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wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID	:	2Y4P
Title	:	Dimeric structure of DAPK-1 catalytic domain
Authors	:	De Diego, I.; Lehmann, F.; Wilmanns, M.
Deposited on	:	2011-01-07
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

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:

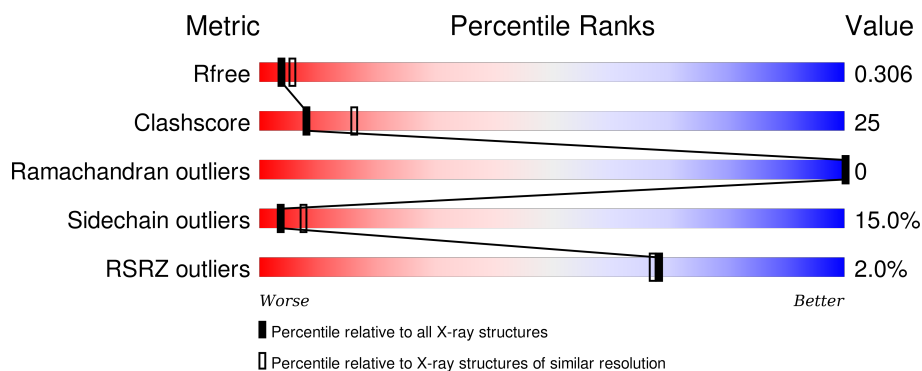|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.306
Clashscore		25
Ramachandran outliers		0
Sidechain outliers		15.0%
RSRZ outliers		2.0%

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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	285	% 60% 23% 5% 12%
1	B	285	37% 21% 7% 35%
1	C	285	3% 56% 30% 7% 7%
1	D	285	2% 36% 25% 8% 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7346 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 DEATH-ASSOCIATED PROTEIN KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total 2024	C 1306	N 330	O 384	S 4	0	0	0
1	B	184	Total 1475	C 958	N 235	O 279	S 3	0	0	0
1	C	264	Total 2122	C 1361	N 353	O 404	S 4	0	0	0
1	D	194	Total 1550	C 1004	N 248	O 295	S 3	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total 51	O 51	0	0
2	B	23	Total 23	O 23	0	0
2	C	58	Total 58	O 58	0	0
2	D	43	Total 43	O 43	0	0

3 Residue-property plots ⓘ

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: DEATH-ASSOCIATED PROTEIN KINASE 1

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D169 PHE GLY ASN GLU PHE LYS ASN ILE PHE GLY T180 P181 E182 F183 V184 I188 E192 I196 M200 Y208 I209 S212 P216 T221 E224 T225 L226 A227 S230 N233 E237 D238 S242 ASN T244 V257 R263 M264 T265 I266 Q267 D268 Q271

I275 K276 PRO LYS ASP THR GLN GLN ALA LEU SER

● Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1

Chain D:

2%

36%   25%   8%   32%

MET THR VAL PHE ARG GLN GLU ASN VAL ASP ASP TYR TYR ASP THR GLY GLU GLU LEU GLY SER GLN GLN PHE ALA VAL VAL LYS LYS CYS ARG GLU LYS SER THR GLY LEU GLN TYR ALA ALA LYS PHE ILE LYS LYS ARG ARG THR LYS SER SER ARG ARG GLY V56 S57 R58 E59 D60

I61 E62 R63 E64 V65 S66 K69 E70 I71 Q72 H73 P74 N75 V76 I77 T78 L79 V82 TYR GLU ASN LYS ASP VAL ILE LEU ILE L93 E94 L95 V96 L101 F102 D103 F104 L105 A106 GLU LYS GLU SER LEU THR E113 E114 E115 A116 T117 E118 F119 L120 K121 Q122 Y129

S132 K141 P142 E143 M146 L147 L148 D149 R150 N151 V152 P153 K154 P155 R156 I157 K158 K167 I168 D169 PHE GLY ASN GLU PHE LYS ASN ILE PHE GLY THR P181 E187 M200 W201 S202 I203 G204 V205 I206 T207 Y208 I209 L210 L211 S212 G213 A214 L218 G219 D220 T221 K222 Q223

E224 T225 N228 V229 S230 N233 Y234 E235 F236 E237 D238 E239 S242 L247 I252 R253 R254 L255 I256 V257 R263 T265 I266 Q267 D268 Q271 H272 P273 W274 I275 K276 PRO LYS ASP THR GLN GLN ALA LEU 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	83.94Å 73.70Å 120.28Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	117.97 – 2.65 62.07 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (117.97-2.65) 98.0 (62.07-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.69 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.252 , 0.312 0.250 , 0.306	Depositor DCC
R_{free} test set	2087 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 41327 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7346	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	1.77	8/2063 (0.4%)	0.89	1/2788 (0.0%)
1	B	1.69	8/1505 (0.5%)	0.85	0/2036
1	C	1.54	8/2162 (0.4%)	0.92	3/2921 (0.1%)
1	D	1.67	6/1582 (0.4%)	0.82	0/2144
All	All	1.67	30/7312 (0.4%)	0.88	4/9889 (0.0%)

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	C	0	3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	275	ILE	C-N	-18.18	0.92	1.34
1	C	91	LEU	CA-C	-9.90	1.27	1.52
1	C	66	SER	N-CA	-9.21	1.27	1.46
1	C	76	VAL	N-CA	-8.43	1.29	1.46
1	B	234	TYR	CD2-CE2	-5.94	1.30	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	91	LEU	CA-C-O	-11.88	95.14	120.10
1	C	91	LEU	CA-C-N	7.01	132.62	117.20
1	A	58	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	91	LEU	O-C-N	5.15	130.94	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	275	ILE	Mainchain
1	C	66	SER	Mainchain
1	C	76	VAL	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	2024	0	2009	72	1
1	B	1475	0	1461	89	0
1	C	2122	0	2105	90	1
1	D	1550	0	1524	108	1
2	A	51	0	0	4	0
2	B	23	0	0	4	0
2	C	58	0	0	12	0
2	D	43	0	0	13	0
All	All	7346	0	7099	352	2

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 25.

The worst 5 of 352 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:180:THR:HG23	1:C:181:PRO:CD	1.35	1.55
1:D:181:PRO:HD2	2:D:2020:HOH:O	1.23	1.34
1:D:78:THR:HG23	1:D:94:GLU:OE2	1.29	1.32
1:D:70:GLU:OE2	1:D:167:LYS:NZ	1.61	1.30
1:A:180:THR:CG2	1:A:181:PRO:HD3	1.64	1.26

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:SER:OG	1:D:219:GLY:O[2_646]	1.37	0.83
1:A:34:SER:O	1:A:271:GLN:NE2[2_647]	1.40	0.80

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	243/285 (85%)	240 (99%)	3 (1%)	0	100	100
1	B	176/285 (62%)	171 (97%)	5 (3%)	0	100	100
1	C	258/285 (90%)	252 (98%)	6 (2%)	0	100	100
1	D	186/285 (65%)	179 (96%)	7 (4%)	0	100	100
All	All	863/1140 (76%)	842 (98%)	21 (2%)	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	219/254 (86%)	189 (86%)	30 (14%)	4	9
1	B	161/254 (63%)	138 (86%)	23 (14%)	4	8
1	C	231/254 (91%)	197 (85%)	34 (15%)	4	8
1	D	169/254 (66%)	139 (82%)	30 (18%)	2	4
All	All	780/1016 (77%)	663 (85%)	117 (15%)	3	7

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	GLN
1	C	62	GLU
1	D	187	GLU
1	C	6	GLN
1	C	45	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	144	ASN
1	C	6	GLN
1	C	190	ASN
1	B	131	HIS
1	D	73	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 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	251/285 (88%)	0.05	3 (1%)	81	80	24, 40, 61, 82	0
1	B	184/285 (64%)	-0.01	0	100	100	25, 50, 74, 81	0
1	C	264/285 (92%)	0.23	8 (3%)	54	52	27, 47, 69, 78	0
1	D	194/285 (68%)	0.16	7 (3%)	46	45	24, 41, 82, 93	0
All	All	893/1140 (78%)	0.11	18 (2%)	68	67	24, 44, 72, 93	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	152	VAL	4.8
1	C	242	SER	3.5
1	D	96	VAL	3.3
1	C	221	THR	2.9
1	A	34	SER	2.8

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.