



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2016 – 10:58 AM EDT

PDB ID : 5A9U
Title : Structure of C1156Y Mutant Human Anaplastic Lymphoma Kinase in Complex with PF-06463922 ((10R)-7-amino-12-fluoro-2,10,16-trimethyl- 15-oxo-10,15,16,17-tetrahydro-2H-8,4-(metheno)pyrazolo(4,3-h)(2,5,11) benzoxadiazacyclotetradecine-3-carbonitrile).
Authors : McTigue, M.; Deng, Y.-L.; Liu, W.; Brooun, A.; Stewart, A.
Deposited on : 2015-07-22
Resolution : 1.60 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

<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

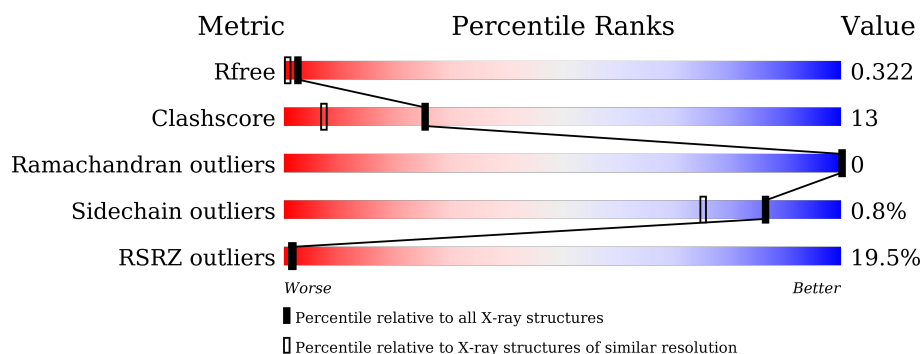
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	327	<div> <div>17%</div> <div>74%</div> <div>15%</div> <div>10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2558 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.

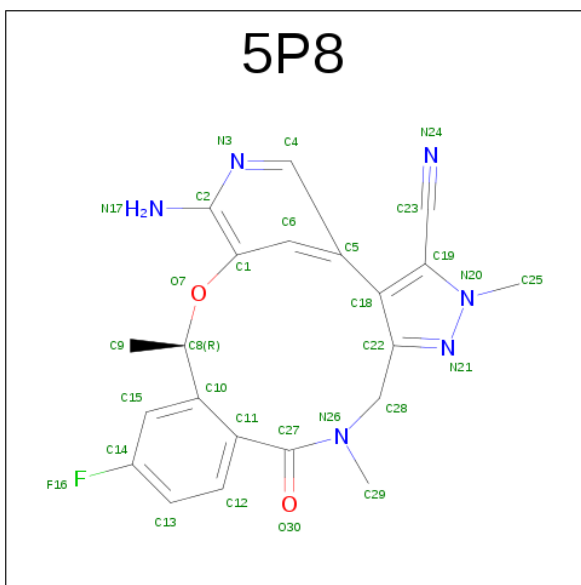
- Molecule 1 is a protein called ALK TYROSINE KINASE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2330	1485	397	426	22	0	3	1

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	MET	-	EXPRESSION TAG	UNP Q9UM73
A	1086	ALA	-	EXPRESSION TAG	UNP Q9UM73
A	1087	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1088	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1089	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1090	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1091	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1092	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1156	TYR	CYS	ENGINEERED MUTATION	UNP Q9UM73

- Molecule 2 is (10R)-7-AMINO-12-FLUORO-2,10,16-TRIMETHYL-15-OXO-10,15,16,17-TETRAHYDRO-2H-8,4-(METHENO)PYRAZOLO[4,3-H][2,5,11]BENZOXADIAZACYCLOTRIDECADECINE-3-CARBONITRILE (three-letter code: 5P8) (formula: C₂₁H₁₉FN₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			30	21	1	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.75Å 57.59Å 104.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.60 38.77 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.64-1.60) 99.2 (38.77-1.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.59Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.215 , 0.258 0.292 , 0.322	Depositor DCC
R_{free} test set	1261 reflections (3.00%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2558	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5P8

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	0.26	0/2386	0.45	0/3233

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	2330	0	2302	59	0
2	A	30	0	19	0	0
3	A	198	0	0	4	0
All	All	2558	0	2321	59	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 13.

All (59) 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:1105:ILE:HG12	1:A:1165:LEU:HD21	1.57	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:ILE:HD11	1:A:1134:GLN:HG3	1.61	0.81
1:A:1105:ILE:HD12	1:A:1105:ILE:H	1.46	0.81
1:A:1165:LEU:O	1:A:1169:LEU:HD13	1.86	0.75
1:A:1105:ILE:HG13	1:A:1165:LEU:HD11	1.70	0.73
1:A:1105:ILE:CG1	1:A:1165:LEU:HD21	2.19	0.71
1:A:1105:ILE:N	1:A:1105:ILE:HD12	2.07	0.68
1:A:1152:LEU:HD21	1:A:1161:GLU:HG2	1.78	0.65
1:A:1365:CYS:O	1:A:1373:ARG:HD2	1.97	0.65
1:A:1093:ASN:HB2	1:A:1105:ILE:HD13	1.78	0.65
1:A:1105:ILE:CD1	1:A:1105:ILE:H	2.10	0.65
1:A:1150:LYS:HE2	1:A:1167:GLU:OE1	1.98	0.64
1:A:1163:ASP:HA	1:A:1275:ARG:HD3	1.80	0.63
1:A:1367:GLN:HB2	1:A:1373:ARG:HG2	1.79	0.62
1:A:1214:ARG:HG3	1:A:1215:PRO:HD2	1.84	0.60
1:A:1163:ASP:CA	1:A:1275:ARG:HD3	2.31	0.60
1:A:1197:GLU:HG2	1:A:1199:MET:HE3	1.85	0.59
1:A:1124:HIS:HB3	1:A:1129:GLU:HA	1.84	0.59
1:A:1248:ARG:CZ	1:A:1277:ILE:HG21	2.33	0.58
1:A:1093:ASN:ND2	1:A:1105:ILE:HD13	2.19	0.58
1:A:1108:LEU:HD11	1:A:1169:LEU:CD1	2.33	0.57
1:A:1093:ASN:HD22	1:A:1105:ILE:HD13	1.68	0.57
1:A:1207:PHE:O	1:A:1211:THR:HG22	2.06	0.56
1:A:1248:ARG:NH1	1:A:1277:ILE:HG21	2.21	0.56
1:A:1382:ARG:HD3	3:A:2177:HOH:O	2.06	0.54
1:A:1383:ILE:O	1:A:1387:THR:HG23	2.08	0.54
1:A:1146:GLN:HG2	1:A:1198:LEU:HD22	1.90	0.53
1:A:1108:LEU:HD11	1:A:1169:LEU:HD12	1.89	0.53
1:A:1244:HIS:HD2	3:A:2006:HOH:O	1.91	0.53
1:A:1211:THR:HG23	1:A:1221:LEU:HD22	1.91	0.52
1:A:1114:LYS:HG3	1:A:1115:ASN:ND2	2.26	0.51
1:A:1279:ARG:HE	1:A:1279:ARG:HA	1.77	0.50
1:A:1124:HIS:HD2	1:A:1130:VAL:H	1.60	0.50
1:A:1124:HIS:CD2	1:A:1129:GLU:HB3	2.47	0.49
1:A:1163:ASP:HB3	1:A:1275:ARG:CZ	2.43	0.48
1:A:1199:MET:HA	1:A:1199:MET:HE2	1.95	0.48
1:A:1197:GLU:HG2	1:A:1199:MET:CE	2.43	0.48
1:A:1247:HIS:O	1:A:1248:ARG:HB2	2.14	0.47
1:A:1122:LEU:HD21	1:A:1132:GLU:HB2	1.97	0.47
1:A:1352:LYS:HD2	1:A:1398:PRO:CB	2.45	0.47
1:A:1325:LEU:HD21	1:A:1397:LEU:HD22	1.95	0.46
1:A:1119:ILE:HD11	1:A:1134:GLN:CG	2.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:MET:HA	1:A:1199:MET:CE	2.47	0.45
1:A:1199:MET:HE1	3:A:2068:HOH:O	2.17	0.45
1:A:1146:GLN:HG2	1:A:1198:LEU:CD2	2.46	0.45
1:A:1352:LYS:HD2	1:A:1398:PRO:HB3	1.99	0.45
1:A:1115:ASN:HD22	1:A:1115:ASN:N	2.15	0.44
1:A:1163:ASP:CB	1:A:1275:ARG:HD3	2.48	0.44
1:A:1279:ARG:HA	1:A:1279:ARG:NE	2.34	0.43
1:A:1118:LEU:HD22	3:A:2002:HOH:O	2.17	0.43
1:A:1186:SER:HB3	1:A:1193:PHE:HB2	2.01	0.43
1:A:1214:ARG:HG3	1:A:1215:PRO:CD	2.47	0.42
1:A:1112:PRO:HG2	1:A:1115:ASN:OD1	2.19	0.42
1:A:1214:ARG:HE	1:A:1400:GLU:HG3	1.85	0.42
1:A:1367:GLN:O	1:A:1373:ARG:HD3	2.19	0.42
1:A:1124:HIS:HB3	1:A:1129:GLU:HG2	2.01	0.41
1:A:1325:LEU:HD22	1:A:1325:LEU:N	2.35	0.41
1:A:1278:TYR:O	1:A:1279:ARG:HB2	2.21	0.40
1:A:1093:ASN:HA	1:A:1094:PRO:HD3	1.85	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	288/327 (88%)	283 (98%)	5 (2%)	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	259/285 (91%)	257 (99%)	2 (1%)	86	75

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1161	GLU
1	A	1214	ARG

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	1093	ASN
1	A	1115	ASN
1	A	1124	HIS
1	A	1134	GLN
1	A	1188	GLN
1	A	1217	GLN
1	A	1243	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 ⓘ

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	5P8	A	2402	-	31,33,33	2.03	9 (29%)	36,49,49	1.48	6 (16%)

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	5P8	A	2402	-	-	0/23/26/26	0/2/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2402	5P8	N21-N20	-3.47	1.34	1.37
2	A	2402	5P8	C6-C1	2.04	1.42	1.38
2	A	2402	5P8	C12-C11	2.50	1.44	1.39
2	A	2402	5P8	C15-C14	2.53	1.42	1.37
2	A	2402	5P8	C2-N17	2.60	1.41	1.34
2	A	2402	5P8	C15-C10	2.97	1.44	1.39
2	A	2402	5P8	O7-C8	3.00	1.47	1.42
2	A	2402	5P8	C11-C10	4.28	1.45	1.40
2	A	2402	5P8	C27-N26	5.53	1.44	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2402	5P8	O30-C27-C11	-3.06	113.91	120.13
2	A	2402	5P8	C6-C5-C4	-2.80	114.49	117.20
2	A	2402	5P8	C29-N26-C27	-2.71	116.46	123.30
2	A	2402	5P8	C1-O7-C8	2.38	121.70	117.82
2	A	2402	5P8	C28-N26-C27	2.40	126.58	120.17
2	A	2402	5P8	C5-C6-C1	2.97	124.32	120.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	293/327 (89%)	1.44	57 (19%) 1 1	17, 30, 61, 77	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1286	GLY	8.6
1	A	1402	GLY	8.5
1	A	1093	ASN	7.9
1	A	1124	HIS	7.4
1	A	1156	TYR	6.8
1	A	1216	SER	5.9
1	A	1279	ARG	5.6
1	A	1277	ILE	5.6
1	A	1217	GLN	5.5
1	A	1129	GLU	5.1
1	A	1400	GLU	5.1
1	A	1101	LYS	4.5
1	A	1401	TYR	4.5
1	A	1165	LEU	4.4
1	A	1399	ILE	4.2
1	A	1218	PRO	3.6
1	A	1214	ARG	3.6
1	A	1385	TYR	3.6
1	A	1157	SER	3.6
1	A	1276	ASP	3.5
1	A	1177	GLN	3.4
1	A	1158	GLU	3.4
1	A	1105	ILE	3.3
1	A	1278	TYR	3.2
1	A	1211	THR	3.1
1	A	1094	PRO	3.0
1	A	1274	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1287	GLY	3.0
1	A	1097[A]	CYS	3.0
1	A	1288	CYS	2.8
1	A	1106	SER	2.8
1	A	1128	GLY	2.7
1	A	1122	LEU	2.7
1	A	1302	MET	2.7
1	A	1155	VAL	2.5
1	A	1162	LEU	2.5
1	A	1099	ALA	2.4
1	A	1262	PRO	2.4
1	A	1255	CYS	2.4
1	A	1261	GLY	2.4
1	A	1220	SER	2.3
1	A	1319	LEU	2.2
1	A	1339	LEU	2.2
1	A	1160	ASP	2.2
1	A	1095	ASN	2.2
1	A	1123	GLY	2.2
1	A	1301	PHE	2.2
1	A	1356	GLY	2.1
1	A	1227	LEU	2.1
1	A	1257	LEU	2.1
1	A	1358	VAL	2.1
1	A	1209	ARG	2.0
1	A	1215	PRO	2.0
1	A	1315	PHE	2.0
1	A	1188	GLN	2.0
1	A	1213	PRO	2.0
1	A	1355	PRO	2.0

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 [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
2	5P8	A	2402	30/30	0.85	0.12	-0.45	23,27,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.