



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 04:34 pm GMT

PDB ID : 3TMH
Title : Crystal structure of dual-specific A-kinase anchoring protein 2 in complex with cAMP-dependent protein kinase A type II alpha and PDZK1
Authors : Sarma, G.N.; Phan, R.H.; Sankaran, B.; Taylor, S.S.
Deposited on : 2011-08-31
Resolution : 3.80 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

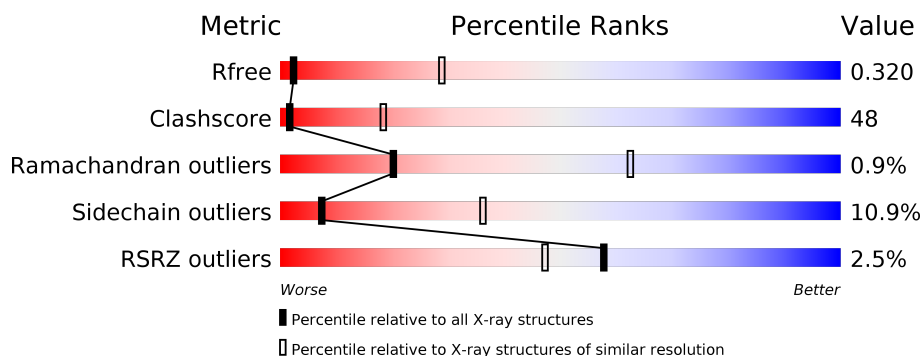
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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 $\leq 5\%$. 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	87	<div> <div>55%</div> <div>37%</div> <div>• 6%</div> </div>
1	E	87	<div> <div>%</div> <div>61%</div> <div>31%</div> <div>• 6%</div> </div>
1	I	87	<div> <div>%</div> <div>62%</div> <div>29%</div> <div>• • 6%</div> </div>
2	B	48	<div> <div>6%</div> <div>31%</div> <div>35%</div> <div>8%</div> <div>25%</div> </div>
2	C	48	<div> <div>2%</div> <div>31%</div> <div>40%</div> <div>10%</div> <div>19%</div> </div>
2	F	48	<div> <div>10%</div> <div>29%</div> <div>35%</div> <div>17%</div> <div>19%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	48	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>25%</div><div>35%</div><div>8%</div><div>31%</div></div></div>
3	D	45	<div><div><div></div><div></div><div></div><div></div></div><div><div>7%</div><div>38%</div><div>18%</div><div>38%</div></div></div>
3	H	45	<div><div><div></div><div></div><div></div><div></div></div><div><div>9%</div><div>29%</div><div>13%</div><div>49%</div></div></div>
3	L	45	<div><div><div></div><div></div><div></div><div></div></div><div><div>9%</div><div>33%</div><div>18%</div><div>40%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3553 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 Na(+)/H(+) exchange regulatory cofactor NHE-RF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	0	0	0
			588	372	98	116	2			
1	E	82	Total	C	N	O	S	0	0	0
			585	371	97	115	2			
1	I	82	Total	C	N	O	S	0	0	0
			564	356	91	115	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLY	-	EXPRESSION TAG	UNP Q5T2W1
A	374	SER	-	EXPRESSION TAG	UNP Q5T2W1
E	373	GLY	-	EXPRESSION TAG	UNP Q5T2W1
E	374	SER	-	EXPRESSION TAG	UNP Q5T2W1
I	373	GLY	-	EXPRESSION TAG	UNP Q5T2W1
I	374	SER	-	EXPRESSION TAG	UNP Q5T2W1

- Molecule 2 is a protein called cAMP-dependent protein kinase type II-alpha regulatory subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	0	0	0
			298	191	51	56			
2	C	39	Total	C	N	O	0	0	0
			321	209	52	60			
2	F	39	Total	C	N	O	0	0	0
			314	204	51	59			
2	G	33	Total	C	N	O	0	0	0
			269	176	42	51			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	EXPRESSION TAG	UNP P12368
B	-2	SER	-	EXPRESSION TAG	UNP P12368
B	-1	HIS	-	EXPRESSION TAG	UNP P12368
B	1	GLY	SER	CONFLICT	UNP P12368
C	-3	GLY	-	EXPRESSION TAG	UNP P12368
C	-2	SER	-	EXPRESSION TAG	UNP P12368
C	-1	HIS	-	EXPRESSION TAG	UNP P12368
C	1	GLY	SER	CONFLICT	UNP P12368
F	-3	GLY	-	EXPRESSION TAG	UNP P12368
F	-2	SER	-	EXPRESSION TAG	UNP P12368
F	-1	HIS	-	EXPRESSION TAG	UNP P12368
F	1	GLY	SER	CONFLICT	UNP P12368
G	-3	GLY	-	EXPRESSION TAG	UNP P12368
G	-2	SER	-	EXPRESSION TAG	UNP P12368
G	-1	HIS	-	EXPRESSION TAG	UNP P12368
G	1	GLY	SER	CONFLICT	UNP P12368

- Molecule 3 is a protein called A-kinase anchor protein 10, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	28	Total	C	N	O	S	0	0	0
			216	136	36	42	2			
3	H	23	Total	C	N	O	S	0	0	0
			179	110	30	37	2			
3	L	27	Total	C	N	O	S	0	0	0
			211	133	35	41	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	618	GLY	-	EXPRESSION TAG	UNP O43572
D	619	SER	-	EXPRESSION TAG	UNP O43572
D	620	PRO	-	EXPRESSION TAG	UNP O43572
D	621	GLU	-	EXPRESSION TAG	UNP O43572
D	622	PHE	-	EXPRESSION TAG	UNP O43572
D	646	VAL	ILE	SEE REMARK 999	UNP O43572
H	618	GLY	-	EXPRESSION TAG	UNP O43572
H	619	SER	-	EXPRESSION TAG	UNP O43572
H	620	PRO	-	EXPRESSION TAG	UNP O43572
H	621	GLU	-	EXPRESSION TAG	UNP O43572
H	622	PHE	-	EXPRESSION TAG	UNP O43572
H	646	VAL	ILE	SEE REMARK 999	UNP O43572
L	618	GLY	-	EXPRESSION TAG	UNP O43572

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	619	SER	-	EXPRESSION TAG	UNP O43572
L	620	PRO	-	EXPRESSION TAG	UNP O43572
L	621	GLU	-	EXPRESSION TAG	UNP O43572
L	622	PHE	-	EXPRESSION TAG	UNP O43572
L	646	VAL	ILE	SEE REMARK 999	UNP O43572

- Molecule 4 is water.

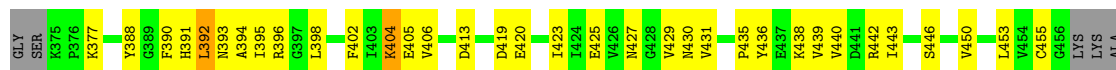
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	3	Total O 3 3	0	0
4	F	1	Total O 1 1	0	0
4	I	2	Total O 2 2	0	0

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.

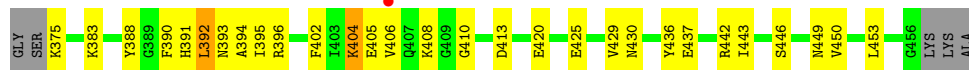
- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF3

Chain A: 



- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF3

Chain E: 



- Molecule 1: Na(+)/H(+) exchange regulatory cofactor NHE-RF3

Chain I: 



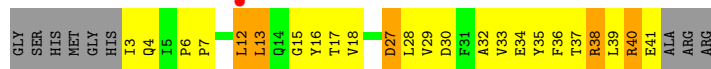
- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain B: 



- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain C: 



- Molecule 2: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.47Å 121.47Å 88.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.04 – 3.80 50.04 – 3.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.04-3.80) 99.2 (50.04-3.69)	Depositor EDS
R_{merge}	0.71	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.268 , 0.328 0.258 , 0.320	Depositor DCC
R_{free} test set	571 reflections (7.45%)	DCC
Wilson B-factor (Å ²)	115.7	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3553	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.78	0/596	0.86	0/809
1	E	0.76	0/593	0.89	0/805
1	I	0.80	0/572	1.17	3/782 (0.4%)
2	B	0.45	0/303	1.17	5/411 (1.2%)
2	C	0.51	0/328	1.59	6/448 (1.3%)
2	F	0.44	0/321	1.20	6/439 (1.4%)
2	G	0.57	0/275	1.32	3/375 (0.8%)
3	D	0.57	0/218	0.71	0/292
3	H	0.50	0/179	0.70	0/237
3	L	0.57	0/213	0.68	0/285
All	All	0.66	0/3598	1.08	23/4883 (0.5%)

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	I	0	2

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	40	ARG	NE-CZ-NH1	-16.06	112.27	120.30
2	C	40	ARG	NE-CZ-NH2	15.51	128.06	120.30
2	C	38	ARG	NE-CZ-NH2	13.53	127.06	120.30
2	G	38	ARG	NE-CZ-NH2	13.51	127.06	120.30
2	G	38	ARG	NE-CZ-NH1	-12.38	114.11	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	395	ILE	Peptide
1	I	397	GLY	Peptide

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	588	0	569	41	0
1	E	585	0	565	44	0
1	I	564	0	512	35	0
2	B	298	0	296	53	0
2	C	321	0	322	59	0
2	F	314	0	310	37	0
2	G	269	0	267	29	0
3	D	216	0	217	46	0
3	H	179	0	184	29	0
3	L	211	0	212	50	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	E	3	0	0	1	0
4	F	1	0	0	0	0
4	I	2	0	0	1	0
All	All	3553	0	3454	334	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 48.

The worst 5 of 334 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:I:393:ASN:HA	3:L:658:LYS:O	1.54	1.07
2:B:40:ARG:HG3	2:C:30:ASP:OD2	1.65	0.94
2:B:36:PHE:C	2:C:33:VAL:HG22	1.86	0.94
2:B:40:ARG:HH12	2:C:33:VAL:HG11	1.30	0.94
3:L:654:GLN:HB3	3:L:655:PRO:HA	1.52	0.92

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	80/87 (92%)	78 (98%)	2 (2%)	0	100	100
1	E	80/87 (92%)	78 (98%)	2 (2%)	0	100	100
1	I	80/87 (92%)	76 (95%)	4 (5%)	0	100	100
2	B	34/48 (71%)	31 (91%)	3 (9%)	0	100	100
2	C	37/48 (77%)	33 (89%)	4 (11%)	0	100	100
2	F	37/48 (77%)	32 (86%)	4 (11%)	1 (3%)	6	43
2	G	31/48 (65%)	30 (97%)	1 (3%)	0	100	100
3	D	26/45 (58%)	19 (73%)	6 (23%)	1 (4%)	4	36
3	H	21/45 (47%)	16 (76%)	4 (19%)	1 (5%)	2	30
3	L	25/45 (56%)	18 (72%)	6 (24%)	1 (4%)	3	34
All	All	451/588 (77%)	411 (91%)	36 (8%)	4 (1%)	20	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	654	GLN
3	D	654	GLN
3	L	654	GLN
2	F	7	PRO

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	61/70 (87%)	58 (95%)	3 (5%)	29	65
1	E	60/70 (86%)	57 (95%)	3 (5%)	28	65
1	I	55/70 (79%)	54 (98%)	1 (2%)	64	85
2	B	32/42 (76%)	28 (88%)	4 (12%)	5	29
2	C	36/42 (86%)	33 (92%)	3 (8%)	13	49
2	F	34/42 (81%)	30 (88%)	4 (12%)	6	32
2	G	30/42 (71%)	27 (90%)	3 (10%)	9	39
3	D	23/39 (59%)	15 (65%)	8 (35%)	0	1
3	H	21/39 (54%)	16 (76%)	5 (24%)	1	6
3	L	23/39 (59%)	16 (70%)	7 (30%)	0	3
All	All	375/495 (76%)	334 (89%)	41 (11%)	7	36

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	383	LYS
2	F	12	LEU
3	L	645	ASP
1	E	392	LEU
1	E	404	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	391	HIS
1	E	393	ASN
3	H	649	GLN
3	D	649	GLN
2	F	14	GLN

5.3.3 RNA ⓘ

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 [i](#)

There are no carbohydrates 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 [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	82/87 (94%)	-0.04	0 100 100	78, 112, 153, 204	0
1	E	82/87 (94%)	-0.05	1 (1%) 79 71	82, 107, 148, 206	0
1	I	82/87 (94%)	-0.17	1 (1%) 79 71	83, 114, 169, 213	0
2	B	36/48 (75%)	0.54	3 (8%) 12 10	154, 201, 260, 279	0
2	C	39/48 (81%)	0.04	1 (2%) 56 46	119, 196, 260, 278	0
2	F	39/48 (81%)	0.34	5 (12%) 4 5	148, 199, 260, 279	0
2	G	33/48 (68%)	-0.10	1 (3%) 51 40	149, 196, 261, 279	0
3	D	28/45 (62%)	-0.22	0 100 100	96, 139, 175, 181	0
3	H	23/45 (51%)	-0.04	0 100 100	99, 138, 174, 180	0
3	L	27/45 (60%)	-0.41	0 100 100	101, 139, 177, 179	0
All	All	471/588 (80%)	-0.02	12 (2%) 58 47	78, 129, 225, 279	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	16	TYR	4.5
1	I	406	VAL	4.0
2	F	22	ARG	3.9
2	G	26	PRO	3.5
2	C	12	LEU	3.3

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 carbohydrates 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.