



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 10:07 AM EDT

PDB ID : 7KFL
Title : Crystal structure of the cargo-binding domain from the plant class XI myosin (MyoXIk)
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Deposited on : 2020-10-14
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	2.18
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)	:	2.18

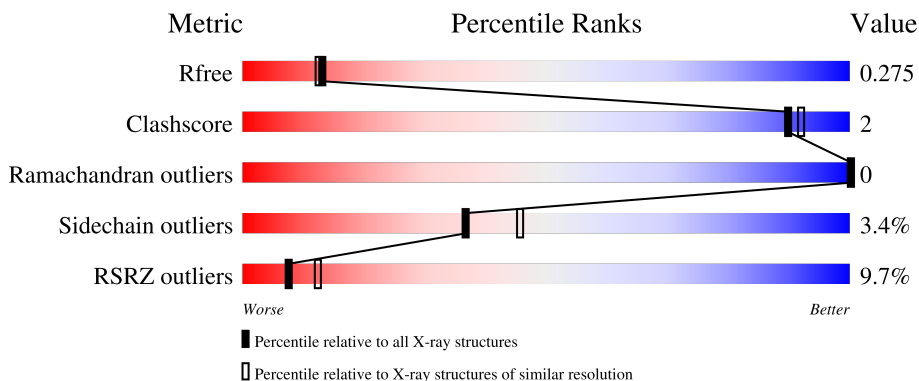
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 of 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	395	<div> <div>6%</div> <div>85%</div> <div>5%</div> <div>10%</div> </div>
1	B	395	<div> <div>11%</div> <div>79%</div> <div>6%</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5619 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-17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2850	1812	491	532	15			
1	B	336	Total	C	N	O	S	0	0	0
			2707	1728	462	502	15			

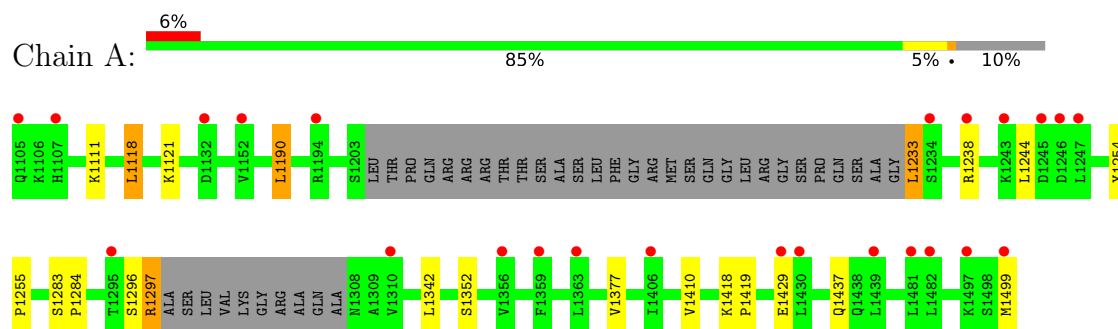
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	25	Total	O	0	0
			25	25		

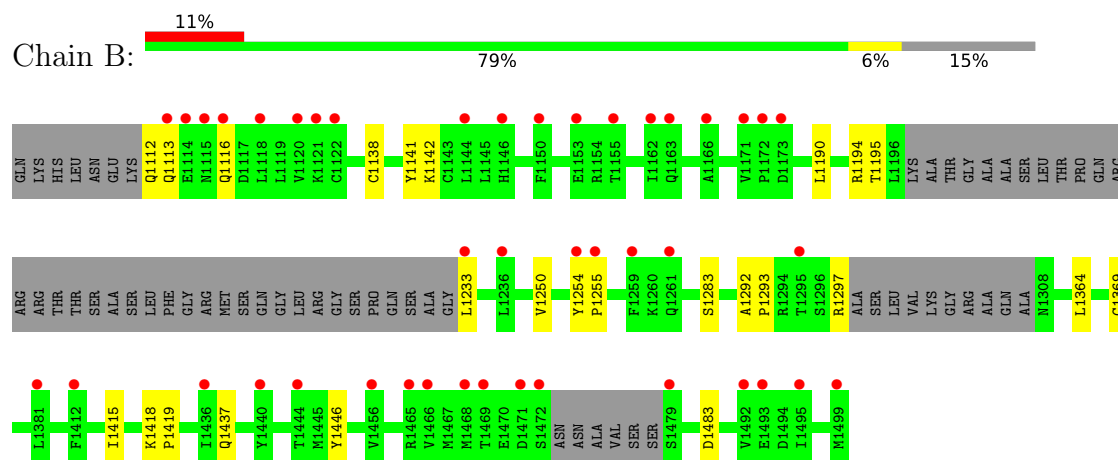
3 Residue-property plots [i](#)

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 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-17



• Molecule 1: Myosin-17



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.06Å 54.33Å 113.43Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	47.36 – 2.35 47.32 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.36-2.35) 99.3 (47.32-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.273 0.235 , 0.275	Depositor DCC
R_{free} test set	1875 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	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	0.95	EDS
Total number of atoms	5619	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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

5.1 Standard geometry

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	0.65	0/2900	0.69	0/3923
1	B	0.65	0/2755	0.68	0/3727
All	All	0.65	0/5655	0.68	0/7650

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2850	0	2877	11	0
1	B	2707	0	2733	9	0
2	A	37	0	0	0	0
2	B	25	0	0	0	0
All	All	5619	0	5610	20	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 2.

All (20) 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:1121:LYS:HE2	1:A:1121:LYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1415:ILE:O	1:B:1418:LYS:NZ	2.43	0.49
1:A:1418:LYS:N	1:A:1419:PRO:CD	2.76	0.48
1:A:1283:SER:HB3	1:A:1284:PRO:HD3	1.98	0.46
1:A:1377:VAL:HG12	1:A:1410:VAL:HG21	1.98	0.46
1:A:1118:LEU:HB3	1:A:1233:LEU:CD1	2.45	0.45
1:A:1190:LEU:HD22	1:A:1190:LEU:O	2.17	0.44
1:B:1418:LYS:N	1:B:1419:PRO:CD	2.81	0.44
1:B:1138:CYS:O	1:B:1142:LYS:HG3	2.17	0.44
1:A:1118:LEU:HB3	1:A:1233:LEU:HD13	1.99	0.43
1:A:1296:SER:O	1:A:1297:ARG:C	2.57	0.42
1:A:1254:TYR:N	1:A:1255:PRO:CD	2.82	0.42
1:B:1418:LYS:HE2	1:B:1446:TYR:CE2	2.56	0.41
1:A:1377:VAL:CG1	1:A:1410:VAL:HG21	2.50	0.41
1:B:1190:LEU:O	1:B:1194:ARG:HG3	2.21	0.41
1:B:1254:TYR:HB2	1:B:1255:PRO:HD3	2.01	0.41
1:B:1292:ALA:N	1:B:1293:PRO:CD	2.83	0.41
1:B:1437:GLN:N	1:B:1437:GLN:OE1	2.53	0.41
1:B:1141:TYR:OH	1:B:1195:THR:HG21	2.21	0.41
1:A:1342:LEU:HD23	1:A:1342:LEU:HA	1.92	0.41

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	350/395 (89%)	338 (97%)	12 (3%)	0	100	100
1	B	328/395 (83%)	314 (96%)	14 (4%)	0	100	100
All	All	678/790 (86%)	652 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	318/347 (92%)	307 (96%)	11 (4%)	36	44
1	B	303/347 (87%)	293 (97%)	10 (3%)	38	46
All	All	621/694 (90%)	600 (97%)	21 (3%)	37	46

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1111	LYS
1	A	1118	LEU
1	A	1190	LEU
1	A	1233	LEU
1	A	1238	ARG
1	A	1244	LEU
1	A	1297	ARG
1	A	1352	SER
1	A	1429	GLU
1	A	1437	GLN
1	A	1499	MET
1	B	1112	GLN
1	B	1113	GLN
1	B	1116	GLN
1	B	1233	LEU
1	B	1250	VAL
1	B	1283	SER
1	B	1297	ARG
1	B	1364	LEU
1	B	1369	CYS
1	B	1483	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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](#)

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	356/395 (90%)	0.74	24 (6%) 17 26	47, 61, 101, 117	0
1	B	336/395 (85%)	0.77	43 (12%) 3 6	48, 68, 112, 131	0
All	All	692/790 (87%)	0.75	67 (9%) 7 12	47, 64, 107, 131	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1172	PRO	5.2
1	B	1254	TYR	5.0
1	B	1295	THR	4.7
1	A	1246	ASP	4.5
1	B	1466	VAL	4.4
1	B	1173	ASP	4.2
1	A	1247	LEU	3.9
1	B	1115	ASN	3.8
1	B	1121	LYS	3.8
1	B	1171	VAL	3.6
1	A	1295	THR	3.6
1	B	1493	GLU	3.3
1	B	1479	SER	3.3
1	B	1118	LEU	3.2
1	B	1114	GLU	3.2
1	B	1113	GLN	3.1
1	B	1166	ALA	3.1
1	A	1245	ASP	3.0
1	B	1116	GLN	3.0
1	B	1440	TYR	3.0
1	B	1495	ILE	2.9
1	A	1107	HIS	2.9
1	B	1472	SER	2.9
1	A	1238	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1499	MET	2.8
1	B	1163	GLN	2.8
1	A	1481	LEU	2.8
1	A	1430	LEU	2.7
1	B	1150	PHE	2.7
1	A	1363	LEU	2.7
1	B	1465	ARG	2.6
1	A	1310	VAL	2.6
1	A	1497	LYS	2.6
1	B	1444	THR	2.6
1	A	1439	LEU	2.5
1	B	1468	MET	2.5
1	B	1144	LEU	2.5
1	B	1162	ILE	2.5
1	B	1499	MET	2.5
1	B	1120	VAL	2.4
1	A	1429	GLU	2.4
1	A	1105	GLN	2.4
1	A	1152	VAL	2.4
1	B	1146	HIS	2.4
1	A	1194	ARG	2.4
1	B	1492	VAL	2.4
1	B	1255	PRO	2.4
1	B	1469	THR	2.4
1	B	1412	PHE	2.4
1	B	1153	GLU	2.3
1	B	1471	ASP	2.3
1	A	1243	LYS	2.3
1	B	1233	LEU	2.2
1	B	1236	LEU	2.2
1	B	1155	THR	2.2
1	B	1261	GLN	2.2
1	A	1234	SER	2.2
1	B	1456	VAL	2.1
1	B	1259	PHE	2.1
1	A	1359	PHE	2.1
1	A	1356	VAL	2.1
1	B	1122	CYS	2.0
1	A	1406	ILE	2.0
1	A	1482	LEU	2.0
1	A	1132	ASP	2.0
1	B	1381	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1436	ILE	2.0

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 monosaccharides 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.