



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:56 AM GMT

PDB ID : 3QGW
Title : Crystal Structure of ITK kinase bound to an inhibitor
Authors : Brown, K.; Cheetham, G.M.T.
Deposited on : 2011-01-25
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/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 (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

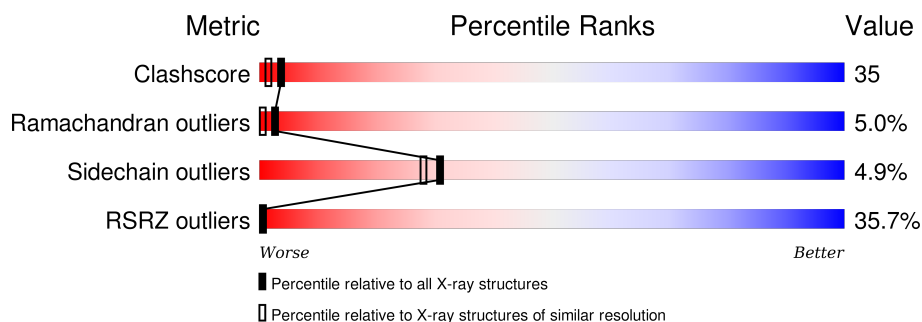
1 Overall quality at a glance

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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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	286	<div> <div>28%</div> <div>50%</div> <div>30%</div> <div>5%</div> <div>15%</div> </div>
1	B	286	<div> <div>33%</div> <div>43%</div> <div>36%</div> <div>5%</div> <div>16%</div> </div>

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
3	L7A	B	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5040 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 Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	1	0
			1956	1251	323	365	17			
1	B	240	Total	C	N	O	S	0	0	0
			1924	1231	319	358	16			

There are 50 discrepancies between the modelled and reference sequences:

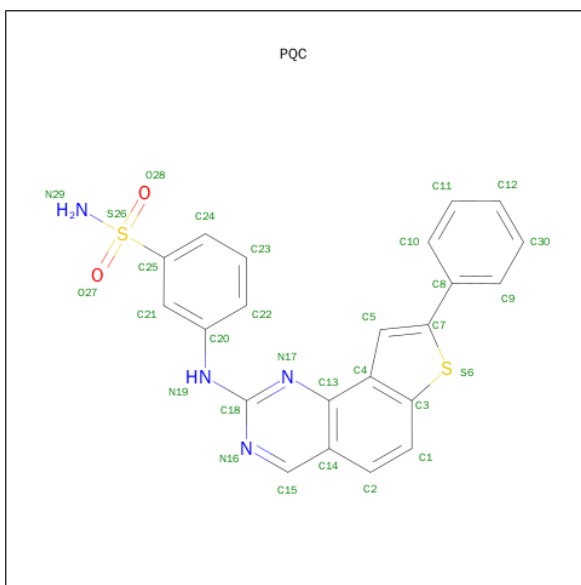
Chain	Residue	Modelled	Actual	Comment	Reference
A	335	MET	-	EXPRESSION TAG	UNP Q08881
A	336	GLY	-	EXPRESSION TAG	UNP Q08881
A	337	SER	-	EXPRESSION TAG	UNP Q08881
A	338	SER	-	EXPRESSION TAG	UNP Q08881
A	339	HIS	-	EXPRESSION TAG	UNP Q08881
A	340	HIS	-	EXPRESSION TAG	UNP Q08881
A	341	HIS	-	EXPRESSION TAG	UNP Q08881
A	342	HIS	-	EXPRESSION TAG	UNP Q08881
A	343	HIS	-	EXPRESSION TAG	UNP Q08881
A	344	HIS	-	EXPRESSION TAG	UNP Q08881
A	345	SER	-	EXPRESSION TAG	UNP Q08881
A	346	SER	-	EXPRESSION TAG	UNP Q08881
A	347	GLY	-	EXPRESSION TAG	UNP Q08881
A	348	LEU	-	EXPRESSION TAG	UNP Q08881
A	349	VAL	-	EXPRESSION TAG	UNP Q08881
A	350	PRO	-	EXPRESSION TAG	UNP Q08881
A	351	ARG	-	EXPRESSION TAG	UNP Q08881
A	352	GLY	-	EXPRESSION TAG	UNP Q08881
A	353	SER	-	EXPRESSION TAG	UNP Q08881
A	354	LEU	-	EXPRESSION TAG	UNP Q08881
A	355	HIS	-	EXPRESSION TAG	UNP Q08881
A	356	MET	-	EXPRESSION TAG	UNP Q08881
A	394	LYS	ARG	CONFLICT	UNP Q08881
A	397	SER	ALA	CONFLICT	UNP Q08881
A	401	ASP	GLU	CONFLICT	UNP Q08881

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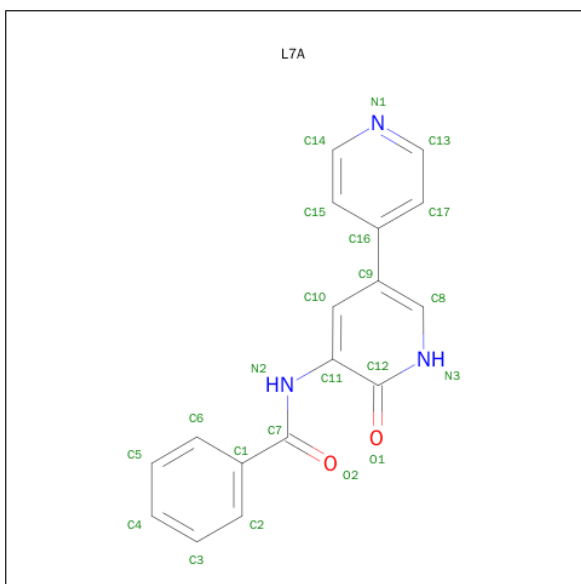
Chain	Residue	Modelled	Actual	Comment	Reference
B	335	MET	-	EXPRESSION TAG	UNP Q08881
B	336	GLY	-	EXPRESSION TAG	UNP Q08881
B	337	SER	-	EXPRESSION TAG	UNP Q08881
B	338	SER	-	EXPRESSION TAG	UNP Q08881
B	339	HIS	-	EXPRESSION TAG	UNP Q08881
B	340	HIS	-	EXPRESSION TAG	UNP Q08881
B	341	HIS	-	EXPRESSION TAG	UNP Q08881
B	342	HIS	-	EXPRESSION TAG	UNP Q08881
B	343	HIS	-	EXPRESSION TAG	UNP Q08881
B	344	HIS	-	EXPRESSION TAG	UNP Q08881
B	345	SER	-	EXPRESSION TAG	UNP Q08881
B	346	SER	-	EXPRESSION TAG	UNP Q08881
B	347	GLY	-	EXPRESSION TAG	UNP Q08881
B	348	LEU	-	EXPRESSION TAG	UNP Q08881
B	349	VAL	-	EXPRESSION TAG	UNP Q08881
B	350	PRO	-	EXPRESSION TAG	UNP Q08881
B	351	ARG	-	EXPRESSION TAG	UNP Q08881
B	352	GLY	-	EXPRESSION TAG	UNP Q08881
B	353	SER	-	EXPRESSION TAG	UNP Q08881
B	354	LEU	-	EXPRESSION TAG	UNP Q08881
B	355	HIS	-	EXPRESSION TAG	UNP Q08881
B	356	MET	-	EXPRESSION TAG	UNP Q08881
B	394	LYS	ARG	CONFLICT	UNP Q08881
B	397	SER	ALA	CONFLICT	UNP Q08881
B	401	ASP	GLU	CONFLICT	UNP Q08881

- Molecule 2 is 3-[(8-PHENYLTHIENO[2,3-H]QUINAZOLIN-2-YL)AMINO]BENZENESULFONAMIDE (three-letter code: PQC) (formula: C₂₂H₁₆N₄O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	22	4	2	2		

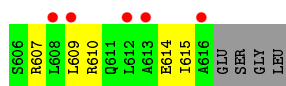
- Molecule 3 is N-(6-OXO-1,6-DIHYDRO-3,4'-BIPYRIDIN-5-YL)BENZAMIDE (three-letter code: L7A) (formula: C₁₇H₁₃N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			22	17	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	485	Total 485	O 485	0	0
4	B	623	Total 623	O 623	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.86 Å 74.38 Å 78.83 Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.93 – 2.09	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 90.3 (19.93-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.09 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.320 0.305 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38915 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5040	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 5.41% 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, 0.375 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: PQC, L7A

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	0.57	0/2005	0.74	1/2707 (0.0%)
1	B	0.57	0/1968	0.75	2/2657 (0.1%)
All	All	0.57	0/3973	0.74	3/5364 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	SER	N-CA-C	5.28	125.25	111.00
1	B	562	ARG	N-CA-C	5.27	125.22	111.00
1	B	530	PHE	CB-CA-C	-5.20	99.99	110.40

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	1956	0	1908	128	1
1	B	1924	0	1885	144	2
2	A	30	0	16	4	0
3	B	22	0	13	2	0
4	A	485	0	0	36	1
4	B	623	0	0	50	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5040	0	3822	275	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 35.

The worst 5 of 275 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:493:ASN:N	1:A:493:ASN:HD22	1.54	1.04
1:B:607:ARG:HH11	1:B:610:ARG:HD2	1.27	0.98
1:B:607:ARG:NH1	1:B:610:ARG:HD2	1.85	0.91
1:B:538:LYS:HE3	4:B:947:HOH:O	1.72	0.88
1:B:430:PRO:HB2	4:B:708:HOH:O	1.73	0.88

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)
1:B:598:ARG:NH2	4:B:979:HOH:O[2_656]	1.99	0.21
1:B:415:HIS:O	4:A:699:HOH:O[4_555]	2.04	0.16
1:A:385:LYS:NZ	4:B:771:HOH:O[4_545]	2.10	0.10

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	241/286 (84%)	216 (90%)	14 (6%)	11 (5%)	3	1
1	B	236/286 (82%)	210 (89%)	13 (6%)	13 (6%)	2	0
All	All	477/572 (83%)	426 (89%)	27 (6%)	24 (5%)	3	0

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	SER
1	A	374	PHE
1	A	428	GLN
1	A	430	PRO
1	A	481	ARG

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	216/252 (86%)	206 (95%)	10 (5%)	33	31
1	B	212/252 (84%)	201 (95%)	11 (5%)	29	25
All	All	428/504 (85%)	407 (95%)	21 (5%)	31	28

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	600	GLU
1	B	363	LEU
1	B	479	ILE
1	A	585	THR
1	B	499	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	493	ASN
1	A	586	HIS
1	B	420	GLN
1	A	450	GLN
1	B	428	GLN

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
2	PQC	A	1	-	30,34,34	5.36	24 (80%)	38,50,50	2.93	16 (42%)
3	L7A	B	1	-	23,24,24	4.04	17 (73%)	28,32,32	2.59	11 (39%)

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	PQC	A	1	-	-	0/14/14/14	0/5/5/5
3	L7A	B	1	-	-	0/12/12/12	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	PQC	C15-C14	-2.70	1.36	1.41
2	A	1	PQC	O28-S26	-2.28	1.40	1.43
2	A	1	PQC	C23-C22	2.32	1.43	1.38
2	A	1	PQC	C30-C12	2.51	1.44	1.38
2	A	1	PQC	C11-C10	2.66	1.44	1.38

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	L7A	C9-C8-N3	-6.17	114.36	124.34
2	A	1	PQC	O28-S26-N29	-5.02	100.78	107.28
2	A	1	PQC	N16-C18-N17	-4.84	121.27	126.62
2	A	1	PQC	C24-C23-C22	-4.74	113.47	120.24
3	B	1	L7A	C15-C14-N1	-4.43	115.92	123.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PQC	4	0
3	B	1	L7A	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 [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	244/286 (85%)	1.75	80 (32%) 0 1	24, 26, 45, 52	0
1	B	240/286 (83%)	1.85	93 (38%) 0 0	23, 26, 42, 46	0
All	All	484/572 (84%)	1.80	173 (35%) 0 0	23, 26, 43, 52	0

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	GLY	7.9
1	B	428	GLN	7.1
1	A	372	GLY	6.3
1	B	358	ILE	6.3
1	A	371	SER	6.0

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, 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(\AA^2)	Q<0.9
3	L7A	B	1	22/22	0.76	0.25	2.22	42,42,42,42	0
2	PQC	A	1	30/30	0.78	0.26	0.61	11,19,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.