



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 05:40 AM EST

PDB ID : 5OQ6  
Title : Structure of CHK1 12-pt. mutant complex with aminopyrimido-benzodiazepine LRRK2 inhibitor  
Authors : Dokurno, P.; Williamson, D.S.; Acheson-Dossang, P.; Chen, I.; Murray, J.B.; Shaw, T.; Surgenor, A.E.  
Deposited on : unknown  
Resolution : 1.95 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
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) : rb-20030345

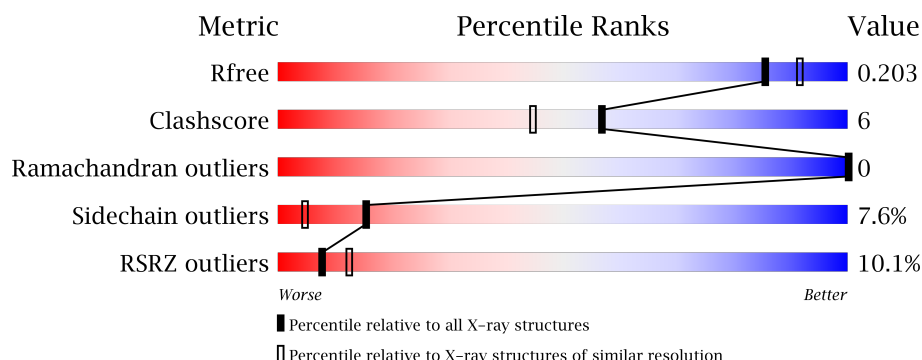
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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  $\geq 3$ , 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	297	<div> <div>9%</div> <div>72%</div> <div>12%</div> <div>13%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2279 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.

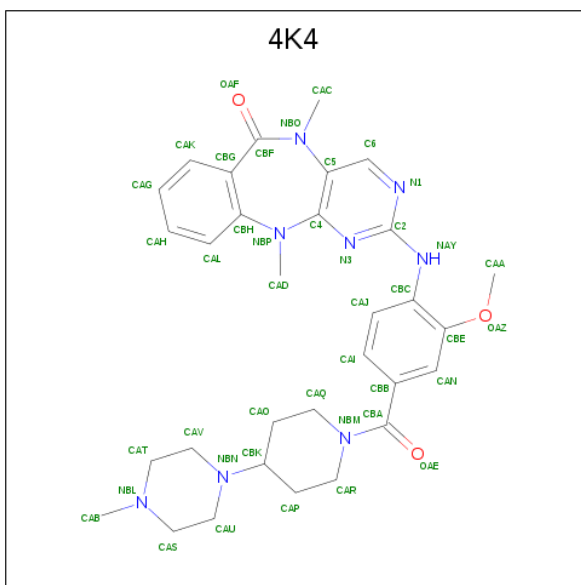
- Molecule 1 is a protein called Serine/threonine-protein kinase Chk1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2071	1329	356	376	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	ALA	engineered mutation	UNP O14757
A	20	PHE	TYR	engineered mutation	UNP O14757
A	59	LEU	ASN	engineered mutation	UNP O14757
A	68	ILE	VAL	engineered mutation	UNP O14757
A	84	MET	LEU	engineered mutation	UNP O14757
A	86	LEU	TYR	engineered mutation	UNP O14757
A	87	ALA	CYS	engineered mutation	UNP O14757
A	91	SER	GLU	engineered mutation	UNP O14757
A	134	HIS	GLU	engineered mutation	UNP O14757
A	147	ALA	SER	engineered mutation	UNP O14757
A	149	TYR	PHE	engineered mutation	UNP O14757
A	150	SER	GLY	engineered mutation	UNP O14757
A	290	HIS	-	expression tag	UNP O14757
A	291	HIS	-	expression tag	UNP O14757
A	292	HIS	-	expression tag	UNP O14757
A	293	HIS	-	expression tag	UNP O14757
A	294	HIS	-	expression tag	UNP O14757
A	295	HIS	-	expression tag	UNP O14757
A	296	HIS	-	expression tag	UNP O14757
A	297	HIS	-	expression tag	UNP O14757

- Molecule 2 is 2-[(2-methoxy-4-{[4-(4-methylpiperazin-1-yl)piperidin-1-yl]carbonyl}phenyl)amino]-5,11-dimethyl-5,11-dihydro-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one (three-letter code: 4K4) (formula: C<sub>31</sub>H<sub>38</sub>N<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	31	8	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

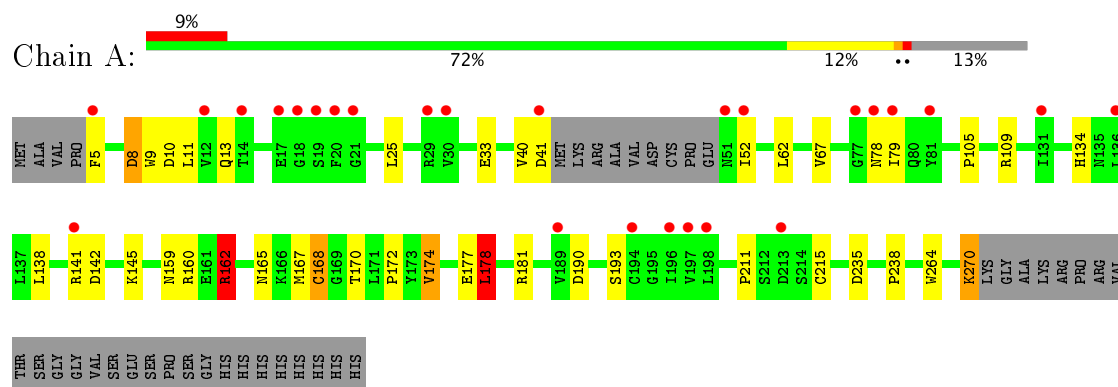
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	165	Total O 165 165	0	0



- Molecule 1: Serine/threonine-protein kinase Chk1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.00Å 66.16Å 54.98Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 28.18 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.95) 98.5 (28.18-1.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.158 , 0.192 0.171 , 0.203	Depositor DCC
$R_{free}$ test set	1164 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4K4, CL

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	0.98	1/2120 (0.0%)	0.99	6/2874 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	SER	CB-OG	-5.31	1.35	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	LEU	CA-CB-CG	8.38	134.56	115.30
1	A	190	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	109	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	A	162	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	235	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	178	LEU	CB-CA-C	5.07	119.82	110.20

There are no chirality outliers.

There are no planarity outliers.

### 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	2071	0	2059	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	42	0	38	2	0
3	A	1	0	0	1	0
4	A	165	0	0	8	3
All	All	2279	0	2097	24	3

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 (24) 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:215:CYS:SG	4:A:531:HOH:O	2.28	0.91
3:A:302:CL:CL	4:A:558:HOH:O	2.26	0.90
1:A:162:ARG:NH1	4:A:401:HOH:O	2.07	0.86
1:A:5:PHE:N	1:A:9:TRP:O	2.24	0.69
1:A:105:PRO:HG2	1:A:270:LYS:HG3	1.72	0.69
1:A:8:ASP:N	1:A:8:ASP:OD1	2.22	0.60
1:A:270:LYS:O	1:A:270:LYS:HD3	2.02	0.60
1:A:142:ASP:OD1	4:A:403:HOH:O	2.17	0.57
1:A:177:GLU:HB2	1:A:181:ARG:HD3	1.87	0.57
1:A:5:PHE:N	1:A:10:ASP:HA	2.20	0.56
1:A:167:MET:SD	1:A:178:LEU:HD13	2.49	0.53
1:A:168:CYS:HB3	4:A:542:HOH:O	2.09	0.52
2:A:301:4K4:H29	2:A:301:4K4:N3	2.24	0.51
1:A:170:THR:HG22	1:A:172:PRO:HD2	1.92	0.51
1:A:159:ASN:HB2	4:A:519:HOH:O	2.11	0.51
1:A:174:VAL:O	1:A:211:PRO:HG3	2.12	0.50
1:A:41:ASP:HB3	1:A:79:ILE:HD13	1.97	0.46
1:A:168:CYS:SG	4:A:542:HOH:O	2.62	0.43
1:A:134:HIS:HD2	4:A:450:HOH:O	2.03	0.42
1:A:270:LYS:O	1:A:270:LYS:CD	2.66	0.42
1:A:78:ASN:HD22	1:A:78:ASN:HA	1.77	0.42
1:A:238:PRO:HD3	1:A:264:TRP:CD1	2.56	0.41
2:A:301:4K4:N3	2:A:301:4K4:CAJ	2.83	0.41
1:A:62:LEU:HD13	1:A:67:VAL:CG1	2.51	0.40

All (3) 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)
4:A:482:HOH:O	4:A:540:HOH:O[2_555]	1.84	0.36
4:A:544:HOH:O	4:A:559:HOH:O[2_555]	2.03	0.17
4:A:416:HOH:O	4:A:430:HOH:O[2_545]	2.11	0.09

## 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	253/297 (85%)	246 (97%)	7 (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	224/261 (86%)	207 (92%)	17 (8%)	15	5

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

Mol	Chain	Res	Type
1	A	8	ASP
1	A	11	LEU
1	A	13	GLN
1	A	25	LEU
1	A	33	GLU
1	A	40	VAL

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Mol	Chain	Res	Type
1	A	52	ILE
1	A	138	LEU
1	A	141	ARG
1	A	145	LYS
1	A	160	ARG
1	A	162	ARG
1	A	165	ASN
1	A	168	CYS
1	A	174	VAL
1	A	178	LEU
1	A	270	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	24	GLN
1	A	73	HIS
1	A	78	ASN
1	A	158	ASN
1	A	165	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](#)

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
2	4K4	A	301	-	40,47,47	1.33	2 (5%)	49,68,68	1.96	9 (18%)

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
2	4K4	A	301	-	-	0/18/38/38	0/5/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	4K4	CBG-CBH	-5.89	1.37	1.41
2	A	301	4K4	CAD-NBP	-3.28	1.44	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	4K4	N1-C2-N3	-3.62	123.04	126.65
2	A	301	4K4	CAA-OAZ-CBE	-2.82	113.48	117.54
2	A	301	4K4	OAE-CBA-NBM	-2.18	118.59	122.36
2	A	301	4K4	NAY-C2-N3	2.15	124.00	116.89
2	A	301	4K4	CAB-NBL-CAT	2.47	114.39	110.67
2	A	301	4K4	C6-N1-C2	2.96	120.71	115.89
2	A	301	4K4	CAR-NBM-CAQ	2.98	118.25	112.61
2	A	301	4K4	CBB-CBA-NBM	3.92	123.84	118.77
2	A	301	4K4	CAK-CBG-CBH	8.90	122.15	118.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	4K4	2	0

## 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	257/297 (86%)	0.19	26 (10%) 8 12	18, 35, 77, 112	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	PHE	8.8
1	A	78	ASN	5.8
1	A	18	GLY	4.1
1	A	17	GLU	4.0
1	A	19	SER	4.0
1	A	12	VAL	3.8
1	A	77	GLY	3.8
1	A	21	GLY	3.5
1	A	131	ILE	3.3
1	A	79	ILE	3.1
1	A	41	ASP	3.0
1	A	81	TYR	2.8
1	A	136	LEU	2.8
1	A	52	ILE	2.8
1	A	197	VAL	2.7
1	A	51	ASN	2.5
1	A	29	ARG	2.5
1	A	30	VAL	2.4
1	A	189	VAL	2.4
1	A	14	THR	2.4
1	A	5	PHE	2.4
1	A	141	ARG	2.3
1	A	213	ASP	2.2
1	A	194	CYS	2.2
1	A	196	ILE	2.1
1	A	198	LEU	2.0

## 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](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	4K4	A	301	42/42	0.91	0.16	0.75	28,43,77,80	10
3	CL	A	302	1/1	0.97	0.08	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.