Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:00 am BST

PDB ID	:	4YXR
Title	:	CRYSTAL STRUCTURE OF PKA IN COMPLEX WITH inhibitor.
Authors	:	Schiffer, A.; Wendt, K.U.
Deposited on	:	2015-03-23
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

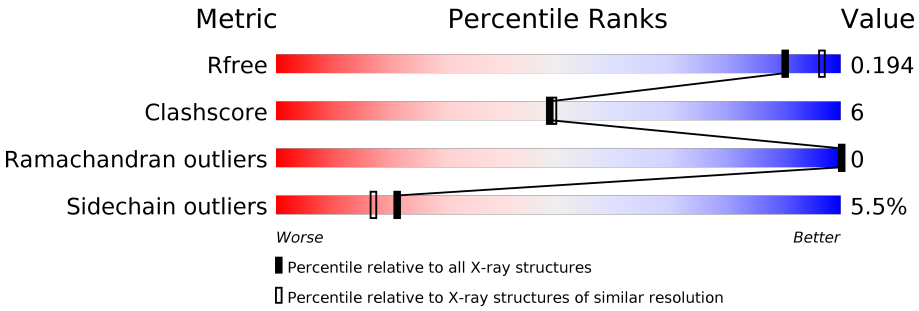
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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%

Mol	Chain	Length	Quality of chain
1	A	350	83% 11% • •
2	I	20	90% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3264 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	P	S	0	0	0
			2780	1803	465	501	2	9			

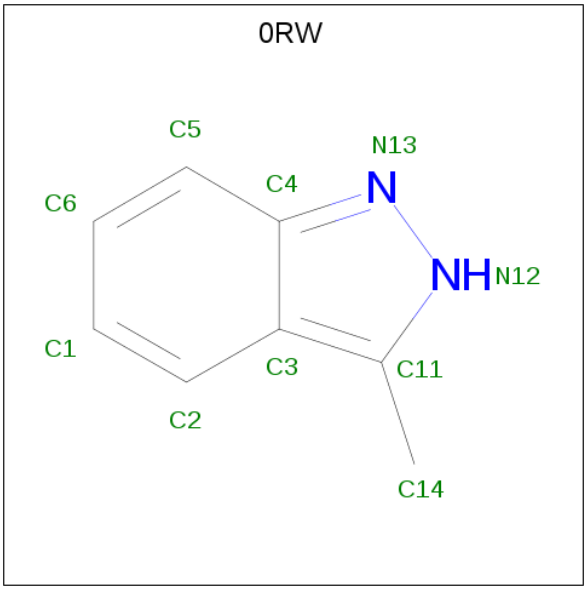
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ASP	ASN	conflict	UNP P00517

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	0	0	0
			157	94	32	31			

- Molecule 3 is 3-methyl-2H-indazole (three-letter code: 0RW) (formula: $C_8H_8N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 8 2	0	0

- Molecule 4 is water.

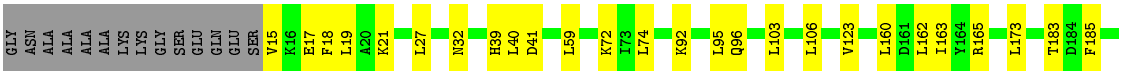
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	287	Total O 287 287	0	0
4	I	30	Total O 30 30	0	0

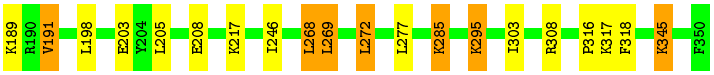
3 Residue-property plots (i)

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. 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. 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: cAMP-dependent protein kinase catalytic subunit alpha

Chain A:





- Molecule 2: cAMP-dependent protein kinase inhibitor alpha

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.84Å 75.06Å 79.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	2.00 – 2.00 19.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (2.00-2.00) 99.8 (19.31-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.01Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	(Not available) , 0.252 0.202 , 0.194	Depositor DCC
R_{free} test set	1528 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3264	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: TPO, 0RW, SEP

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	0.34	0/2830	0.58	0/3812
2	I	0.36	0/159	0.56	0/212
All	All	0.34	0/2989	0.58	0/4024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2780	0	2759	35	0
2	I	157	0	146	3	0
3	A	10	0	8	1	0
4	A	287	0	0	3	0
4	I	30	0	0	0	0
All	All	3264	0	2913	35	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 6.

All (35) 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:A:163:ILE:HG12	1:A:217:LYS:HD3	1.51	0.92
1:A:345:LYS:H	1:A:345:LYS:HE3	1.44	0.81
1:A:123:VAL:H	3:A:401:0RW:H5	1.34	0.76
1:A:39:HIS:HD2	1:A:41:ASP:H	1.38	0.70
1:A:173:LEU:HD12	1:A:183:THR:HG21	1.74	0.69
1:A:308:ARG:HG3	4:A:504:HOH:O	1.95	0.65
1:A:268:LEU:HD22	1:A:272:LEU:HD22	1.82	0.60
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.69	0.57
1:A:285:LYS:NZ	1:A:285:LYS:H	2.04	0.56
1:A:189:LYS:HG2	1:A:191:VAL:HG22	1.88	0.55
1:A:18:PHE:HD2	1:A:19:LEU:HD22	1.72	0.54
1:A:173:LEU:CD1	1:A:183:THR:HG21	2.41	0.50
1:A:208:GLU:HG2	1:A:277:LEU:HD11	1.94	0.49
1:A:72:LYS:HE2	1:A:74:LEU:HD11	1.95	0.49
1:A:205:LEU:HD11	2:I:22:ILE:HD11	1.94	0.49
1:A:285:LYS:HZ3	1:A:285:LYS:H	1.62	0.48
1:A:39:HIS:CD2	1:A:41:ASP:H	2.25	0.48
1:A:316:PRO:HB2	1:A:318:PHE:CZ	2.49	0.48
1:A:17:GLU:O	1:A:21:LYS:HD3	2.15	0.47
1:A:15:VAL:O	1:A:19:LEU:HD23	2.14	0.47
1:A:303:ILE:N	1:A:303:ILE:HD12	2.30	0.47
1:A:15:VAL:N	4:A:501:HOH:O	2.48	0.46
1:A:173:LEU:HD12	1:A:183:THR:CG2	2.45	0.46
1:A:123:VAL:HB	1:A:173:LEU:HD13	1.97	0.46
1:A:246:ILE:HD11	2:I:15:ARG:HD2	1.98	0.45
1:A:203:GLU:OE2	2:I:15:ARG:HD3	2.18	0.44
1:A:303:ILE:H	1:A:303:ILE:HD12	1.83	0.43
1:A:295:LYS:H	1:A:295:LYS:CD	2.32	0.43
1:A:308:ARG:NH2	4:A:503:HOH:O	2.51	0.43
1:A:295:LYS:HD3	1:A:295:LYS:N	2.35	0.42
1:A:103:LEU:HD22	1:A:185:PHE:CZ	2.53	0.42
1:A:295:LYS:H	1:A:295:LYS:HD3	1.86	0.41
1:A:163:ILE:HG22	1:A:165:ARG:HG3	2.03	0.40
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.94	0.40
1:A:96:GLN:HB3	1:A:106:LEU:HD23	2.03	0.40

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	332/350 (95%)	322 (97%)	10 (3%)	0	100	100
2	I	18/20 (90%)	18 (100%)	0	0	100	100
All	All	350/370 (95%)	340 (97%)	10 (3%)	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	295/303 (97%)	278 (94%)	17 (6%)	20	15
2	I	15/15 (100%)	15 (100%)	0	100	100
All	All	310/318 (98%)	293 (94%)	17 (6%)	21	17

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	ASN
1	A	40	LEU
1	A	59	LEU
1	A	92	LYS
1	A	95	LEU
1	A	160	LEU
1	A	162	LEU

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Mol	Chain	Res	Type
1	A	191	VAL
1	A	198	LEU
1	A	268	LEU
1	A	269	LEU
1	A	272	LEU
1	A	285	LYS
1	A	295	LYS
1	A	317	LYS
1	A	345	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	39	HIS
1	A	62	HIS
1	A	113	ASN
1	A	271	ASN
1	A	307	GLN
2	I	20	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	SEP	A	338	1	8,9,10	1.93	3 (37%)	8,12,14	1.58	1 (12%)
1	TPO	A	197	1	8,10,11	2.57	3 (37%)	10,14,16	0.87	0

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	SEP	A	338	1	-	2/5/8/10	-
1	TPO	A	197	1	-	1/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	TPO	P-OG1	-6.24	1.47	1.59
1	A	338	SEP	P-OG	-4.06	1.47	1.60
1	A	197	TPO	P-O2P	-2.29	1.46	1.54
1	A	197	TPO	P-O3P	-2.27	1.46	1.54
1	A	338	SEP	P-O2P	-2.25	1.46	1.54
1	A	338	SEP	P-O3P	-2.18	1.46	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	SEP	OG-CB-CA	3.52	111.57	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	N-CA-CB-OG
1	A	338	SEP	CA-CB-OG-P
1	A	197	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	0RW	A	401	-	9,11,11	1.55	2 (22%)	8,15,15	1.44	2 (25%)

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	0RW	A	401	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	0RW	C5-C4	-2.36	1.37	1.41
3	A	401	0RW	C1-C2	2.00	1.41	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	0RW	C5-C4-N13	3.27	135.52	130.19
3	A	401	0RW	C14-C11-N12	2.20	124.49	119.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	0RW	1	0

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.