wwPDB X-ray Structure Validation Summary Report (i)

Jan 16, 2023 – 01:55 pm GMT

PDB ID	:	1HKX
Title	:	Crystal structure of calcium/calmodulin-dependent protein kinase
Authors	:	Hoelz, A.; Nairn, A.C.; Kuriyan, J.
Deposited on	:	2003-03-12
Resolution	:	2.65 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 (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:

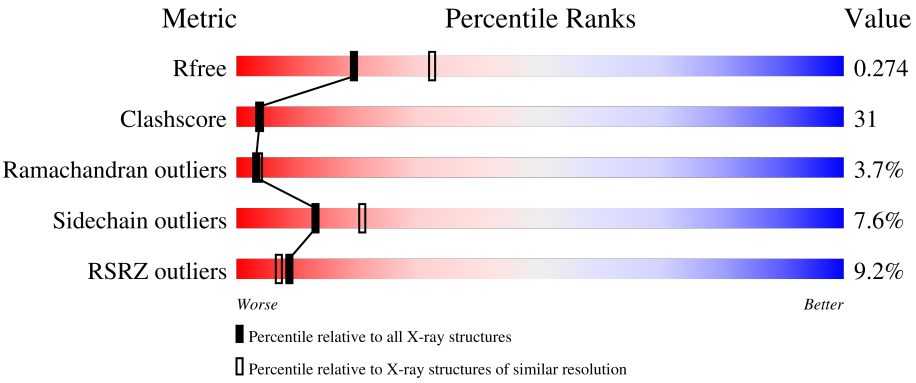
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	147	9% 57% 33% 6% •
1	B	147	5% 56% 31% 5% • 7%
1	C	147	8% 48% 40% 6% 5%
1	D	147	12% 46% 41% 6% • 6%
1	E	147	10% 56% 37% 5% •

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Mol	Chain	Length	Quality of chain
1	F	147	10% 53% 33% 7% • 5%
1	G	147	7% 55% 31% 6% • 7%
1	H	147	14% 55% 35% 7% • •
1	I	147	7% 52% 31% 7% • 8%
1	J	147	9% 41% 46% 7% 5%
1	K	147	7% 41% 44% 5% • 8%
1	L	147	7% 43% 39% 9% • 8%
1	M	147	7% 48% 39% 8% 5%
1	N	147	8% 53% 33% 7% 7%

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
2	DTT	A	1475	X	X	X	X
3	CL	I	1475	-	-	X	-
4	TBR	A	2000	-	-	X	-

2 Entry composition (i)

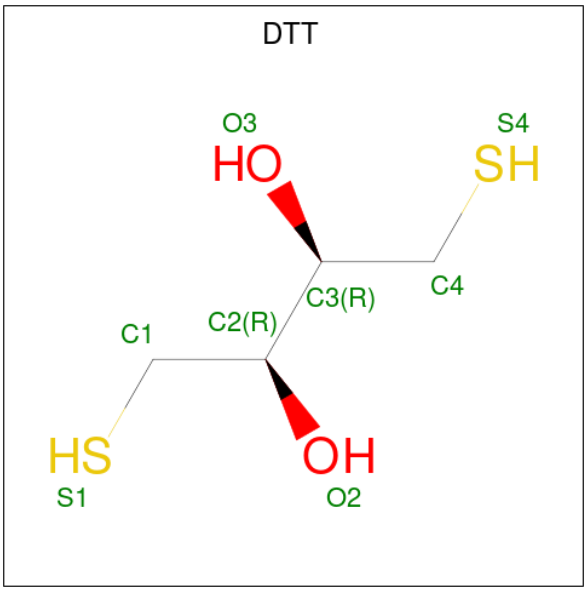
There are 5 unique types of molecules in this entry. The entry contains 15690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	1
			1135	713	201	215	6			
1	B	136	Total	C	N	O	S	0	0	1
			1096	689	196	206	5			
1	C	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	D	138	Total	C	N	O	S	0	0	1
			1113	700	198	210	5			
1	E	144	Total	C	N	O	S	0	0	1
			1156	726	206	218	6			
1	F	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	G	136	Total	C	N	O	S	0	0	1
			1096	689	196	206	5			
1	H	143	Total	C	N	O	S	0	0	1
			1152	724	205	217	6			
1	I	135	Total	C	N	O	S	0	0	1
			1088	685	195	203	5			
1	J	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	K	135	Total	C	N	O	S	0	0	1
			1088	685	195	203	5			
1	L	135	Total	C	N	O	S	0	0	1
			1088	685	195	203	5			
1	M	139	Total	C	N	O	S	0	0	1
			1120	704	199	212	5			
1	N	136	Total	C	N	O	S	0	0	1
			1096	689	196	206	5			

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 8 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0

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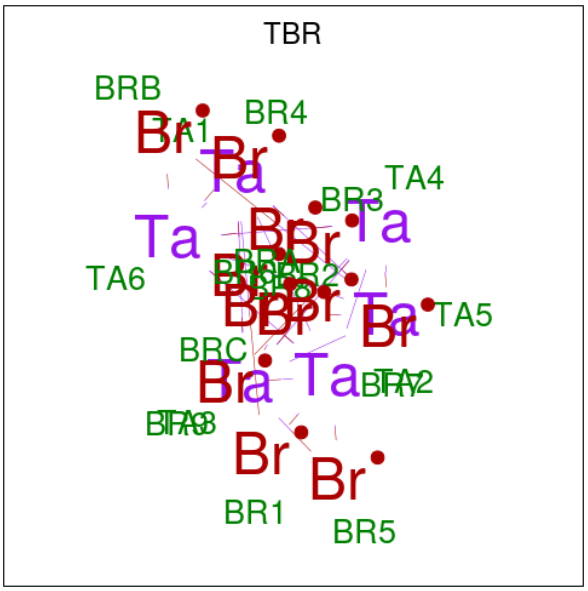
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Cl 1 1	0	0
3	M	1	Total Cl 1 1	0	0
3	N	1	Total Cl 1 1	0	0

- Molecule 4 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Br Ta 18 12 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	4	Total O 4 4	0	0
5	C	5	Total O 5 5	0	0
5	D	4	Total O 4 4	0	0
5	E	4	Total O 4 4	0	0

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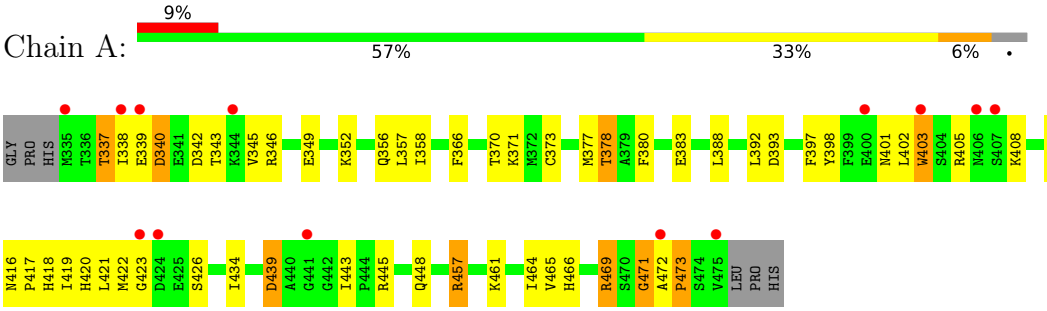
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	4	Total O 4 4	0	0
5	G	7	Total O 7 7	0	0
5	H	6	Total O 6 6	0	0
5	I	2	Total O 2 2	0	0
5	J	3	Total O 3 3	0	0
5	K	4	Total O 4 4	0	0
5	L	5	Total O 5 5	0	0
5	M	4	Total O 4 4	0	0
5	N	4	Total O 4 4	0	0

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.

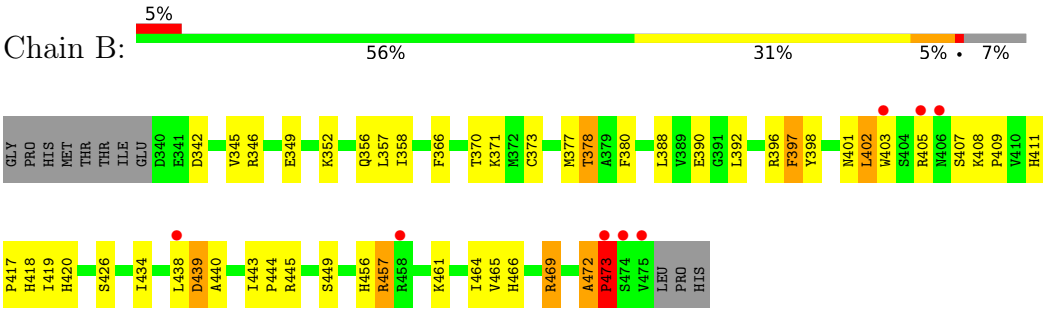
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain A:



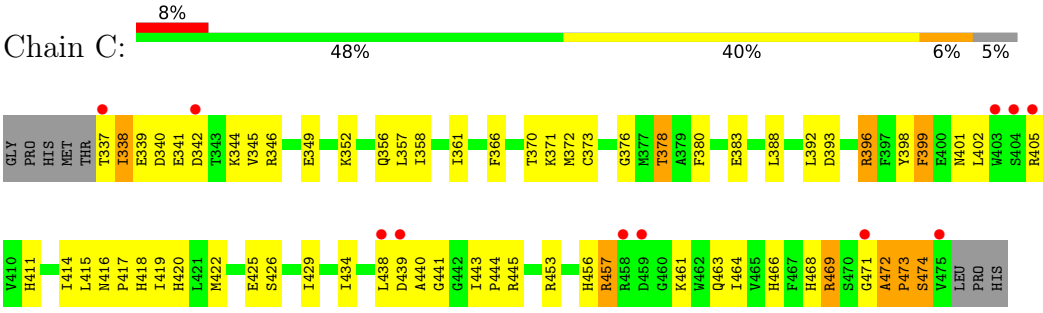
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain B:



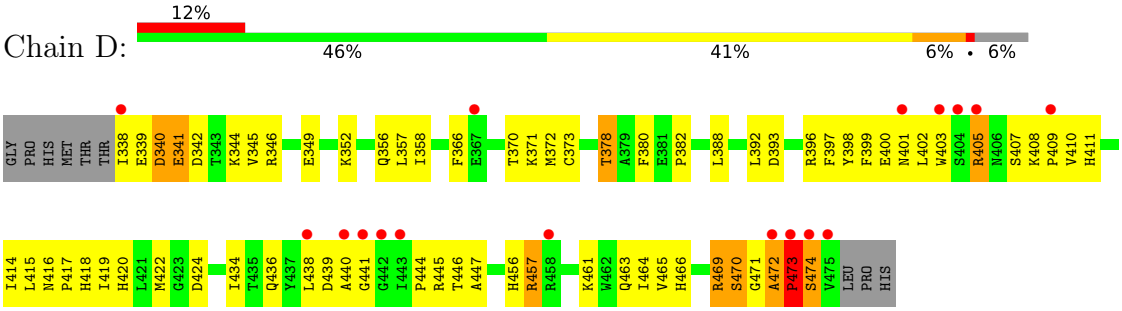
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain C:



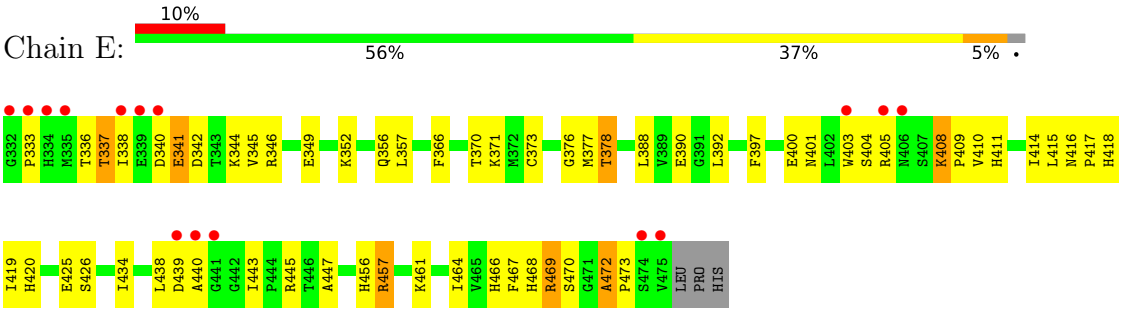
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain D:



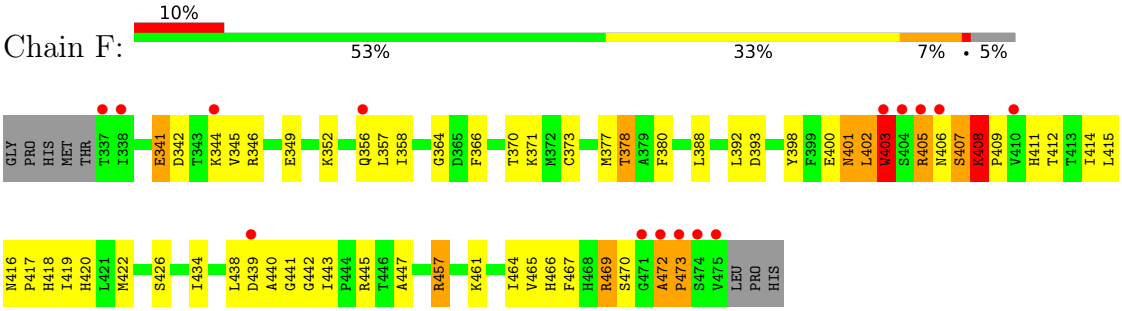
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain E:



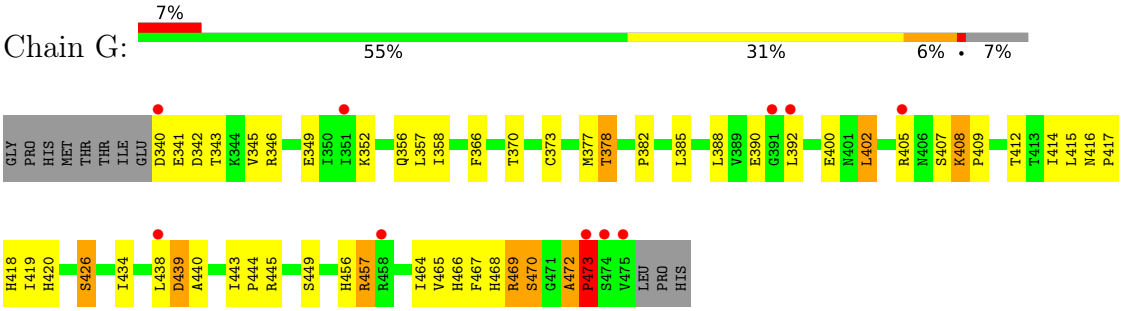
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain F:



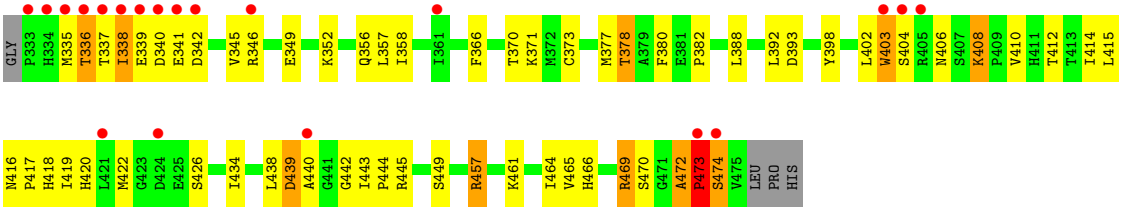
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain G:



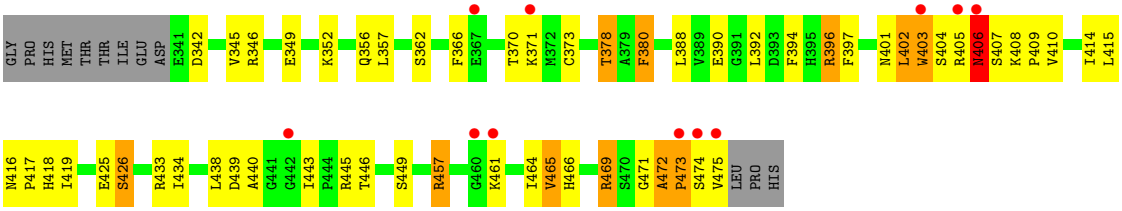
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain H:



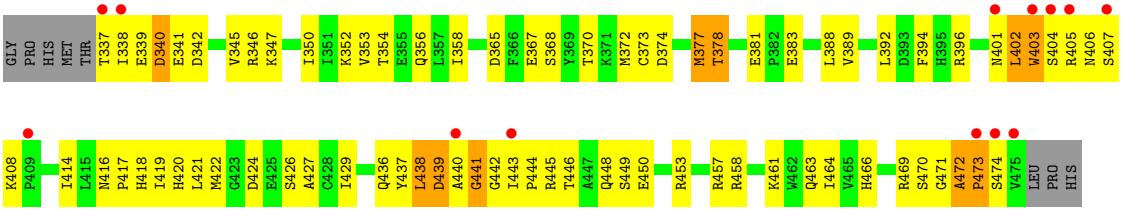
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain I:



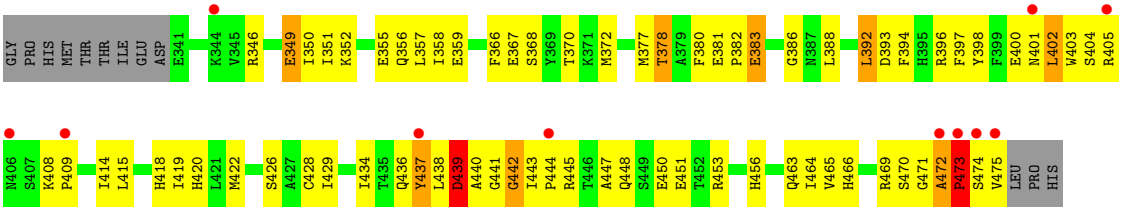
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain J:



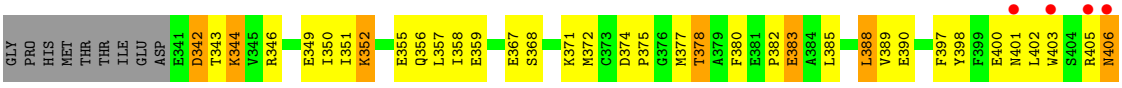
• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

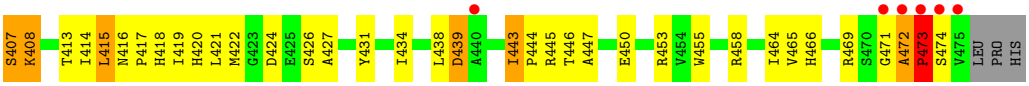
Chain K:



• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

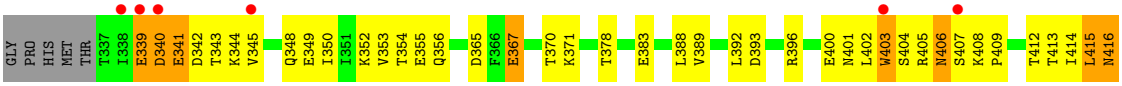
Chain L:

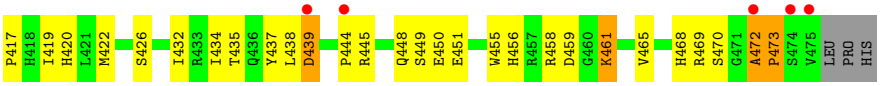




• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

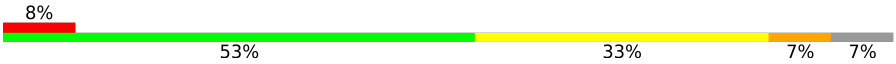
Chain M:

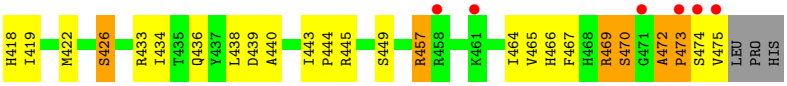




• Molecule 1: CALCIUM/CALMODULIN-DEPENDENT PROTEIN KINASE TYPE II ALPHA CHAIN

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.95Å 118.04Å 157.82Å 90.00° 110.91° 90.00°	Depositor
Resolution (Å)	19.84 – 2.65 89.76 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.84-2.65) 96.2 (89.76-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.279 0.243 , 0.274	Depositor DCC
R_{free} test set	6774 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15690	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TBR, DTT, CL

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	0.46	0/1163	0.70	3/1575 (0.2%)
1	B	0.43	0/1124	0.64	0/1522
1	C	0.41	0/1148	0.61	0/1555
1	D	0.42	0/1141	0.62	0/1545
1	E	0.41	0/1186	0.59	0/1607
1	F	0.42	0/1148	0.62	0/1555
1	G	0.41	0/1124	0.63	0/1522
1	H	0.42	0/1182	0.67	0/1601
1	I	0.41	0/1116	0.65	0/1511
1	J	0.46	0/1148	0.69	0/1555
1	K	0.44	0/1116	0.66	0/1511
1	L	0.45	0/1116	0.69	1/1511 (0.1%)
1	M	0.44	0/1148	0.67	0/1555
1	N	0.41	0/1124	0.62	0/1522
All	All	0.43	0/15984	0.65	4/21647 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	471	GLY	N-CA-C	-5.38	99.64	113.10
1	A	439	ASP	N-CA-CB	5.31	120.16	110.60
1	L	421	LEU	CA-CB-CG	5.25	127.37	115.30

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	1135	0	1089	72	0
1	B	1096	0	1049	69	0
1	C	1120	0	1073	72	0
1	D	1113	0	1066	91	0
1	E	1156	0	1106	68	0
1	F	1120	0	1073	86	0
1	G	1096	0	1049	68	0
1	H	1152	0	1104	72	0
1	I	1088	0	1045	71	0
1	J	1120	0	1073	88	0
1	K	1088	0	1045	91	0
1	L	1088	0	1045	83	0
1	M	1120	0	1073	58	0
1	N	1096	0	1049	65	0
2	A	8	0	8	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	2	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	18	0	0	4	0
5	A	6	0	0	1	0
5	B	4	0	0	0	0
5	C	5	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
5	G	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	6	0	0	1	0
5	I	2	0	0	1	0
5	J	3	0	0	0	0
5	K	4	0	0	0	0
5	L	5	0	0	0	0
5	M	4	0	0	0	0
5	N	4	0	0	0	0
All	All	15690	0	14947	955	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 31.

The worst 5 of 955 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:E:378:THR:HG22	1:E:466:HIS:ND1	1.63	1.12
1:B:378:THR:HG22	1:B:466:HIS:ND1	1.65	1.11
1:N:378:THR:HG22	1:N:466:HIS:ND1	1.65	1.09
1:C:409:PRO:HD2	1:C:438:LEU:HD12	1.31	1.07
1:M:458:ARG:HH11	1:M:458:ARG:HB2	1.14	1.07

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	139/147 (95%)	129 (93%)	7 (5%)	3 (2%)	6	9
1	B	134/147 (91%)	121 (90%)	10 (8%)	3 (2%)	6	9
1	C	137/147 (93%)	124 (90%)	9 (7%)	4 (3%)	4	6
1	D	136/147 (92%)	122 (90%)	10 (7%)	4 (3%)	4	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	142/147 (97%)	123 (87%)	14 (10%)	5 (4%)	3	4
1	F	137/147 (93%)	122 (89%)	8 (6%)	7 (5%)	2	2
1	G	134/147 (91%)	121 (90%)	8 (6%)	5 (4%)	3	4
1	H	141/147 (96%)	128 (91%)	6 (4%)	7 (5%)	2	2
1	I	133/147 (90%)	116 (87%)	14 (10%)	3 (2%)	6	8
1	J	137/147 (93%)	120 (88%)	11 (8%)	6 (4%)	2	2
1	K	133/147 (90%)	111 (84%)	16 (12%)	6 (4%)	2	2
1	L	133/147 (90%)	119 (90%)	9 (7%)	5 (4%)	3	3
1	M	137/147 (93%)	118 (86%)	12 (9%)	7 (5%)	2	2
1	N	134/147 (91%)	123 (92%)	6 (4%)	5 (4%)	3	4
All	All	1907/2058 (93%)	1697 (89%)	140 (7%)	70 (4%)	3	4

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ALA
1	B	397	PHE
1	C	472	ALA
1	C	473	PRO
1	C	474	SER

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	123/129 (95%)	113 (92%)	10 (8%)	11	17
1	B	118/129 (92%)	110 (93%)	8 (7%)	16	24
1	C	121/129 (94%)	114 (94%)	7 (6%)	20	31
1	D	120/129 (93%)	110 (92%)	10 (8%)	11	16
1	E	125/129 (97%)	118 (94%)	7 (6%)	21	33
1	F	121/129 (94%)	110 (91%)	11 (9%)	9	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	118/129 (92%)	110 (93%)	8 (7%)	16 24
1	H	125/129 (97%)	115 (92%)	10 (8%)	12 18
1	I	117/129 (91%)	107 (92%)	10 (8%)	10 15
1	J	121/129 (94%)	114 (94%)	7 (6%)	20 31
1	K	117/129 (91%)	109 (93%)	8 (7%)	16 24
1	L	117/129 (91%)	104 (89%)	13 (11%)	6 8
1	M	121/129 (94%)	110 (91%)	11 (9%)	9 13
1	N	118/129 (92%)	111 (94%)	7 (6%)	19 30
All	All	1682/1806 (93%)	1555 (92%)	127 (8%)	13 21

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	457	ARG
1	M	341	GLU
1	I	378	THR
1	M	339	GLU
1	M	461	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	411	HIS
1	M	348	GLN
1	J	436	GLN
1	L	348	GLN
1	M	418	HIS

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)

Of 16 ligands modelled in this entry, 14 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	$\#\|Z\| > 2$
4	TBR	A	2000	-	0,36,36	-	-	-		
2	DTT	A	1475	-	7,7,7	6.33	4 (57%)	4,8,8	4.71	4 (100%)

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
2	DTT	A	1475	-	2/2/2/2	2/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1475	DTT	O2-C2	-15.43	1.10	1.43
2	A	1475	DTT	C4-S4	-4.53	1.72	1.81
2	A	1475	DTT	O3-C3	-3.14	1.36	1.43
2	A	1475	DTT	C4-C3	-2.77	1.43	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1475	DTT	C3-C4-S4	-6.80	94.70	114.47
2	A	1475	DTT	C2-C1-S1	-4.52	101.31	114.47
2	A	1475	DTT	O2-C2-C3	4.08	118.10	109.72
2	A	1475	DTT	O3-C3-C2	-2.30	105.01	109.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1475	DTT	C3
2	A	1475	DTT	C2

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1475	DTT	O2-C2-C3-C4
2	A	1475	DTT	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2000	TBR	4	0
2	A	1475	DTT	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

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, 95^{th} 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	141/147 (95%)	0.78	13 (9%) 9 7	31, 56, 105, 116	0
1	B	136/147 (92%)	0.60	8 (5%) 22 19	30, 56, 102, 124	0
1	C	139/147 (94%)	0.78	12 (8%) 10 8	32, 58, 110, 126	0
1	D	138/147 (93%)	0.92	17 (12%) 4 2	31, 58, 114, 122	0
1	E	144/147 (97%)	0.87	15 (10%) 6 4	31, 58, 122, 159	0
1	F	139/147 (94%)	0.88	15 (10%) 5 4	30, 56, 107, 127	0
1	G	136/147 (92%)	0.66	10 (7%) 14 12	32, 55, 101, 117	0
1	H	143/147 (97%)	0.78	20 (13%) 2 2	33, 57, 110, 117	0
1	I	135/147 (91%)	0.60	11 (8%) 12 9	32, 57, 100, 119	0
1	J	139/147 (94%)	0.55	13 (9%) 8 6	28, 53, 113, 142	0
1	K	135/147 (91%)	0.63	11 (8%) 12 9	32, 57, 99, 120	0
1	L	135/147 (91%)	0.44	10 (7%) 14 12	26, 54, 92, 113	0
1	M	139/147 (94%)	0.45	11 (7%) 12 10	26, 48, 105, 130	0
1	N	136/147 (92%)	0.78	12 (8%) 10 8	31, 56, 102, 116	0
All	All	1935/2058 (94%)	0.70	178 (9%) 9 7	26, 56, 109, 159	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	332	GLY	15.3
1	F	475	VAL	11.3
1	D	473	PRO	11.2
1	L	475	VAL	10.9
1	K	473	PRO	10.3

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)

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, 95^{th} 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(Å^2)	Q<0.9
3	CL	D	1475	1/1	0.68	0.19	68,68,68,68	0
2	DTT	A	1475	8/8	0.77	0.49	72,75,77,79	0
3	CL	H	1475	1/1	0.83	0.16	66,66,66,66	0
3	CL	E	1475	1/1	0.84	0.19	68,68,68,68	0
3	CL	K	1475	1/1	0.86	0.17	62,62,62,62	0
3	CL	L	1475	1/1	0.86	0.10	60,60,60,60	0
3	CL	F	1475	1/1	0.90	0.23	53,53,53,53	0
3	CL	C	1475	1/1	0.92	0.18	65,65,65,65	0
3	CL	N	1475	1/1	0.92	0.21	55,55,55,55	0
3	CL	J	1475	1/1	0.94	0.12	52,52,52,52	0
3	CL	G	1475	1/1	0.94	0.18	56,56,56,56	0
3	CL	A	1476	1/1	0.94	0.11	54,54,54,54	0
3	CL	I	1475	1/1	0.94	0.15	58,58,58,58	0
3	CL	M	1475	1/1	0.95	0.13	55,55,55,55	0
3	CL	B	1475	1/1	0.95	0.18	58,58,58,58	0
4	TBR	A	2000	18/18	0.95	0.08	50,53,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.