wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:07 PM GMT

PDB ID	:	3SYV
Title	:	Crystal structure of mPACSIN 3 F-BAR domain mutant
Authors	:	Bai, X.
Deposited on	:	2011-07-18
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

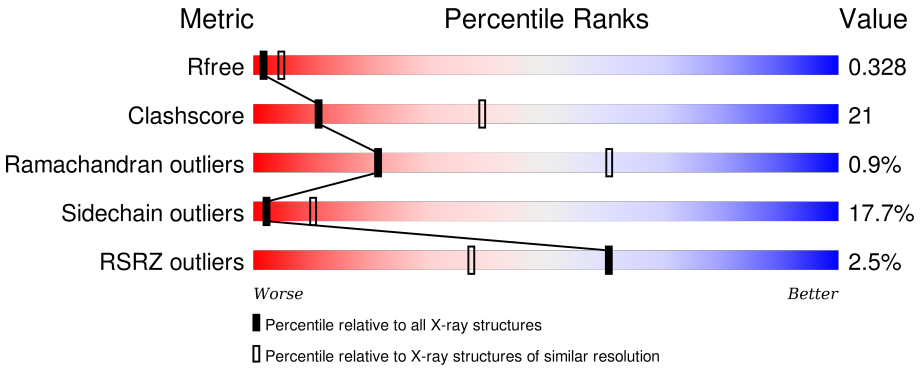
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	347	2% 43% 24% 5% 28%
1	B	347	2% 44% 25% 5% 26%
1	C	347	% 41% 26% 7% 26%
1	D	347	% 39% 29% 5% 27%
1	E	347	3% 39% 29% 6% 27%

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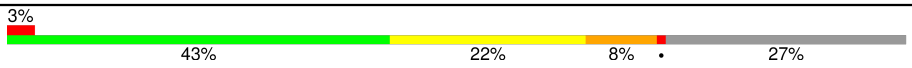
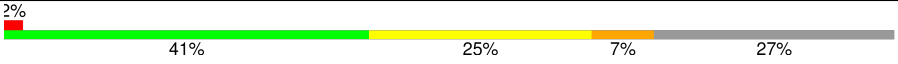
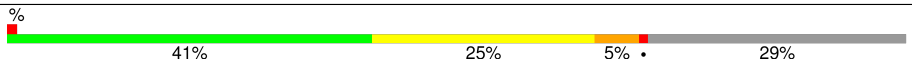
Mol	Chain	Length	Quality of chain
1	F	347	
1	G	347	
1	H	347	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16470 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 Protein kinase C and casein kinase II substrate protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			2047	1284	384	372	7			
1	B	257	Total	C	N	O	S	0	0	0
			2115	1317	403	387	8			
1	C	257	Total	C	N	O	S	0	0	0
			2061	1284	390	379	8			
1	D	255	Total	C	N	O	S	0	0	0
			2085	1304	396	378	7			
1	E	255	Total	C	N	O	S	0	0	1
			2044	1278	387	374	5			
1	F	255	Total	C	N	O	S	0	0	0
			2050	1283	392	369	6			
1	G	254	Total	C	N	O	S	0	0	0
			1978	1231	374	368	5			
1	H	247	Total	C	N	O	S	0	0	0
			1981	1236	378	364	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
A	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
A	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
A	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
A	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
A	0	HIS	-	EXPRESSION TAG	UNP Q99JB8
A	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8
B	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
B	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
B	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
B	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
B	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
B	0	HIS	-	EXPRESSION TAG	UNP Q99JB8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8
C	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
C	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
C	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
C	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
C	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
C	0	HIS	-	EXPRESSION TAG	UNP Q99JB8
C	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8
D	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
D	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
D	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
D	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
D	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
D	0	HIS	-	EXPRESSION TAG	UNP Q99JB8
D	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8
E	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
E	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
E	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
E	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
E	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
E	0	HIS	-	EXPRESSION TAG	UNP Q99JB8
E	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8
F	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
F	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
F	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
F	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
F	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
F	0	HIS	-	EXPRESSION TAG	UNP Q99JB8
F	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8
G	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
G	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
G	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
G	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
G	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
G	0	HIS	-	EXPRESSION TAG	UNP Q99JB8
G	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8
H	-5	HIS	-	EXPRESSION TAG	UNP Q99JB8
H	-4	HIS	-	EXPRESSION TAG	UNP Q99JB8
H	-3	HIS	-	EXPRESSION TAG	UNP Q99JB8
H	-2	HIS	-	EXPRESSION TAG	UNP Q99JB8
H	-1	HIS	-	EXPRESSION TAG	UNP Q99JB8
H	0	HIS	-	EXPRESSION TAG	UNP Q99JB8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	121	GLN	PRO	ENGINEERED MUTATION	UNP Q99JB8

- Molecule 2 is water.

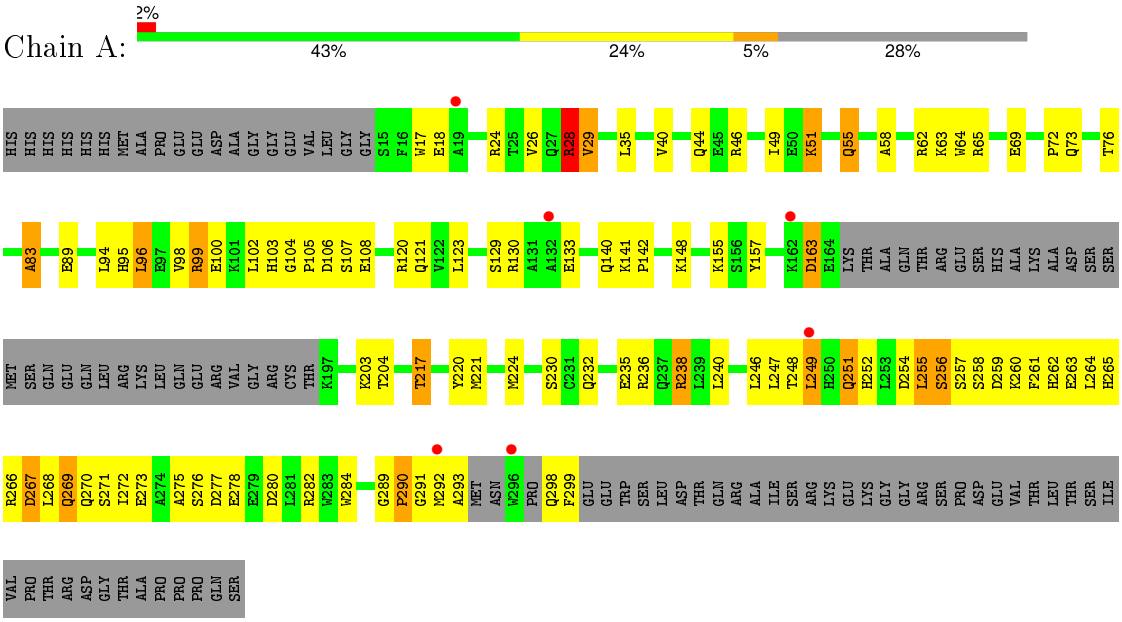
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	13	Total O 13 13	0	0
2	C	19	Total O 19 19	0	0
2	D	12	Total O 12 12	0	0
2	E	12	Total O 12 12	0	0
2	F	16	Total O 16 16	0	0
2	G	10	Total O 10 10	0	0
2	H	13	Total O 13 13	0	0

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 errors 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.

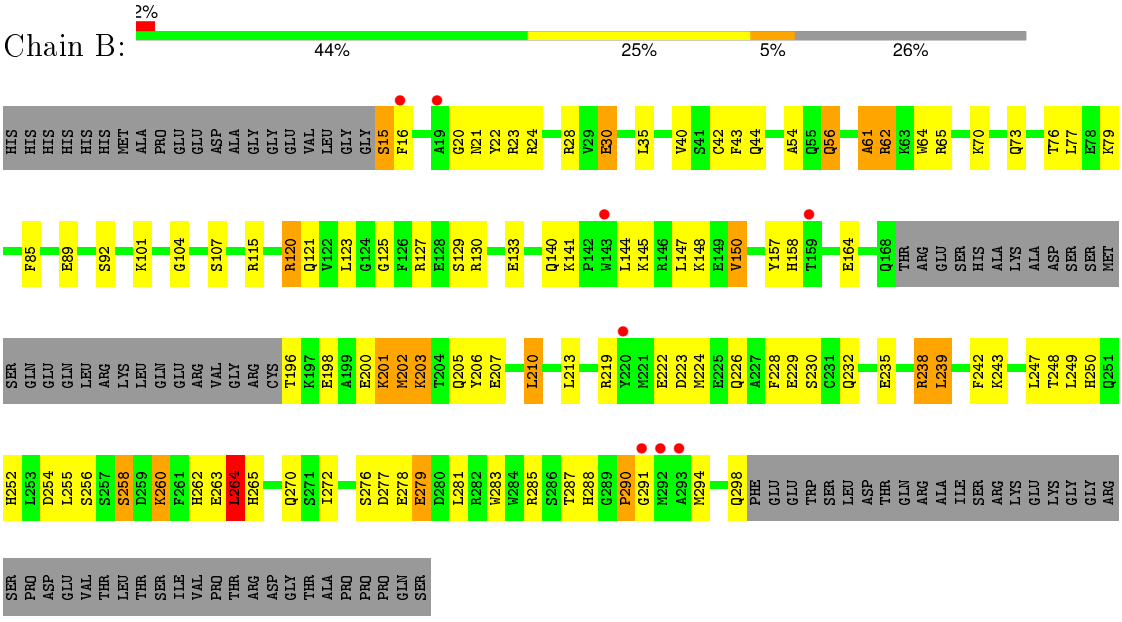
• Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain A:



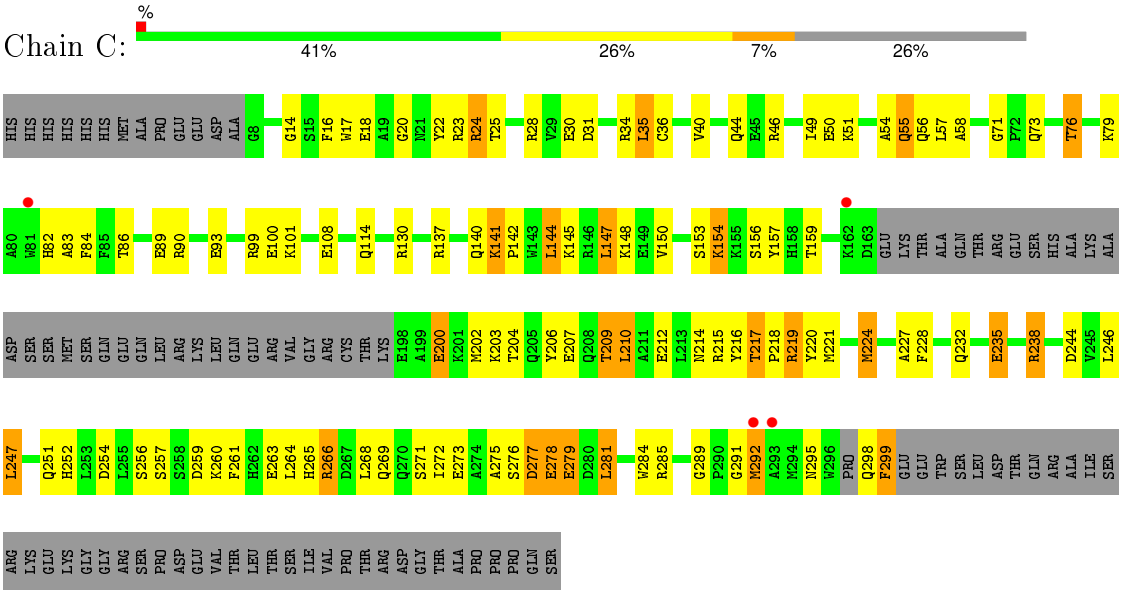
• Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain B:



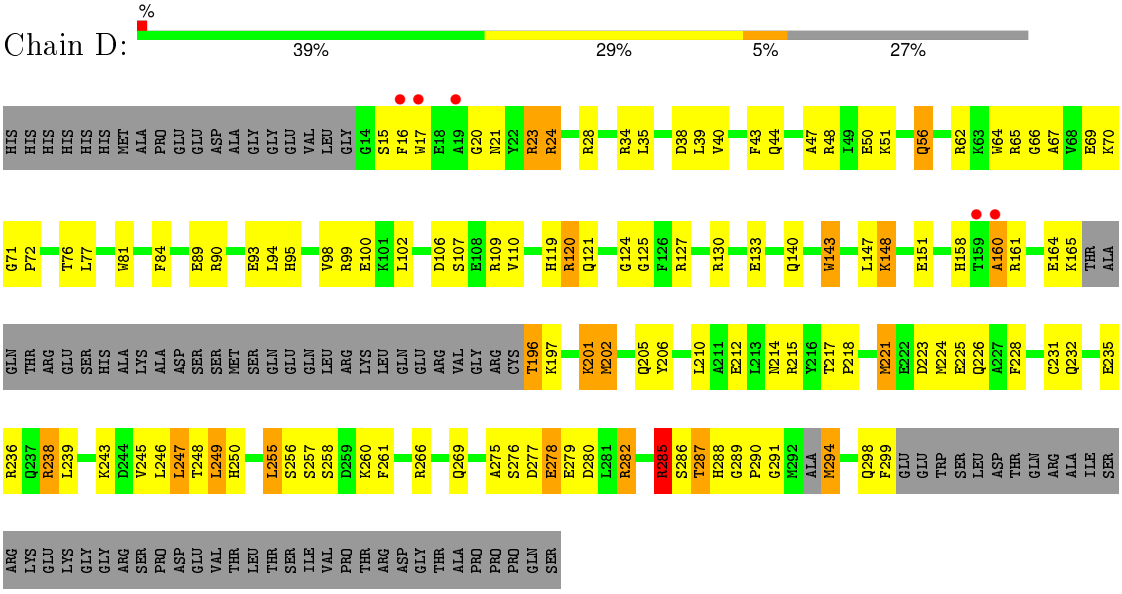
- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain C:



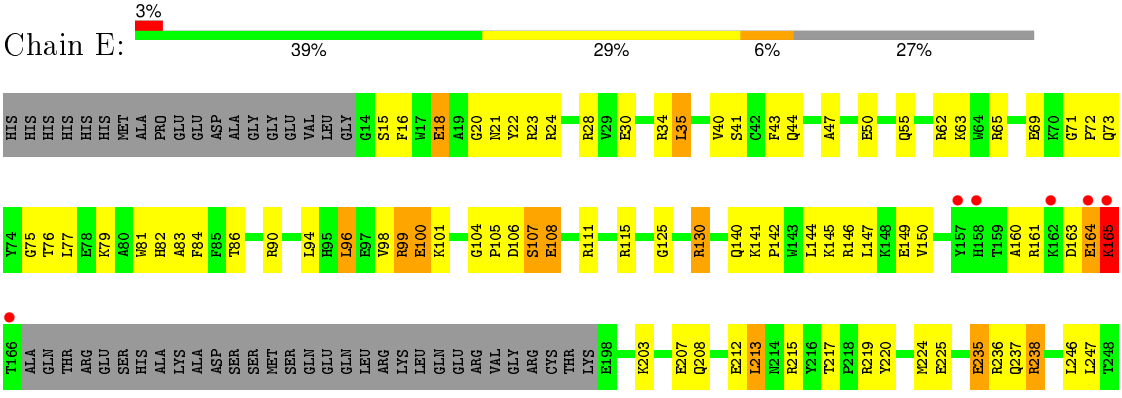
- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

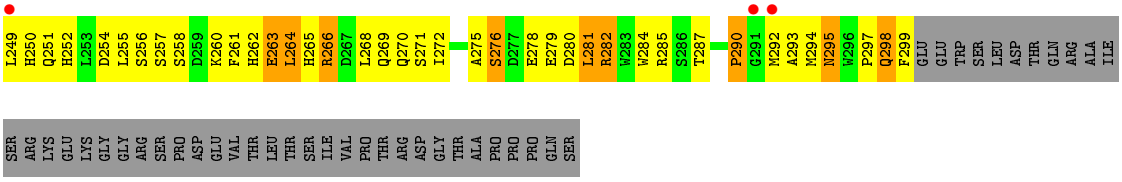
Chain D:



- Molecule 1: Protein kinase C and casein kinase II substrate protein 3

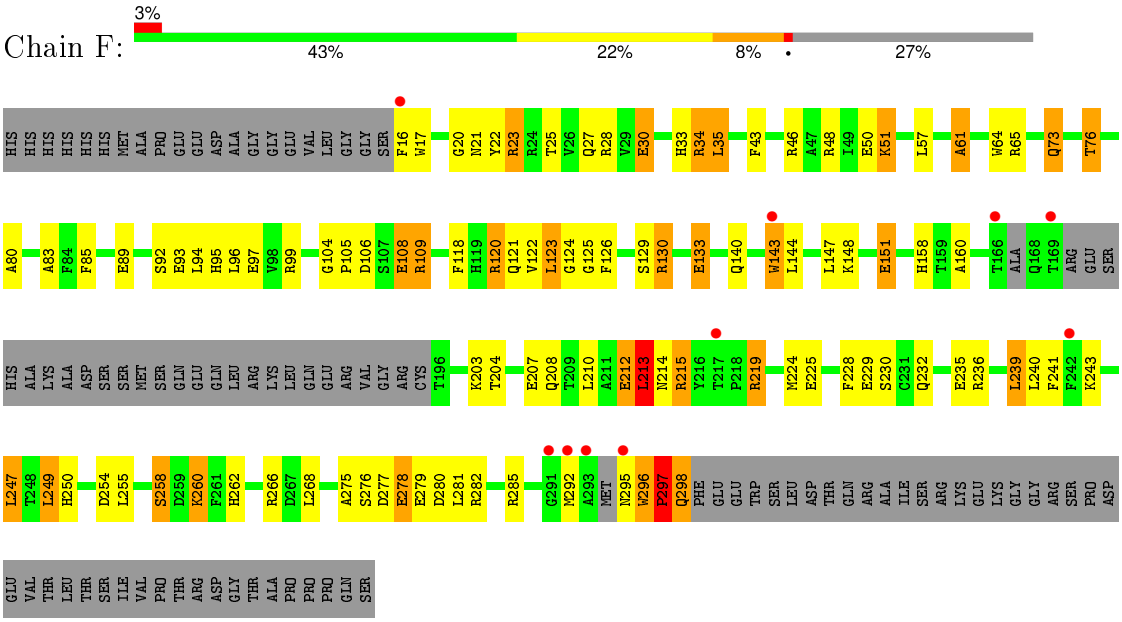
Chain E:





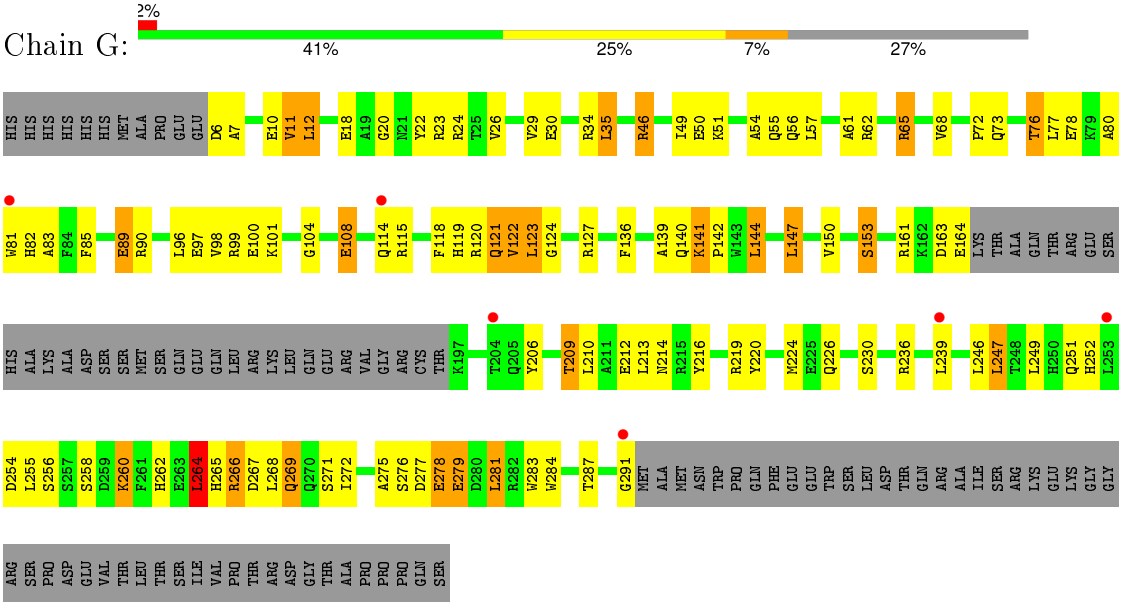
• Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain F:



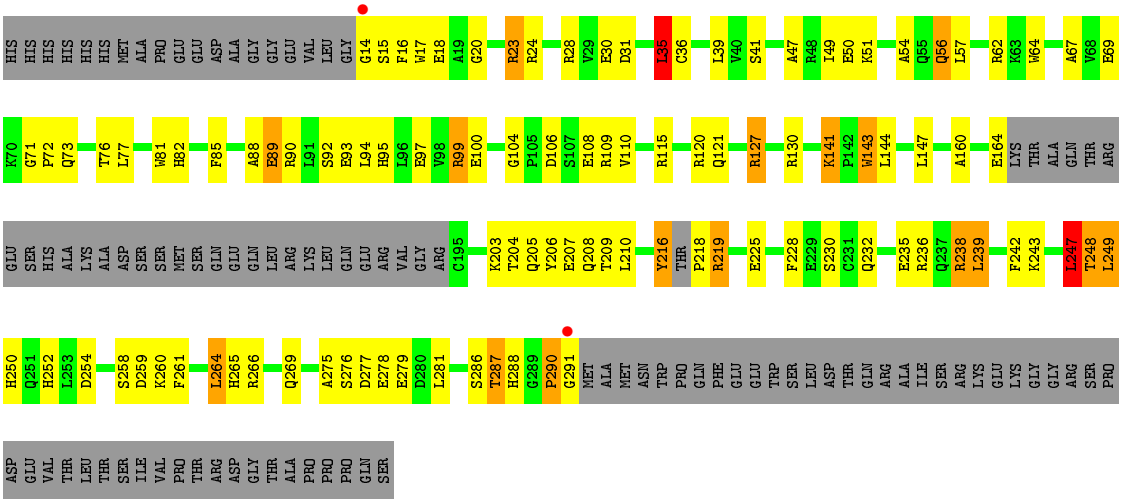
• Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain G:



• Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain H:


HIS HIS HIS HIS HIS HIS MET ALA PRO GLU GLU ASP ALA GLY GLY GLU VAL LEU GLY G14 S15 F16 W17 E18 A19 G20 R23 R24 R28 V29 E30 D31 L35 C36 L39 V40 S41 A47 R48 I49 E50 K51 A54 Q55 Q56 L57 R62 K63 W64 A67 V68 E69
K70 G71 F72 Q73 T76 L77 W81 H82 F85 A88 E89 R90 I91 S92 E93 L94 H95 L96 E97 Y98 R99 E100 G104 P105 D106 S107 E108 R109 V110 R115 R120 Q121 R127 R130 K141 P142 W143 L144 L147 A160 E164 LYS THR ALA GLN THR ARG
GLU SER HIS ALA LYS ALA ASP SER SER MET SER GLN GLU GLN LEU ARG LYS LEU GLN GLU ARG VAL GLY ARG C195 K203 T204 Q205 Y206 E207 Q208 T209 L210 Y216 THR P218 R219 E225 F228 E229 S230 C231 Q232 E235 R236 Q237 R238 L239 F242 K243 L247 T248 L249
H250 Q251 H252 L253 D254 S258 D259 K260 F261 L264 H265 R266 Q269 A275 S276 D277 E278 E279 D280 L281 S286 T287 H288 G289 P290 G291 MET ALA MET ASN TRP PRO GLN PHE GLU GLU TRP SER LEU ASP THR GLN ARG ALA ILE SER ARG LYS GLU LYS GLY GLY ARG SER PRO
ASP GLU VAL THR LEU THR SER ILE VAL PRO THR ARG ASP GLY THR ALA PRO PRO PRO GLN SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.57Å 108.90Å 222.32Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	48.90 – 3.10 48.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.90-3.10) 98.5 (48.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.60 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.281 , 0.337 0.274 , 0.328	Depositor DCC
R_{free} test set	5196 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.0	EDS
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Outliers	17 of 103398 reflections (0.016%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16470	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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 50.83 % 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 6.1201e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.12	6/2094 (0.3%)	1.01	5/2811 (0.2%)
1	B	1.14	7/2160 (0.3%)	1.00	2/2895 (0.1%)
1	C	1.12	8/2104 (0.4%)	1.00	4/2821 (0.1%)
1	D	1.26	11/2133 (0.5%)	1.06	4/2862 (0.1%)
1	E	1.17	6/2092 (0.3%)	1.02	6/2813 (0.2%)
1	F	1.22	12/2097 (0.6%)	1.05	2/2821 (0.1%)
1	G	1.14	3/2021 (0.1%)	1.03	5/2724 (0.2%)
1	H	1.28	12/2025 (0.6%)	1.08	9/2725 (0.3%)
All	All	1.18	65/16726 (0.4%)	1.03	37/22472 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	108	GLU	CG-CD	10.46	1.67	1.51
1	H	108	GLU	CG-CD	10.14	1.67	1.51
1	D	160	ALA	C-O	9.96	1.42	1.23
1	H	97	GLU	CG-CD	9.93	1.66	1.51
1	A	108	GLU	CG-CD	8.23	1.64	1.51

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	D	161	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	28	ARG	NE-CZ-NH1	6.89	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	219	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	E	238	ARG	NE-CZ-NH2	-6.84	116.88	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	160	ALA	Mainchain

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	2047	0	1943	82	0
1	B	2115	0	2020	76	0
1	C	2061	0	1930	97	0
1	D	2085	0	1982	110	0
1	E	2044	0	1900	111	0
1	F	2050	0	1898	93	0
1	G	1978	0	1807	89	0
1	H	1981	0	1827	84	0
2	A	14	0	0	1	0
2	B	13	0	0	2	0
2	C	19	0	0	0	0
2	D	12	0	0	3	0
2	E	12	0	0	0	0
2	F	16	0	0	2	0
2	G	10	0	0	0	0
2	H	13	0	0	1	0
All	All	16470	0	15307	658	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 21.

The worst 5 of 658 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:D:196:THR:CG2	1:D:196:THR:CB	1.76	1.59
1:D:121:GLN:HE22	1:D:130:ARG:CD	1.42	1.33
1:D:121:GLN:NE2	1:D:130:ARG:HD3	1.46	1.30
1:E:76:THR:CG2	1:E:275:ALA:HA	1.69	1.23
1:A:76:THR:CG2	1:A:275:ALA:HA	1.74	1.18

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	243/347 (70%)	229 (94%)	10 (4%)	4 (2%)	12	44
1	B	253/347 (73%)	236 (93%)	14 (6%)	3 (1%)	16	52
1	C	251/347 (72%)	231 (92%)	20 (8%)	0	100	100
1	D	249/347 (72%)	230 (92%)	17 (7%)	2 (1%)	24	63
1	E	249/347 (72%)	232 (93%)	16 (6%)	1 (0%)	39	75
1	F	247/347 (71%)	224 (91%)	21 (8%)	2 (1%)	24	63
1	G	250/347 (72%)	222 (89%)	25 (10%)	3 (1%)	16	52
1	H	241/347 (70%)	224 (93%)	14 (6%)	3 (1%)	16	52
All	All	1983/2776 (71%)	1828 (92%)	137 (7%)	18 (1%)	21	61

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	213	LEU
1	F	297	PRO
1	B	290	PRO
1	D	71	GLY
1	H	71	GLY

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	201/294 (68%)	173 (86%)	28 (14%)	4 19
1	B	210/294 (71%)	177 (84%)	33 (16%)	3 13
1	C	197/294 (67%)	154 (78%)	43 (22%)	1 5
1	D	205/294 (70%)	172 (84%)	33 (16%)	3 13
1	E	196/294 (67%)	157 (80%)	39 (20%)	1 7
1	F	193/294 (66%)	157 (81%)	36 (19%)	2 8
1	G	182/294 (62%)	143 (79%)	39 (21%)	1 5
1	H	186/294 (63%)	159 (86%)	27 (14%)	4 16
All	All	1570/2352 (67%)	1292 (82%)	278 (18%)	2 10

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	248	THR
1	E	212	GLU
1	H	56	GLN
1	D	266	ARG
1	E	41	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	251	GLN
1	E	262	HIS
1	H	208	GLN
1	D	265	HIS
1	E	226	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	250/347 (72%)	0.40	6 (2%)	62	39	37, 61, 103, 129	0
1	B	257/347 (74%)	0.44	8 (3%)	52	28	25, 55, 120, 137	0
1	C	257/347 (74%)	0.42	4 (1%)	74	55	42, 59, 97, 112	0
1	D	255/347 (73%)	0.41	5 (1%)	68	46	34, 54, 120, 135	0
1	E	255/347 (73%)	0.43	9 (3%)	48	23	39, 59, 108, 127	0
1	F	255/347 (73%)	0.50	10 (3%)	43	21	32, 55, 101, 114	0
1	G	254/347 (73%)	0.37	6 (2%)	62	39	41, 59, 83, 98	0
1	H	247/347 (71%)	0.42	2 (0%)	87	75	35, 53, 89, 102	0
All	All	2030/2776 (73%)	0.42	50 (2%)	61	37	25, 57, 103, 137	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	MET	7.7
1	C	293	ALA	6.6
1	F	293	ALA	5.9
1	E	291	GLY	5.1
1	E	166	THR	5.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.