W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:58 AM GMT

PDB ID	:	2JIV
Title	:	Crystal structure of EGFR kinase domain T790M mutation in compex with HKI-272
Authors	:	Yun, C.-H.; Mengwasser, K.E.; Toms, A.V.; Li, Y.; Woo, M.S.; Greulich, H.; Wong, K.-K.; Meyerson, M.; Eck, M.J.
Deposited on	:	2007-07-02
Resolution	:	3.50 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.
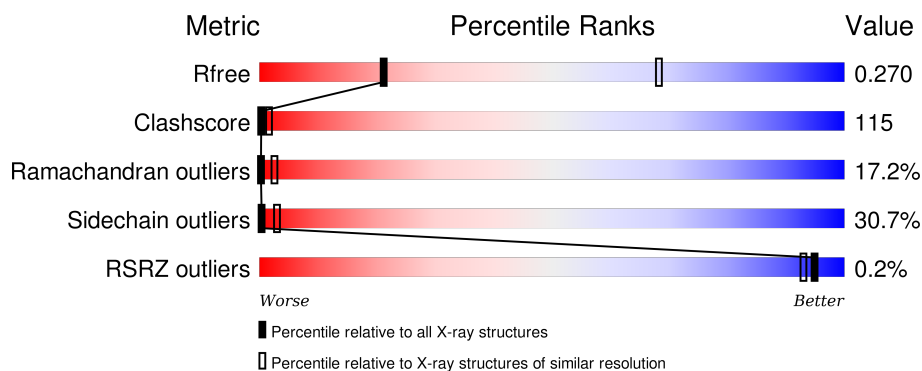
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	328	9% 41% 28% • 18%
1	B	328	12% 46% 23% • 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HKI	A	1797	-	-	X	-
2	HKI	B	1797	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4427 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 EPIDERMAL GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total 2137	C 1384	N 364	O 373	S 16	0	0	0
1	B	272	Total 2146	C 1391	N 363	O 376	S 16	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	790	MET	THR	ENGINEERED MUTATION	UNP P00533
B	790	MET	THR	ENGINEERED MUTATION	UNP P00533

- Molecule 2 is N-(4-{[3-CHLORO-4-(PYRIDIN-2-YLMETHOXY)PHENYL]AMINO}-3-CYANO-7-ETHOXYQUINOLIN-6-YL)-4-(DIMETHYLAMINO)BUTANAMIDE (three-letter code: HKI) (formula: $C_{30}H_{31}ClN_6O_3$).
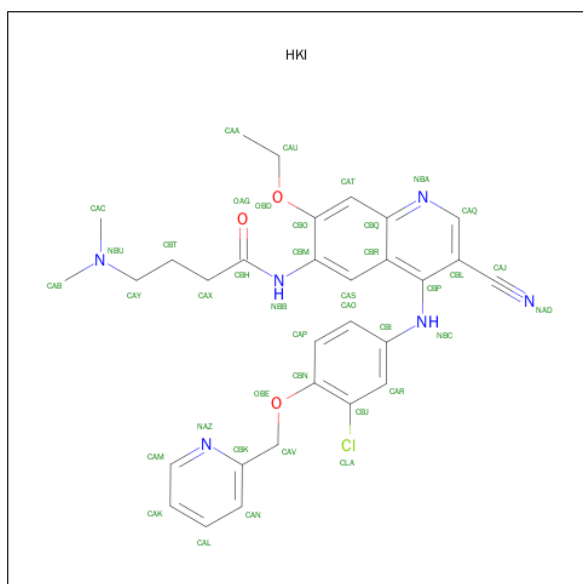
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			40	30	1	6	3		
2	B	1	Total	C	Cl	N	O	0	0
			40	30	1	6	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	19	Total	O	0	0
			19	19		

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: EPIDERMAL GROWTH FACTOR RECEPTOR

• Molecule 1: EPIDERMAL GROWTH FACTOR RECEPTOR

I946 M947 V948 K949 C950 W951 M952 I953 D954 A955 D956 S957 R958 F961 R962 E963 L964 I965 I966 E967 F968 S969 K970 M971 A972 R973 D974 P975 Q976 R977 Y978 L979 V980 I981 Q982 GLY ASP GLU ARG MET HIS LEU PRO SER PRO THR ASP SER ASN PHE TYR ARG ALA LEU MET ASP GLU GLU ASP

MET ASP ASP VAL VAL ASP ALA ASP GLU TYR LEU ILE PRO GLN GLN GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.09Å 98.99Å 73.33Å 90.00° 109.94° 90.00°	Depositor
Resolution (Å)	25.00 – 3.50 24.75 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.2 (25.00-3.50) 90.3 (24.75-3.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.87 (at 3.54Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, R_{free}	0.251 , 0.284 0.246 , 0.270	Depositor DCC
R_{free} test set	428 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 72.1	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.47, <L^2> = 0.29$	Xtriage
Outliers	0 of 8640 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4427	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 6.33% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: HKI, 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	0.44	1/2182 (0.0%)	0.55	1/2951 (0.0%)
1	B	0.42	0/2195	0.53	1/2972 (0.0%)
All	All	0.43	1/4377 (0.0%)	0.54	2/5923 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	797	CYS	C-N	5.24	1.46	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	PRO	N-CA-CB	5.91	110.40	103.30
1	B	699	PRO	N-CA-CB	5.62	110.05	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	932	ARG	Sidechain

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	2137	0	2181	546	0
1	B	2146	0	2183	453	0
2	A	40	0	30	22	0
2	B	40	0	30	23	0
3	B	2	0	0	0	0
4	A	43	0	0	1	0
4	B	19	0	0	0	0
All	All	4427	0	4424	1012	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 115.

The worst 5 of 1012 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)
2:A:1797:HKI:H17	2:A:1797:HKI:CAX	1.49	1.28
2:A:1797:HKI:H23	2:A:1797:HKI:CAC	1.52	1.26
1:A:835:HIS:CE1	1:A:856:PHE:HB3	1.70	1.25
1:A:798:LEU:O	1:A:802:VAL:HG23	1.33	1.23
1:A:743:ALA:O	1:A:744:ILE:HG12	1.32	1.23

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	264/328 (80%)	150 (57%)	66 (25%)	48 (18%)	0	2
1	B	267/328 (81%)	168 (63%)	55 (21%)	44 (16%)	0	3
All	All	531/656 (81%)	318 (60%)	121 (23%)	92 (17%)	0	2

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	702	ALA
1	A	714	LYS
1	A	738	VAL
1	A	739	LYS
1	A	796	GLY

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	230/288 (80%)	153 (66%)	77 (34%)	0	2
1	B	230/288 (80%)	165 (72%)	65 (28%)	0	3
All	All	460/576 (80%)	318 (69%)	142 (31%)	0	3

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	933	LEU
1	B	705	ARG
1	B	932	ARG
1	A	939	CYS
1	A	971	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	835	HIS

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Mol	Chain	Res	Type
1	A	842	ASN
1	B	816	ASN
1	A	816	ASN
1	B	756	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	HKI	A	1797	1	43,43,43	1.27	5 (11%)	56,58,58	1.69	13 (23%)
2	HKI	B	1797	1	43,43,43	1.27	5 (11%)	56,58,58	1.72	13 (23%)

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	HKI	A	1797	1	-	0/24/24/24	0/4/4/4
2	HKI	B	1797	1	-	0/24/24/24	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1797	HKI	CBM-NBB	-4.55	1.33	1.41
2	B	1797	HKI	CBM-NBB	-4.44	1.33	1.41
2	B	1797	HKI	CBI-NBC	-3.46	1.33	1.40
2	A	1797	HKI	CBI-NBC	-3.39	1.33	1.40
2	B	1797	HKI	CBP-CBR	-2.58	1.39	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1797	HKI	CAU-OBD-CBO	-4.63	109.36	118.01
2	A	1797	HKI	CAU-OBD-CBO	-4.51	109.58	118.01
2	B	1797	HKI	CAV-OBE-CBN	-4.46	108.98	117.82
2	A	1797	HKI	CAV-OBE-CBN	-4.05	109.80	117.82
2	B	1797	HKI	OBD-CBO-CAT	-2.81	120.02	125.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1797	HKI	22	0
2	B	1797	HKI	23	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, 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	270/328 (82%)	-0.46	1 (0%)	93	90	28, 47, 54, 61	0
1	B	272/328 (82%)	-0.46	0	100	100	31, 46, 55, 61	0
All	All	542/656 (82%)	-0.46	1 (0%)	95	93	28, 47, 55, 61	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	ALA	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HKI	A	1797	40/40	0.88	0.23	0.31	29,35,38,38	0
2	HKI	B	1797	40/40	0.90	0.21	-0.12	29,31,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	CL	B	1984	1/1	0.92	0.12	-	12,12,12,12	0
3	CL	B	1985	1/1	0.67	0.26	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.