



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:30 am GMT

PDB ID : 5OOT
Title : Structure of CHK1 10-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 : 2017-08-08
Resolution : 2.10 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

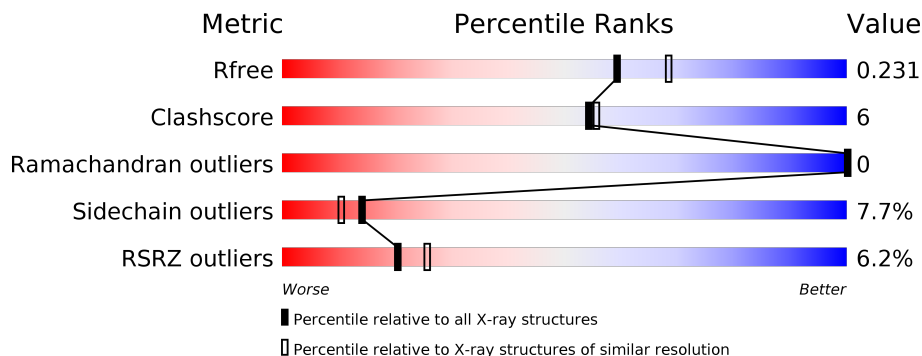
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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	297	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2246 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.

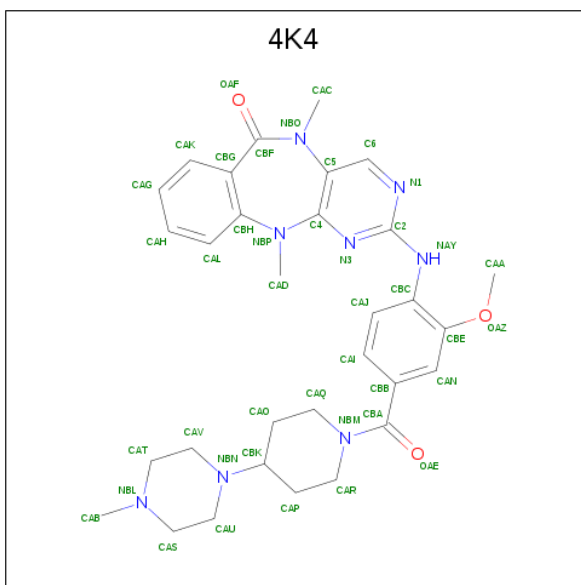
- Molecule 1 is a protein called Serine/threonine-protein kinase Chk1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2078	1332	357	379	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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: C₃₁H₃₈N₈O₃).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	126	Total O 126 126	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.27Å 66.28Å 54.92Å 90.00° 101.99° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 38.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (40.00-2.10) 96.5 (38.30-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.176 , 0.224 0.188 , 0.231	Depositor DCC
R_{free} test set	919 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2246	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% 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](#)

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

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	0.82	0/2127	0.93	2/2886 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	95	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	156	ARG	NE-CZ-NH2	-5.13	117.74	120.30

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	2078	0	2053	23	0
2	A	42	0	38	1	0
3	A	126	0	0	9	0
All	All	2246	0	2091	24	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 (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	3:A:522:HOH:O	2.37	0.81
1:A:162:ARG:NH1	3:A:402:HOH:O	2.19	0.75
1:A:213:ASP:OD1	1:A:222:LYS:NZ	2.18	0.73
1:A:232:LYS:HE3	3:A:496:HOH:O	1.92	0.69
2:A:301:4K4:OAE	3:A:401:HOH:O	2.10	0.69
1:A:8:ASP:N	1:A:8:ASP:OD1	2.27	0.67
1:A:68:ILE:O	1:A:68:ILE:HD12	2.00	0.60
1:A:8:ASP:HB3	3:A:514:HOH:O	2.06	0.56
1:A:13:GLN:O	1:A:24:GLN:NE2	2.41	0.54
1:A:213:ASP:HA	3:A:426:HOH:O	2.08	0.54
1:A:11:LEU:N	1:A:11:LEU:HD12	2.25	0.52
1:A:270:LYS:O	1:A:270:LYS:HG2	2.09	0.51
1:A:13:GLN:C	1:A:24:GLN:HE22	2.13	0.51
1:A:174:VAL:O	1:A:211:PRO:HG3	2.11	0.51
1:A:9:TRP:HZ3	1:A:33:GLU:O	1.94	0.50
1:A:270:LYS:O	1:A:270:LYS:CG	2.61	0.49
1:A:217:GLU:N	3:A:405:HOH:O	2.48	0.46
1:A:170:THR:HG22	1:A:172:PRO:HD2	1.97	0.45
1:A:26:ALA:HB2	1:A:37:VAL:CG2	2.48	0.44
1:A:13:GLN:C	1:A:24:GLN:NE2	2.71	0.44
1:A:104:GLU:N	1:A:105:PRO:CD	2.84	0.41
1:A:140:GLU:OE2	1:A:141:ARG:NH2	2.53	0.41
1:A:232:LYS:CE	3:A:496:HOH:O	2.59	0.41
1:A:168:CYS:SG	3:A:511:HOH:O	2.13	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	256/297 (86%)	244 (95%)	12 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	222/260 (85%)	205 (92%)	17 (8%)	14	10

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

Mol	Chain	Res	Type
1	A	8	ASP
1	A	12	VAL
1	A	13	GLN
1	A	15	LEU
1	A	25	LEU
1	A	40	VAL
1	A	65	GLU
1	A	100	ILE
1	A	138	LEU
1	A	141	ARG
1	A	145	LYS
1	A	165	ASN
1	A	174	VAL
1	A	198	LEU
1	A	215	CYS
1	A	232	LYS
1	A	239	LEU

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	143	ASN
1	A	158	ASN
1	A	165	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	216	GLN

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](#)

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	$\# Z > 2$
2	4K4	A	301	-	40,47,47	1.33	3 (7%)	49,68,68	2.04	11 (22%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	4K4	CBB-CBA	-5.60	1.41	1.50
2	A	301	4K4	C2-NAY	2.01	1.40	1.36
2	A	301	4K4	CAR-NBM	2.03	1.50	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	4K4	N1-C2-N3	-2.75	123.92	126.63
2	A	301	4K4	C2-N3-C4	2.27	117.70	115.11
2	A	301	4K4	CAV-CAT-NBL	2.77	113.95	110.80
2	A	301	4K4	CAP-CAR-NBM	2.84	115.00	110.81
2	A	301	4K4	CAO-CAQ-NBM	2.97	115.19	110.81
2	A	301	4K4	CBB-CBA-NBM	3.01	122.63	118.75
2	A	301	4K4	CAS-NBL-CAT	3.04	113.86	109.53
2	A	301	4K4	C6-N1-C2	3.43	121.38	115.84
2	A	301	4K4	CAU-NBN-CBK	3.46	122.65	112.56
2	A	301	4K4	CAR-NBM-CAQ	4.49	121.09	112.61
2	A	301	4K4	CAK-CBG-CBH	7.94	121.70	118.04

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
2	A	301	4K4	1	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 [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	260/297 (87%)	-0.03	16 (6%)	20 26	20, 35, 77, 97	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	TYR	3.3
1	A	81	TYR	3.3
1	A	17	GLU	3.2
1	A	19	ALA	3.0
1	A	6	VAL	2.9
1	A	79	ILE	2.9
1	A	27	VAL	2.6
1	A	18	GLY	2.5
1	A	74	ARG	2.5
1	A	78	ASN	2.4
1	A	4	PRO	2.4
1	A	21	GLY	2.3
1	A	12	VAL	2.3
1	A	31	THR	2.1
1	A	30	VAL	2.1
1	A	83	PHE	2.1

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

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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	4K4	A	301	42/42	0.95	0.16	28,44,105,109	0

6.5 Other polymers

There are no such residues in this entry.