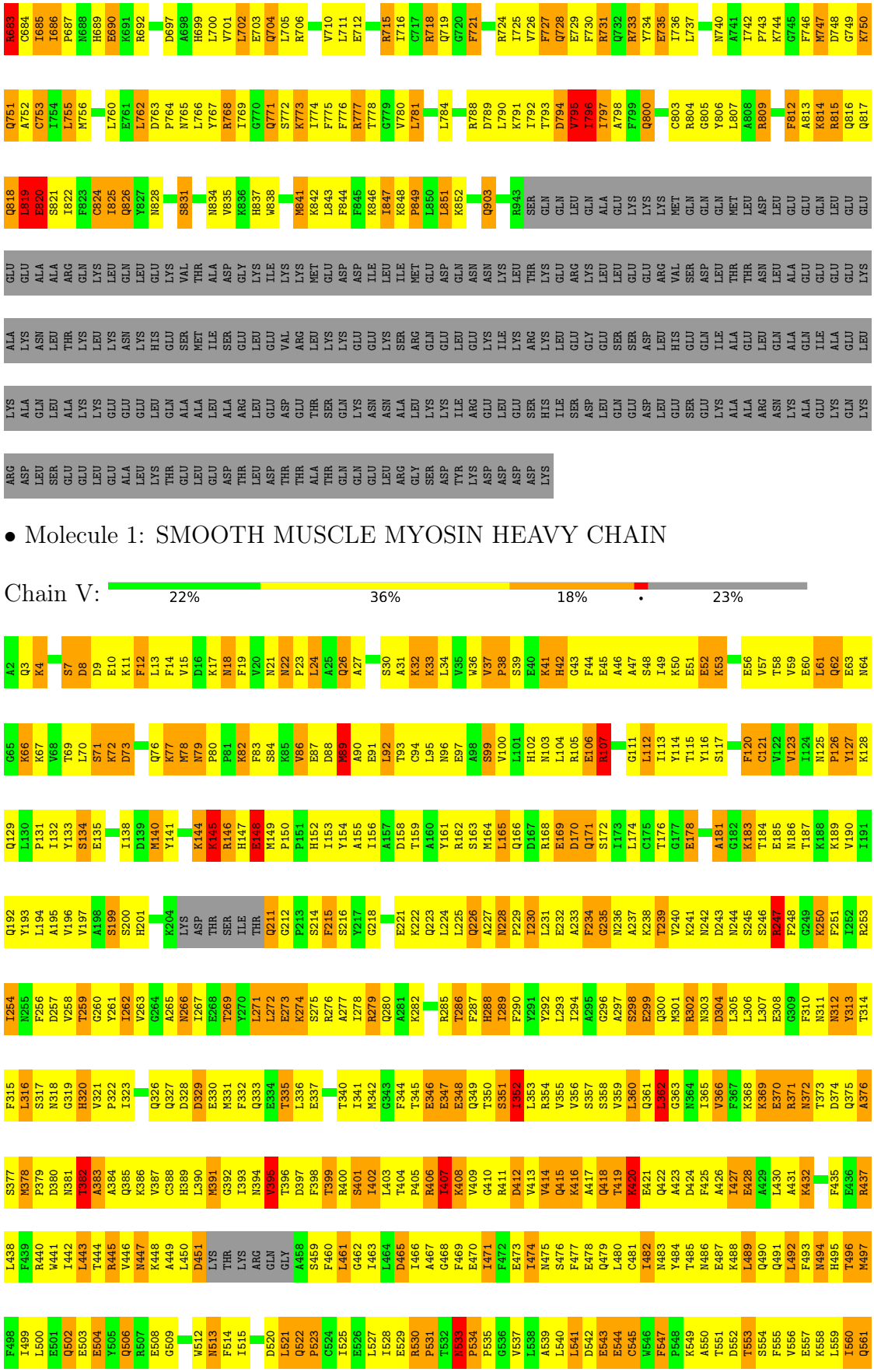
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: SMOOTH MUSCLE MYOSIN HEAVY CHAIN

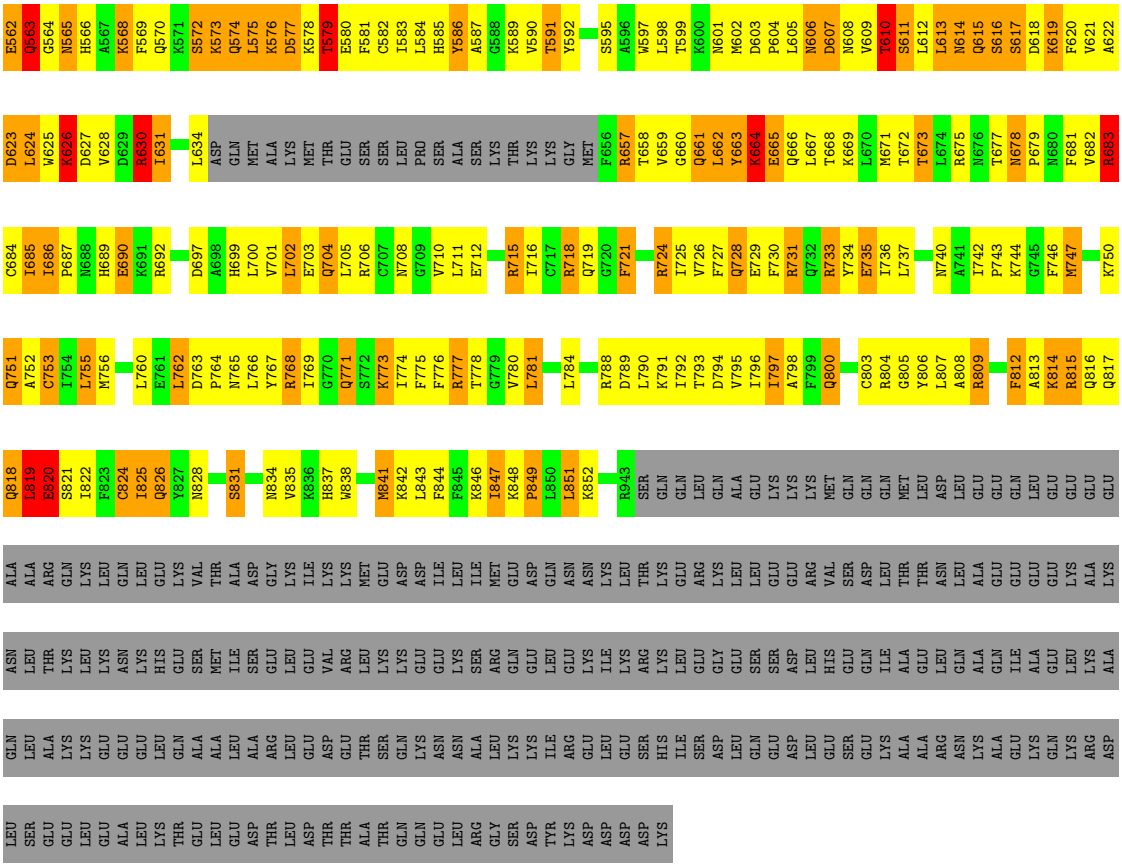
Chain S: 21% 36% 18% • 23%





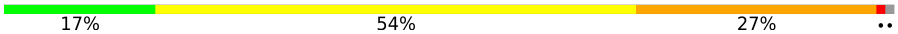
• Molecule 1: SMOOTH MUSCLE MYOSIN HEAVY CHAIN

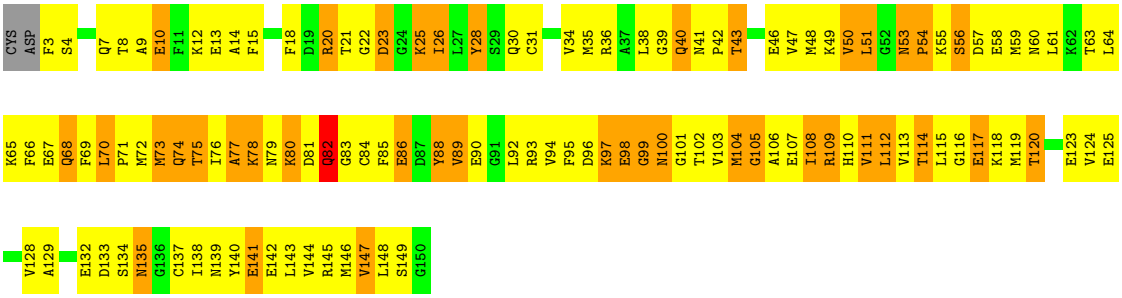
Chain V: 22% 36% 18% • 23%



• Molecule 2: SMOOTH MUSCLE MYOSIN ESSENTIAL LIGHT CHAIN

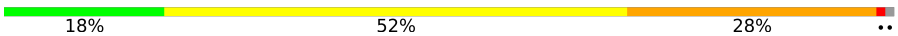
Chain T:

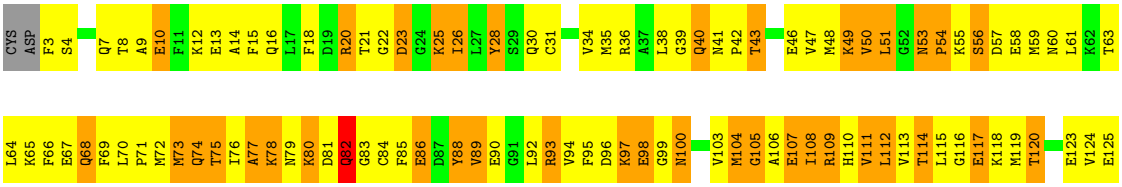




• Molecule 2: SMOOTH MUSCLE MYOSIN ESSENTIAL LIGHT CHAIN

Chain W:



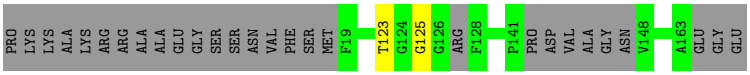


• Molecule 3: SMOOTH MUSCLE MYOSIN REGULATORY LIGHT CHAIN

Chain U:

• Molecule 3: SMOOTH MUSCLE MYOSIN REGULATORY LIGHT CHAIN

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 1 2	Depositor
Cell constants a, b, c, α, β, γ	133.00Å 304.00Å 200.00Å 90.00° 90.00° 91.50°	Depositor
Resolution (Å)	(Not available) – 20.00 303.90 – 19.32	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-20.00) 40.9 (303.90-19.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 100.1	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.48	EDS
Total number of atoms	16580	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]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)

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

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	S	0.76	5/7076 (0.1%)	1.06	18/9501 (0.2%)
1	V	0.68	2/7076 (0.0%)	0.87	13/9501 (0.1%)
2	T	0.46	0/1175	0.60	0/1575
2	W	0.46	0/1175	0.60	0/1575
All	All	0.69	7/16502 (0.0%)	0.92	31/22152 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	819	LEU	C-N	26.74	1.95	1.34
1	S	819	LEU	C-N	26.72	1.95	1.34
1	S	903	GLN	C-N	22.86	1.86	1.34
1	S	796	ILE	C-N	16.86	1.72	1.34
1	S	795	VAL	C-N	7.35	1.50	1.34

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	796	ILE	O-C-N	-45.91	49.24	122.70
1	S	819	LEU	O-C-N	-34.53	67.45	122.70
1	V	819	LEU	O-C-N	-34.51	67.48	122.70
1	S	903	GLN	O-C-N	-32.87	70.11	122.70
1	V	819	LEU	CA-C-N	16.41	153.29	117.20

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	S	6992	0	6742	974	88
1	V	6992	0	6738	1072	0
2	T	1160	0	1117	277	0
2	W	1160	0	1126	150	4
3	U	138	0	0	3	0
3	Z	138	0	0	3	0
All	All	16580	0	15723	2234	92

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 71.

The worst 5 of 2234 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)
2:T:102:THR:CG2	1:V:617:SER:H	1.12	1.60
1:S:258:VAL:CG1	1:V:406:ARG:HH12	1.06	1.59
2:T:94:VAL:HA	1:V:396:THR:CG2	1.26	1.56
2:T:94:VAL:CA	1:V:396:THR:HG21	1.42	1.49
1:S:258:VAL:HG13	1:V:406:ARG:NH1	1.30	1.46

The worst 5 of 92 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:S:61:LEU:O	1:S:70:LEU:CD1[2_665]	0.35	1.85
1:S:47:ALA:C	1:S:68:VAL:C[2_665]	0.39	1.81
1:S:38:PRO:CA	1:S:64:ASN:CB[2_665]	0.41	1.79
1:S:38:PRO:CB	1:S:64:ASN:CA[2_665]	0.60	1.60
1:S:37:VAL:CA	1:S:66:LYS:CB[2_665]	0.72	1.48

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 PDB entries followed by that with respect to all EM entries.

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	S	891/1184 (75%)	649 (73%)	178 (20%)	64 (7%)	1 14
1	V	891/1184 (75%)	651 (73%)	178 (20%)	62 (7%)	1 14
2	T	146/150 (97%)	101 (69%)	31 (21%)	14 (10%)	0 10
2	W	146/150 (97%)	101 (69%)	31 (21%)	14 (10%)	0 10
All	All	2074/2668 (78%)	1502 (72%)	418 (20%)	154 (7%)	2 14

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	145	LYS
1	S	170	ASP
1	S	383	ALA
1	S	395	VAL
1	S	414	VAL

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 PDB entries followed by that with respect to all EM entries.

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	S	717/1047 (68%)	470 (66%)	247 (34%)	0 1
1	V	717/1047 (68%)	470 (66%)	247 (34%)	0 1
2	T	127/129 (98%)	86 (68%)	41 (32%)	0 2
2	W	127/129 (98%)	86 (68%)	41 (32%)	0 2
All	All	1688/2352 (72%)	1112 (66%)	576 (34%)	1 1

5 of 576 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	595	SER
2	W	135	ASN
1	V	626	LYS
1	V	591	THR
1	V	797	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	26	GLN
1	V	783	HIS
1	V	244	ASN
1	V	771	GLN
1	V	661	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	MLY	S	842	1	9,10,11	1.16	1 (11%)	6,11,13	0.30	0
1	MLY	V	842	1	9,10,11	1.16	1 (11%)	6,11,13	0.32	0
1	MLY	S	836	1	9,10,11	0.70	0	6,11,13	0.48	0
1	MLY	S	848	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	V	846	1	9,10,11	0.61	0	6,11,13	0.55	0
1	MLY	S	846	1	9,10,11	0.59	0	6,11,13	0.55	0
1	MLY	V	836	1	9,10,11	0.69	0	6,11,13	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLY	V	848	1	9,10,11	0.72	0	6,11,13	0.78	0

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
1	MLY	S	842	1	-	6/8/9/11	-
1	MLY	V	842	1	-	6/8/9/11	-
1	MLY	S	836	1	-	0/8/9/11	-
1	MLY	S	848	1	-	3/8/9/11	-
1	MLY	V	846	1	-	5/8/9/11	-
1	MLY	S	846	1	-	5/8/9/11	-
1	MLY	V	836	1	-	0/8/9/11	-
1	MLY	V	848	1	-	3/8/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	842	MLY	CB-CA	-2.33	1.50	1.53
1	S	842	MLY	CB-CA	-2.33	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S	842	MLY	CD-CE-NZ-CH1
1	S	842	MLY	CD-CE-NZ-CH2
1	S	846	MLY	CD-CE-NZ-CH1
1	S	846	MLY	CD-CE-NZ-CH2
1	S	848	MLY	CD-CE-NZ-CH2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S	848	MLY	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	V	846	MLY	1	0
1	S	846	MLY	1	0
1	V	848	MLY	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	S	6
1	V	4

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	852:LYS	C	853:VAL	N	5.40
1	V	903:GLN	C	904:ALA	N	3.37
1	S	860:MET	C	861:GLN	N	2.66
1	V	852:LYS	C	853:VAL	N	2.29
1	S	854:THR	C	855:ARG	N	2.18