



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 09:15 AM GMT

PDB ID : 3DDP
Title : Structure of phosphorylated Thr160 CDK2/cyclin A in complex with the inhibitor CR8
Authors : Echalier, A.; Endicott, J.A.
Deposited on : 2008-06-06
Resolution : 2.70 Å (reported)

This is a wwPDB 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/ValidationPDFNotes.html>

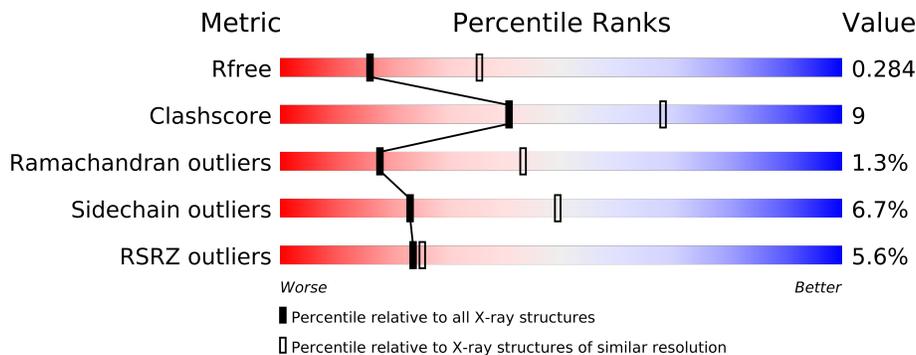
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	299	
1	C	299	
2	B	268	
2	D	268	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9299 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	298	Total	C	N	O	P	S	0	1	0
			2404	1559	409	427	1	8			
1	C	299	Total	C	N	O	P	S	0	0	0
			2407	1562	409	427	1	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	262	Total	C	N	O	S	0	1	0
			2118	1371	344	393	10			
2	D	268	Total	C	N	O	S	0	0	0
			2172	1403	362	397	10			

There are 12 discrepancies between the modelled and reference sequences:

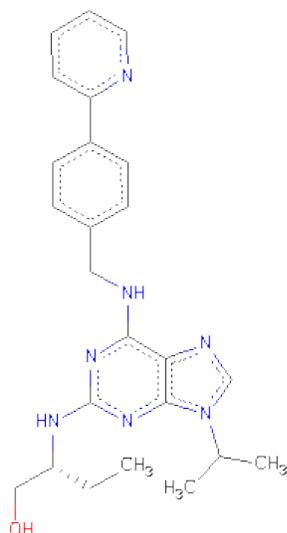
Chain	Residue	Modelled	Actual	Comment	Reference
B	433	HIS	-	EXPRESSION TAG	UNP P30274
B	434	HIS	-	EXPRESSION TAG	UNP P30274
B	435	HIS	-	EXPRESSION TAG	UNP P30274
B	436	HIS	-	EXPRESSION TAG	UNP P30274
B	437	HIS	-	EXPRESSION TAG	UNP P30274
B	438	HIS	-	EXPRESSION TAG	UNP P30274
D	433	HIS	-	EXPRESSION TAG	UNP P30274
D	434	HIS	-	EXPRESSION TAG	UNP P30274
D	435	HIS	-	EXPRESSION TAG	UNP P30274
D	436	HIS	-	EXPRESSION TAG	UNP P30274

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	437	HIS	-	EXPRESSION TAG	UNP P30274
D	438	HIS	-	EXPRESSION TAG	UNP P30274

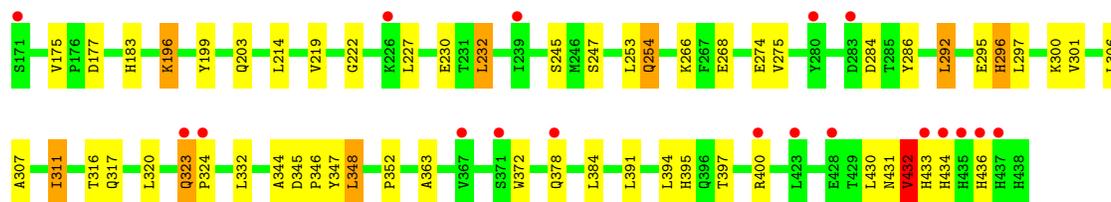
- Molecule 3 is (2R)-2-({9-(1-METHYLETHYL)-6-[(4-PYRIDIN-2-YLBENZYL)AMINO]-9H-PURIN-2-YL}AMINO)BUTAN-1-OL (three-letter code: RC8) (formula: C₂₄H₂₉N₇O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
3	A	1	Total	C	N	O	0	0
			32	24	7	1		
3	C	1	Total	C	N	O	0	0
			32	24	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	28	Total	O	0	0
			28	28		
4	C	33	Total	O	0	0
			33	33		
4	D	20	Total	O	0	0
			20	20		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.32Å 135.16Å 168.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.70) 93.0 (19.98-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.71Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.270 0.235 , 0.284	Depositor DCC
R_{free} test set	2226 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	49.5	Xtrriage
Anisotropy	0.364	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.5	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Outliers	0 of 44100 reflections	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, RC8

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	0.50	0/2457	0.62	0/3333
1	C	0.44	0/2457	0.61	0/3333
2	B	0.44	0/2171	0.59	0/2952
2	D	0.40	0/2228	0.56	0/3030
All	All	0.45	0/9313	0.60	0/12648

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	70	ILE	Peptide
1	C	89	LYS	Peptide

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2404	0	2449	53	0
1	C	2407	0	2454	67	0
2	B	2118	0	2136	24	0
2	D	2172	0	2172	39	0
3	A	32	0	29	2	0
3	C	32	0	29	2	0
4	A	53	0	0	3	0
4	B	28	0	0	3	0
4	C	33	0	0	6	0
4	D	20	0	0	3	0
All	All	9299	0	9269	171	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 171 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:41:THR:CB	1:C:42:GLU:HA	1.77	1.14
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.32	1.12
1:C:41:THR:HB	1:C:42:GLU:HA	1.39	1.04
1:A:41:THR:HA	4:A:336:HOH:O	1.62	0.99
1:C:41:THR:HB	1:C:42:GLU:CA	2.00	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	296/299 (99%)	281 (95%)	9 (3%)	6 (2%)	11 28
1	C	296/299 (99%)	268 (90%)	21 (7%)	7 (2%)	9 22
2	B	261/268 (97%)	254 (97%)	6 (2%)	1 (0%)	43 76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	266/268 (99%)	260 (98%)	5 (2%)	1 (0%)	43 76
All	All	1119/1134 (99%)	1063 (95%)	41 (4%)	15 (1%)	18 43

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	C	39	THR
1	C	295	HIS
2	D	432	VAL
1	A	39	THR

5.3.2 Protein sidechains ⓘ

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	263/263 (100%)	249 (95%)	14 (5%)	32 62
1	C	263/263 (100%)	238 (90%)	25 (10%)	12 28
2	B	236/241 (98%)	224 (95%)	12 (5%)	33 64
2	D	241/241 (100%)	225 (93%)	16 (7%)	24 50
All	All	1003/1008 (100%)	936 (93%)	67 (7%)	23 49

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	37	LEU
1	C	122	ARG
2	D	348	LEU
1	C	41	THR
1	C	89	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	396	GLN
1	C	62	ASN
2	D	317	GLN
2	B	395	HIS
2	D	323	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	160	1	10,10,11	5.96	1 (10%)	12,14,16	1.36	2 (16%)
1	TPO	C	160	1	10,10,11	5.70	1 (10%)	12,14,16	1.46	1 (8%)

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	160	1	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	O-C	18.64	1.24	1.11
1	C	160	TPO	O-C	17.83	1.23	1.11

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	160	TPO	OG1-CB-CG2	-2.87	105.32	110.13
1	A	160	TPO	CB-CA-N	-2.77	105.72	109.60
1	A	160	TPO	OG1-CB-CG2	-2.38	106.15	110.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands 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$
3	RC8	A	299	-	35,35,35	1.14	4 (11%)	48,48,48	2.32	15 (31%)
3	RC8	C	299	-	35,35,35	1.09	4 (11%)	48,48,48	2.20	15 (31%)

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
3	RC8	A	299	-	-	0/21/21/21	0/2/4/4
3	RC8	C	299	-	-	0/21/21/21	0/2/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	299	RC8	C4-N9	-3.44	1.32	1.37
3	A	299	RC8	C4-N9	-3.40	1.32	1.37
3	C	299	RC8	C5-C4	3.00	1.47	1.40
3	C	299	RC8	C6-C5	2.59	1.49	1.44
3	A	299	RC8	C5-C4	2.54	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	299	RC8	C8-N9-C9	6.08	131.65	125.43
3	C	299	RC8	C9-N9-C4	-5.36	119.61	127.17
3	A	299	RC8	C9-N9-C4	-5.05	120.04	127.17
3	A	299	RC8	C8-N9-C9	5.01	130.55	125.43
3	C	299	RC8	C2-N3-C4	4.72	121.07	115.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 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	298/299 (99%)	0.26	9 (3%) 48 54	42, 54, 67, 80	0
1	C	299/299 (100%)	0.35	30 (10%) 8 8	45, 55, 81, 115	0
2	B	262/268 (97%)	0.06	6 (2%) 57 64	41, 55, 66, 85	0
2	D	268/268 (100%)	0.23	18 (6%) 17 19	44, 57, 68, 82	0
All	All	1127/1134 (99%)	0.23	63 (5%) 24 25	41, 55, 73, 115	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	435	HIS	5.4
1	C	40	GLU	5.0
1	C	251	VAL	4.9
2	D	434	HIS	4.8
1	C	297	ARG	4.7

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.15	-0.34	47,51,53,53	0
1	TPO	A	160	11/12	0.15	-0.78	49,53,57,57	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	RC8	C	299	32/32	0.22	0.41	51,56,62,62	0
3	RC8	A	299	32/32	0.22	0.21	43,47,55,55	0

6.5 Other polymers

There are no such residues in this entry.