wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2017 – 02:03 AM EST

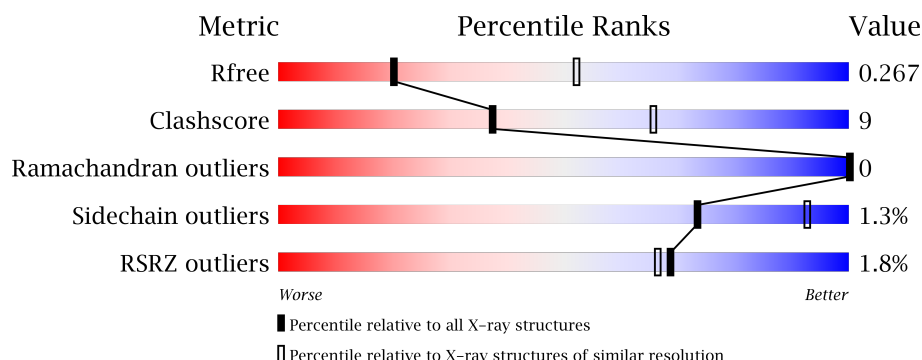|		
PDB ID	:	5E4H
Title	:	Crystal Structure of Apoenzyme Alpha-kinase Domain of Myosin-II Heavy Chain Kinase A
Authors	:	Ye, Q.; Cote, G.P.; Jia, Z.
Deposited on	:	unknown
Resolution	:	2.90 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		1.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 <=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	307	64% 18% 18%
1	B	307	3% 64% 16% • 20%
1	C	307	2% 63% 17% 20%
1	D	307	66% 17% 17%
1	E	307	2% 63% 19% 19%

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Mol	Chain	Length	Quality of chain
1	F	307	.% 67% 14% · 18%
1	G	307	.% 67% 16% 17%
1	H	307	2% 64% 16% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16069 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-II heavy chain kinase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	P	S	0	0	0
			2004	1280	334	376	2	12			
1	B	247	Total	C	N	O	P	S	0	0	0
			1972	1260	328	370	2	12			
1	C	245	Total	C	N	O	P	S	0	0	0
			1957	1252	326	365	2	12			
1	D	256	Total	C	N	O	P	S	0	0	0
			2039	1301	340	384	2	12			
1	E	250	Total	C	N	O	P	S	0	0	0
			1990	1271	332	373	2	12			
1	F	253	Total	C	N	O	P	S	0	0	0
			2012	1286	335	377	2	12			
1	G	256	Total	C	N	O	P	S	0	0	0
			2039	1301	340	384	2	12			
1	H	249	Total	C	N	O	P	S	0	0	0
			1984	1268	331	371	2	12			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	MET	-	expression tag	UNP P42527
A	536	GLY	-	expression tag	UNP P42527
A	537	GLY	-	expression tag	UNP P42527
A	538	HIS	-	expression tag	UNP P42527
A	539	HIS	-	expression tag	UNP P42527
A	540	HIS	-	expression tag	UNP P42527
A	541	HIS	-	expression tag	UNP P42527
A	542	HIS	-	expression tag	UNP P42527
A	543	HIS	-	expression tag	UNP P42527
A	544	GLY	-	expression tag	UNP P42527
A	545	GLU	-	expression tag	UNP P42527
A	546	ASN	-	expression tag	UNP P42527
A	547	LEU	-	expression tag	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
A	548	TYR	-	expression tag	UNP P42527
A	549	PHE	-	expression tag	UNP P42527
A	550	GLN	-	expression tag	UNP P42527
A	551	GLY	-	expression tag	UNP P42527
B	535	MET	-	expression tag	UNP P42527
B	536	GLY	-	expression tag	UNP P42527
B	537	GLY	-	expression tag	UNP P42527
B	538	HIS	-	expression tag	UNP P42527
B	539	HIS	-	expression tag	UNP P42527
B	540	HIS	-	expression tag	UNP P42527
B	541	HIS	-	expression tag	UNP P42527
B	542	HIS	-	expression tag	UNP P42527
B	543	HIS	-	expression tag	UNP P42527
B	544	GLY	-	expression tag	UNP P42527
B	545	GLU	-	expression tag	UNP P42527
B	546	ASN	-	expression tag	UNP P42527
B	547	LEU	-	expression tag	UNP P42527
B	548	TYR	-	expression tag	UNP P42527
B	549	PHE	-	expression tag	UNP P42527
B	550	GLN	-	expression tag	UNP P42527
B	551	GLY	-	expression tag	UNP P42527
C	535	MET	-	expression tag	UNP P42527
C	536	GLY	-	expression tag	UNP P42527
C	537	GLY	-	expression tag	UNP P42527
C	538	HIS	-	expression tag	UNP P42527
C	539	HIS	-	expression tag	UNP P42527
C	540	HIS	-	expression tag	UNP P42527
C	541	HIS	-	expression tag	UNP P42527
C	542	HIS	-	expression tag	UNP P42527
C	543	HIS	-	expression tag	UNP P42527
C	544	GLY	-	expression tag	UNP P42527
C	545	GLU	-	expression tag	UNP P42527
C	546	ASN	-	expression tag	UNP P42527
C	547	LEU	-	expression tag	UNP P42527
C	548	TYR	-	expression tag	UNP P42527
C	549	PHE	-	expression tag	UNP P42527
C	550	GLN	-	expression tag	UNP P42527
C	551	GLY	-	expression tag	UNP P42527
D	535	MET	-	expression tag	UNP P42527
D	536	GLY	-	expression tag	UNP P42527
D	537	GLY	-	expression tag	UNP P42527
D	538	HIS	-	expression tag	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
D	539	HIS	-	expression tag	UNP P42527
D	540	HIS	-	expression tag	UNP P42527
D	541	HIS	-	expression tag	UNP P42527
D	542	HIS	-	expression tag	UNP P42527
D	543	HIS	-	expression tag	UNP P42527
D	544	GLY	-	expression tag	UNP P42527
D	545	GLU	-	expression tag	UNP P42527
D	546	ASN	-	expression tag	UNP P42527
D	547	LEU	-	expression tag	UNP P42527
D	548	TYR	-	expression tag	UNP P42527
D	549	PHE	-	expression tag	UNP P42527
D	550	GLN	-	expression tag	UNP P42527
D	551	GLY	-	expression tag	UNP P42527
E	535	MET	-	expression tag	UNP P42527
E	536	GLY	-	expression tag	UNP P42527
E	537	GLY	-	expression tag	UNP P42527
E	538	HIS	-	expression tag	UNP P42527
E	539	HIS	-	expression tag	UNP P42527
E	540	HIS	-	expression tag	UNP P42527
E	541	HIS	-	expression tag	UNP P42527
E	542	HIS	-	expression tag	UNP P42527
E	543	HIS	-	expression tag	UNP P42527
E	544	GLY	-	expression tag	UNP P42527
E	545	GLU	-	expression tag	UNP P42527
E	546	ASN	-	expression tag	UNP P42527
E	547	LEU	-	expression tag	UNP P42527
E	548	TYR	-	expression tag	UNP P42527
E	549	PHE	-	expression tag	UNP P42527
E	550	GLN	-	expression tag	UNP P42527
E	551	GLY	-	expression tag	UNP P42527
F	535	MET	-	expression tag	UNP P42527
F	536	GLY	-	expression tag	UNP P42527
F	537	GLY	-	expression tag	UNP P42527
F	538	HIS	-	expression tag	UNP P42527
F	539	HIS	-	expression tag	UNP P42527
F	540	HIS	-	expression tag	UNP P42527
F	541	HIS	-	expression tag	UNP P42527
F	542	HIS	-	expression tag	UNP P42527
F	543	HIS	-	expression tag	UNP P42527
F	544	GLY	-	expression tag	UNP P42527
F	545	GLU	-	expression tag	UNP P42527
F	546	ASN	-	expression tag	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
F	547	LEU	-	expression tag	UNP P42527
F	548	TYR	-	expression tag	UNP P42527
F	549	PHE	-	expression tag	UNP P42527
F	550	GLN	-	expression tag	UNP P42527
F	551	GLY	-	expression tag	UNP P42527
G	535	MET	-	expression tag	UNP P42527
G	536	GLY	-	expression tag	UNP P42527
G	537	GLY	-	expression tag	UNP P42527
G	538	HIS	-	expression tag	UNP P42527
G	539	HIS	-	expression tag	UNP P42527
G	540	HIS	-	expression tag	UNP P42527
G	541	HIS	-	expression tag	UNP P42527
G	542	HIS	-	expression tag	UNP P42527
G	543	HIS	-	expression tag	UNP P42527
G	544	GLY	-	expression tag	UNP P42527
G	545	GLU	-	expression tag	UNP P42527
G	546	ASN	-	expression tag	UNP P42527
G	547	LEU	-	expression tag	UNP P42527
G	548	TYR	-	expression tag	UNP P42527
G	549	PHE	-	expression tag	UNP P42527
G	550	GLN	-	expression tag	UNP P42527
G	551	GLY	-	expression tag	UNP P42527
H	535	MET	-	expression tag	UNP P42527
H	536	GLY	-	expression tag	UNP P42527
H	537	GLY	-	expression tag	UNP P42527
H	538	HIS	-	expression tag	UNP P42527
H	539	HIS	-	expression tag	UNP P42527
H	540	HIS	-	expression tag	UNP P42527
H	541	HIS	-	expression tag	UNP P42527
H	542	HIS	-	expression tag	UNP P42527
H	543	HIS	-	expression tag	UNP P42527
H	544	GLY	-	expression tag	UNP P42527
H	545	GLU	-	expression tag	UNP P42527
H	546	ASN	-	expression tag	UNP P42527
H	547	LEU	-	expression tag	UNP P42527
H	548	TYR	-	expression tag	UNP P42527
H	549	PHE	-	expression tag	UNP P42527
H	550	GLN	-	expression tag	UNP P42527
H	551	GLY	-	expression tag	UNP P42527

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	O 9	0	0
3	B	13	Total 13	O 13	0	0
3	C	5	Total 5	O 5	0	0
3	D	9	Total 9	O 9	0	0
3	E	7	Total 7	O 7	0	0
3	F	7	Total 7	O 7	0	0
3	G	11	Total 11	O 11	0	0
3	H	3	Total 3	O 3	0	0

3 Residue-property plots (i)

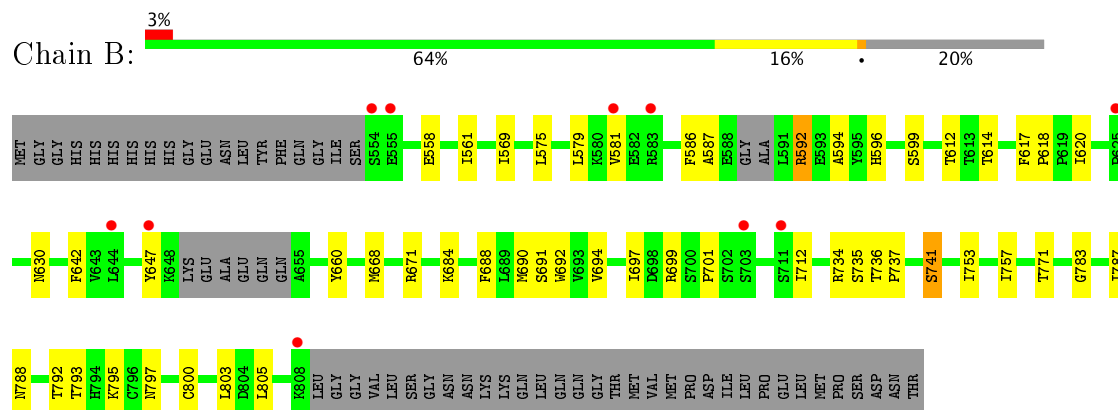These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.
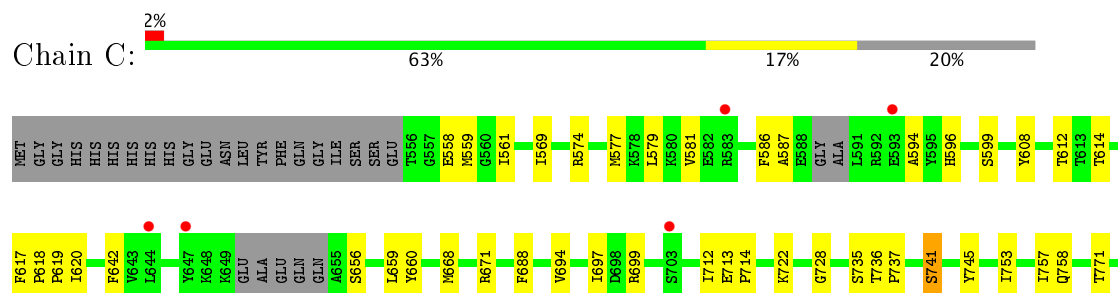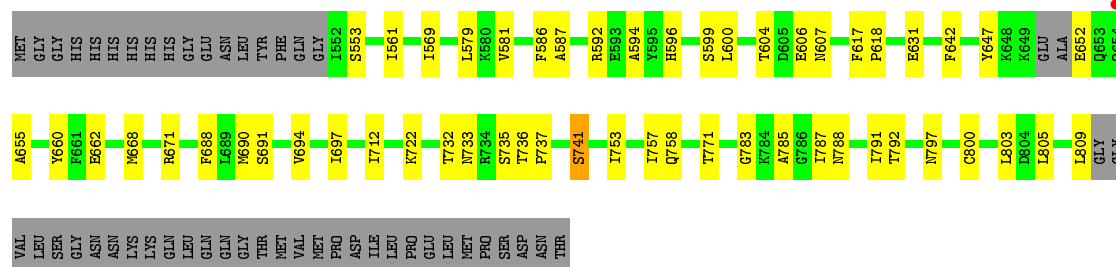
- Molecule 1: Myosin-II heavy chain kinase A
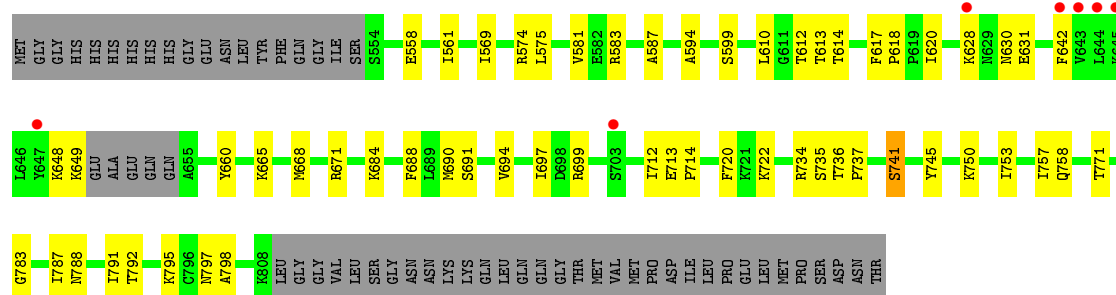
Chain A:

- Molecule 1: Myosin-II heavy chain kinase A
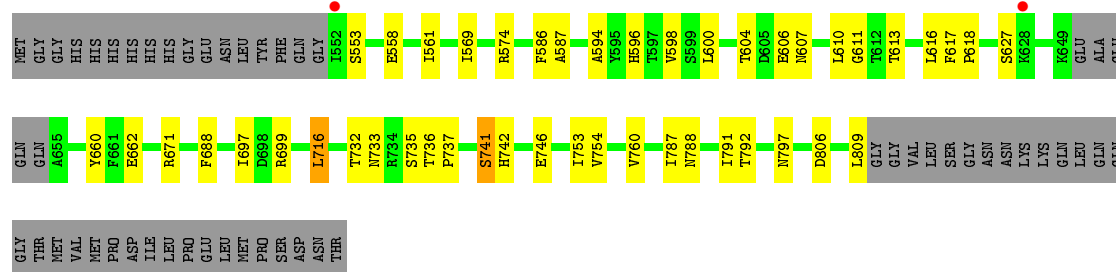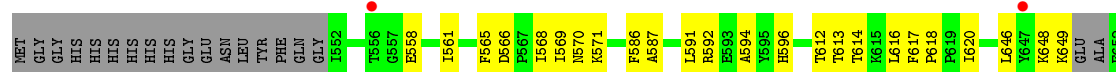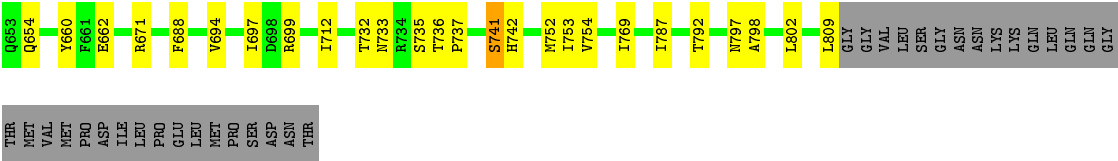
Chain B:

- Molecule 1: Myosin-II heavy chain kinase A

Chain C:

G783 I787 N788 I791 T792 T793 H794 K795 C796 N797 V807 LYS LEU GLY GLY VAL LEU SER GLY ASN ASN LYS LYS GLN LEU GLN GLN GLY THR MET VAL MET PRO ASP ILE LEU PRO GLU LEU MET PRO SER ASP ASN THR

• Molecule 1: Myosin-II heavy chain kinase A

Chain D:

66%   17%   17%

MET GLY GLY HIS HIS HIS HIS HIS HIS GLY GLU ASN LEU TYR PHE GLN GLY I552 S553 I561 I569 L579 K580 V581 F586 A587 R592 E593 A594 Y595 H596 S599 L600 T604 D605 E606 N607 F617 P618 E631 F642 Y647 K648 K649 GLU ALA E652 Q653 Q654

A655 Y660 F661 E662 M668 R671 F688 L689 M690 S691 V694 I697 I712 K722 T732 N733 R734 S735 T736 P737 S741 I753 I757 Q758 T771 G783 K784 A785 G786 I787 N788 I791 T792 N797 C800 L803 D804 L805 L809 GLY GLY

VAL LEU SER GLY ASN ASN LYS LYS GLN LEU GLN GLN GLY THR MET VAL MET PRO ASP ILE LEU PRO GLU LEU MET PRO SER ASP ASN THR

• Molecule 1: Myosin-II heavy chain kinase A

Chain E:

2%

63%   19%   19%

MET GLY GLY HIS HIS HIS HIS HIS HIS GLY GLU ASN LEU TYR PHE GLN GLY ILE SER S554 E558 I561 I569 R574 L575 V581 E582 R583 A587 A594 S599 L610 G611 T612 T613 T614 F617 P618 P619 I620 K628 N629 N630 E631 F642 V643 L644 K645

L646 Y647 K648 K649 GLU ALA GLU GLN GLN A655 Y660 K665 M668 R671 K684 F688 L689 M690 S691 V694 I697 D698 R699 S703 I712 E713 P714 F720 K721 K722 R734 S735 T736 P737 S741 Y745 K750 I753 I757 Q758 T771

G783 I787 N788 I791 T792 K795 C796 N797 A798 K808 LEU GLY GLY VAL LEU SER GLY ASN ASN LYS LYS GLN LEU GLN GLN GLY THR MET VAL MET PRO ASP ILE LEU PRO GLU LEU MET PRO SER ASP ASN THR

• Molecule 1: Myosin-II heavy chain kinase A

Chain F:

.%

67%   14%   •   18%

MET GLY GLY HIS HIS HIS HIS HIS HIS GLY GLU ASN LEU TYR PHE GLN GLY I552 S553 E558 I561 I569 R574 F586 A587 A594 S595 H596 T597 V598 S599 L600 T604 D605 E606 N607 L610 G611 T612 T613 L616 F617 P618 S627 K628 K649 GLU ALA GLU

GLN GLN A655 Y660 F661 E662 R671 F688 I697 D698 R699 L716 T732 N733 R734 S735 T736 P737 S741 H742 E746 I753 V754 V760 I787 N788 I791 T792 N797 D806 L809 GLY VAL LEU SER GLY ASN ASN LYS LYS GLN LEU GLN GLN

GLY THR MET VAL MET PRO ASP ILE LEU PRO GLU LEU MET PRO SER ASP ASN THR

• Molecule 1: Myosin-II heavy chain kinase A

Chain G:

.%

67%   16%   17%

MET GLY GLY HIS HIS HIS HIS HIS HIS GLY GLU ASN LEU TYR PHE GLN GLY I552 T556 G557 E558 I561 F565 D566 P567 I568 I569 N570 K571 F586 A587 L591 R592 E593 A594 Y595 H596 T612 T613 T614 K615 L616 F617 P618 P619 I620 L646 Y647 K648 K649 GLU ALA E652

Q653 Q654 Y660 F661 E662 R671 F688 V694 I697 D698 R699 I712 T732 N733 R734 S735 T736 P737 S741 H742 M752 I753 V754 I769 I787 T792 N797 A798 L802 L809 GLY GLY VAL LEU SER GLY ASN ASN LYS LYS GLN LEU GLN GLY GLY

THR MET VAL MET PRO ASP ILE LEU PRO GLU LEU MET PRO SER ASP ASN THR

• Molecule 1: Myosin-II heavy chain kinase A

Chain H:

2%

64%   16%   19%

MET GLY GLY HIS HIS HIS HIS HIS HIS GLY GLU ASN LEU TYR PHE GLN GLY ILE SER SER E555 T556 G557 E558 I561 R574 K584 P585 F586 A587 A590 L591 R592 E593 A594 Y595 H596 S599 T604 D605 E606 N607 T612 T613 T614 K615 I616 F617 P618 P619 I620 F642

V643 L644 Y647 K648 K649 GLU ALA GLU GLN GLN A655 Y660 R671 F688 V694 I697 D698 R699 S703 I712 K722 S735 T736 P737 S741 Y745 I753 I757 Q758 T771 P772 G783 K784 I787 I791 T792 K795 C796 N797 C800

L803 D804 L805 K808 LEU GLY GLY VAL LEU SER GLY ASN ASN LYS LYS GLN LEU GLN GLY GLN GLY THR MET VAL MET PRO ASP ILE LEU PRO GLU LEU MET PRO SER ASP ASN THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.30Å 103.47Å 167.81Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 38.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (40.00-2.90) 97.4 (38.93-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.241 , 0.268 0.241 , 0.267	Depositor DCC
R_{free} test set	3125 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	75.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.0	EDS
L-test for twinning[2]	$< |L| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16069	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.00 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.9391e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]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: TPO, ZN, PHD

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	0.53	0/2022	0.81	1/2725 (0.0%)
1	B	0.52	0/1989	0.80	0/2680
1	C	0.51	0/1974	0.78	2/2660 (0.1%)
1	D	0.49	0/2057	0.77	0/2772
1	E	0.53	0/2008	0.81	2/2706 (0.1%)
1	F	0.51	0/2030	0.82	1/2736 (0.0%)
1	G	0.52	0/2057	0.77	0/2772
1	H	0.53	0/2002	0.80	1/2698 (0.0%)
All	All	0.52	0/16139	0.80	7/21749 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	577	MET	CG-SD-CE	6.71	110.94	100.20
1	A	583	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	E	583	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	F	716	LEU	CB-CG-CD1	5.25	119.92	111.00
1	E	610	LEU	N-CA-C	5.21	125.08	111.00

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	2004	0	2017	48	0
1	B	1972	0	1980	37	0
1	C	1957	0	1969	31	0
1	D	2039	0	2050	38	0
1	E	1990	0	2002	45	0
1	F	2012	0	2028	26	0
1	G	2039	0	2050	39	0
1	H	1984	0	1997	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	9	0	0	2	0
3	B	13	0	0	1	0
3	C	5	0	0	0	0
3	D	9	0	0	1	0
3	E	7	0	0	2	0
3	F	7	0	0	0	0
3	G	11	0	0	0	0
3	H	3	0	0	0	0
All	All	16069	0	16093	281	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 9.

The worst 5 of 281 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:C:614:THR:HG21	1:C:619:PRO:HA	1.22	1.17
1:H:614:THR:HG21	1:H:619:PRO:HA	1.39	1.03
1:F:716:LEU:HD21	1:F:760:VAL:HG23	1.54	0.87
1:G:566:ASP:OD2	1:G:569:ILE:HD12	1.76	0.85
1:A:630:ASN:HD21	1:A:633:MET:HG2	1.44	0.81

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	246/307 (80%)	239 (97%)	7 (3%)	0	100	100
1	B	239/307 (78%)	229 (96%)	10 (4%)	0	100	100
1	C	237/307 (77%)	229 (97%)	8 (3%)	0	100	100
1	D	250/307 (81%)	241 (96%)	9 (4%)	0	100	100
1	E	244/307 (80%)	236 (97%)	8 (3%)	0	100	100
1	F	247/307 (80%)	238 (96%)	9 (4%)	0	100	100
1	G	250/307 (81%)	243 (97%)	7 (3%)	0	100	100
1	H	243/307 (79%)	232 (96%)	11 (4%)	0	100	100
All	All	1956/2456 (80%)	1887 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 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	222/268 (83%)	220 (99%)	2 (1%)	82	95
1	B	219/268 (82%)	215 (98%)	4 (2%)	64	89
1	C	217/268 (81%)	215 (99%)	2 (1%)	82	95
1	D	226/268 (84%)	223 (99%)	3 (1%)	73	93
1	E	220/268 (82%)	218 (99%)	2 (1%)	82	95
1	F	223/268 (83%)	218 (98%)	5 (2%)	57	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	226/268 (84%)	223 (99%)	3 (1%)	73	93
1	H	219/268 (82%)	217 (99%)	2 (1%)	82	95
All	All	1772/2144 (83%)	1749 (99%)	23 (1%)	73	93

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	741	SER
1	E	741	SER
1	H	660	TYR
1	E	660	TYR
1	F	598	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	596	HIS
1	C	738	GLN
1	F	596	HIS
1	C	570	ASN
1	E	758	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)

16 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	TPO	A	612	1	9,10,11	0.62	0	10,14,16	1.50	2 (20%)
1	PHD	A	663	1	10,11,12	0.91	1 (10%)	12,15,17	2.10	4 (33%)
1	TPO	B	612	1	9,10,11	1.02	0	10,14,16	1.18	1 (10%)
1	PHD	B	663	1	10,11,12	1.04	1 (10%)	12,15,17	2.14	4 (33%)
1	TPO	C	612	1	9,10,11	1.31	2 (22%)	10,14,16	1.16	0
1	PHD	C	663	1	10,11,12	1.09	1 (10%)	12,15,17	2.02	4 (33%)
1	TPO	D	612	1	9,10,11	0.77	0	10,14,16	1.60	3 (30%)
1	PHD	D	663	1	10,11,12	0.79	0	12,15,17	2.14	4 (33%)
1	TPO	E	612	1	9,10,11	1.09	1 (11%)	10,14,16	1.49	1 (10%)
1	PHD	E	663	1	10,11,12	0.82	1 (10%)	12,15,17	2.10	4 (33%)
1	TPO	F	612	1	9,10,11	0.57	0	10,14,16	1.71	2 (20%)
1	PHD	F	663	1	10,11,12	0.90	1 (10%)	12,15,17	2.11	4 (33%)
1	TPO	G	612	1	9,10,11	0.65	0	10,14,16	1.64	3 (30%)
1	PHD	G	663	1	10,11,12	0.96	1 (10%)	12,15,17	2.13	5 (41%)
1	TPO	H	612	1	9,10,11	1.15	1 (11%)	10,14,16	1.33	0
1	PHD	H	663	1	10,11,12	1.09	1 (10%)	12,15,17	2.04	4 (33%)

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	TPO	A	612	1	-	0/8/11/13	0/0/0/0
1	PHD	A	663	1	-	0/7/11/13	0/0/0/0
1	TPO	B	612	1	-	0/8/11/13	0/0/0/0
1	PHD	B	663	1	-	0/7/11/13	0/0/0/0
1	TPO	C	612	1	-	0/8/11/13	0/0/0/0
1	PHD	C	663	1	-	0/7/11/13	0/0/0/0
1	TPO	D	612	1	-	0/8/11/13	0/0/0/0
1	PHD	D	663	1	-	0/7/11/13	0/0/0/0
1	TPO	E	612	1	-	0/8/11/13	0/0/0/0
1	PHD	E	663	1	-	0/7/11/13	0/0/0/0
1	TPO	F	612	1	-	0/8/11/13	0/0/0/0
1	PHD	F	663	1	-	0/7/11/13	0/0/0/0
1	TPO	G	612	1	-	0/8/11/13	0/0/0/0
1	PHD	G	663	1	-	0/7/11/13	0/0/0/0
1	TPO	H	612	1	-	0/8/11/13	0/0/0/0
1	PHD	H	663	1	-	0/7/11/13	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	612	TPO	CA-C	-2.60	1.46	1.50
1	C	612	TPO	CB-CA	-2.54	1.49	1.53
1	E	612	TPO	CA-C	-2.52	1.47	1.50
1	C	612	TPO	CA-C	-2.49	1.47	1.50
1	E	663	PHD	P-OD1	2.21	1.63	1.59

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	663	PHD	CB-CA-C	-3.31	105.04	111.41
1	H	663	PHD	OD2-CG-CB	-3.30	117.26	124.70
1	E	663	PHD	OD2-CG-CB	-3.28	117.30	124.70
1	D	663	PHD	CB-CA-C	-3.28	105.09	111.41
1	C	663	PHD	OD2-CG-CB	-3.25	117.36	124.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	612	TPO	1	0
1	B	612	TPO	2	0
1	C	612	TPO	2	0
1	E	612	TPO	2	0
1	G	612	TPO	1	0
1	H	612	TPO	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	250/307 (81%)	0.01	1 (0%)	92	92	50, 72, 118, 139	0
1	B	245/307 (79%)	0.10	10 (4%)	38	32	50, 78, 122, 146	0
1	C	243/307 (79%)	0.14	5 (2%)	64	60	50, 80, 127, 147	0
1	D	254/307 (82%)	-0.02	1 (0%)	92	92	45, 69, 116, 155	0
1	E	248/307 (80%)	0.10	7 (2%)	53	48	51, 77, 125, 143	0
1	F	251/307 (81%)	-0.00	2 (0%)	86	85	47, 68, 114, 159	0
1	G	254/307 (82%)	0.02	2 (0%)	86	85	48, 72, 125, 156	0
1	H	247/307 (80%)	0.16	7 (2%)	53	48	51, 82, 127, 155	0
All	All	1992/2456 (81%)	0.06	35 (1%)	69	66	45, 74, 124, 159	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	703	SER	4.2
1	B	554	SER	3.8
1	H	703	SER	3.7
1	B	808	LYS	3.3
1	B	711	SER	3.2

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPO	C	612	11/12	0.95	0.14	-	63,71,79,81	0
1	TPO	A	612	11/12	0.97	0.12	-	52,62,68,68	0
1	TPO	G	612	11/12	0.97	0.18	-	49,60,66,68	0
1	TPO	B	612	11/12	0.98	0.12	-	56,63,72,73	0
1	PHD	E	663	12/13	0.93	0.12	-	71,80,95,98	0
1	TPO	F	612	11/12	0.97	0.16	-	51,61,71,76	0
1	PHD	A	663	12/13	0.92	0.16	-	61,87,102,105	0
1	TPO	E	612	11/12	0.97	0.15	-	56,66,77,79	0
1	PHD	C	663	12/13	0.93	0.15	-	64,80,95,102	0
1	PHD	B	663	12/13	0.93	0.11	-	73,82,93,96	0
1	TPO	H	612	11/12	0.95	0.15	-	69,75,83,86	0
1	PHD	D	663	12/13	0.89	0.17	-	59,84,104,110	0
1	PHD	G	663	12/13	0.88	0.19	-	59,87,106,107	0
1	PHD	F	663	12/13	0.92	0.15	-	56,84,99,100	0
1	PHD	H	663	12/13	0.92	0.12	-	69,80,97,100	0
1	TPO	D	612	11/12	0.96	0.18	-	51,57,60,64	0

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. 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	D	901	1/1	0.99	0.16	-0.16	72,72,72,72	0
2	ZN	A	901	1/1	0.99	0.17	-0.18	76,76,76,76	0
2	ZN	G	901	1/1	0.97	0.17	-0.23	77,77,77,77	0
2	ZN	F	901	1/1	1.00	0.17	-0.28	72,72,72,72	0
2	ZN	E	901	1/1	0.99	0.17	-0.37	77,77,77,77	0
2	ZN	C	901	1/1	1.00	0.17	-0.42	63,63,63,63	0
2	ZN	H	901	1/1	0.99	0.12	-1.27	69,69,69,69	0
2	ZN	B	901	1/1	0.99	0.09	-1.72	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.