Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 01:59 pm BST

PDB ID	:	5IUI
Title	:	Crystal Structure of Anaplastic Lyphoma Kinase (ALK) in complex with 4
Authors	:	Tu, C.H.; Wu, S.Y.
Deposited on	:	2016-03-18
Resolution	:	1.88 Å(reported)

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

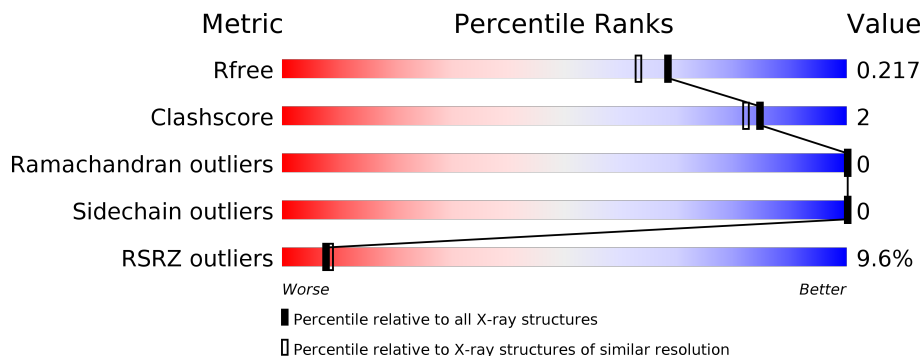|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.88 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	Percentile Ranks	Value
Rfree		0.217
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		9.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 respectively. 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	327	9% ... 88% ... · 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2578 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
1	A	303	Total	C	N	O	S	0	3	0
			2362	1503	400	438	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1097	SER	CYS	engineered mutation	UNP Q9UM73

- Molecule 2 is N-[3-(4-amino-3-methylphenyl)-1H-pyrazol-5-yl]-4-[(4-methylpiperazin-1-yl)m ethyl]benzamide (three-letter code: 45Q) (formula: $C_{23}H_{28}N_6O$).
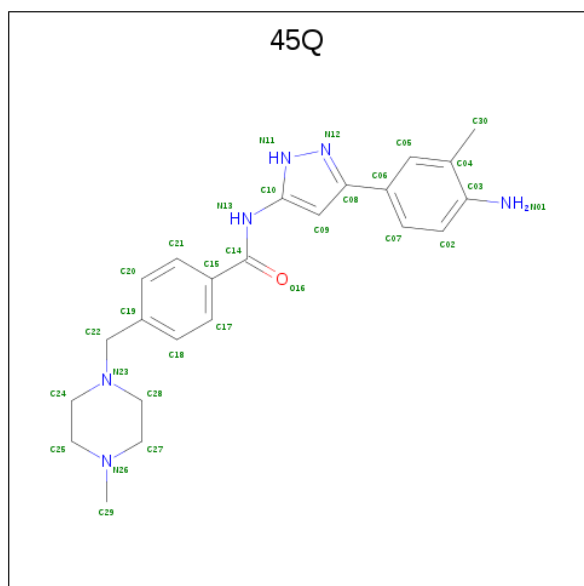
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	23	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	186	Total O 186 186	0	0

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 the various outlier classes 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: ALK tyrosine kinase receptor
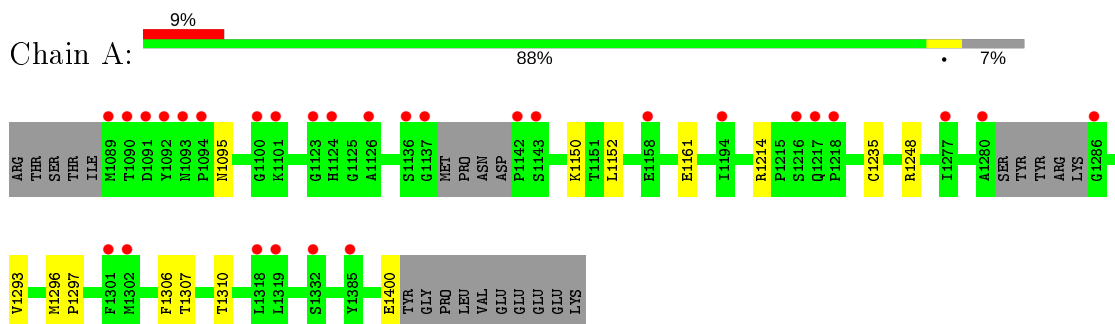
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.85Å 57.43Å 105.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.63 – 1.88 23.63 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.9 (23.63-1.88) 97.9 (23.63-1.88)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.11 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.179 , 0.205 0.191 , 0.217	Depositor DCC
R_{free} test set	1285 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.1	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2578	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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, 0.333 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: 45Q

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	0.30	0/2427	0.51	0/3292

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 (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	2362	0	2328	11	0
2	A	30	0	0	1	0
3	A	186	0	0	2	0
All	All	2578	0	2328	11	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 2.

All (11) 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:1293:VAL:HA	1:A:1296:MET:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:ASN:ND2	3:A:1602:HOH:O	2.37	0.57
1:A:1150:LYS:HD2	2:A:1501:45Q:C30	2.40	0.51
1:A:1293:VAL:HA	1:A:1296:MET:CE	2.43	0.48
1:A:1248:ARG:CD	1:A:1306:PHE:CD1	2.99	0.45
1:A:1214:ARG:NH2	1:A:1400:GLU:OE1	2.49	0.45
1:A:1297:PRO:HG3	1:A:1310:THR:HG22	1.99	0.44
1:A:1307:THR:O	1:A:1310:THR:OG1	2.32	0.43
1:A:1235[A]:CYS:SG	3:A:1764:HOH:O	2.34	0.43
1:A:1152:LEU:HD21	1:A:1161:GLU:HG2	1.99	0.42
1:A:1248:ARG:NE	1:A:1306:PHE:CD1	2.88	0.42

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	300/327 (92%)	291 (97%)	9 (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	261/286 (91%)	261 (100%)	0	100　100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	45Q	A	1501	-	32,33,33	3.95	21 (65%)	42,46,46	2.07	11 (26%)

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	45Q	A	1501	-	-	4/14/26/26	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	45Q	C22-N23	-9.21	1.29	1.47
2	A	1501	45Q	C29-N26	-7.21	1.30	1.46
2	A	1501	45Q	C05-C04	5.91	1.48	1.39
2	A	1501	45Q	C21-C20	5.67	1.49	1.38
2	A	1501	45Q	C21-C15	5.62	1.48	1.39
2	A	1501	45Q	C17-C15	5.49	1.48	1.39
2	A	1501	45Q	C18-C17	5.11	1.48	1.38
2	A	1501	45Q	C07-C02	4.93	1.47	1.38
2	A	1501	45Q	C28-N23	-4.43	1.34	1.46
2	A	1501	45Q	C25-N26	-4.27	1.37	1.46
2	A	1501	45Q	C18-C19	4.26	1.48	1.38
2	A	1501	45Q	C05-C06	4.20	1.47	1.39
2	A	1501	45Q	C20-C19	4.09	1.47	1.38
2	A	1501	45Q	C09-C08	-3.90	1.33	1.40
2	A	1501	45Q	C27-N26	-3.89	1.38	1.46
2	A	1501	45Q	N12-N11	-3.44	1.30	1.37
2	A	1501	45Q	O16-C14	-3.25	1.16	1.23
2	A	1501	45Q	C02-C03	3.09	1.47	1.40
2	A	1501	45Q	C07-C06	2.93	1.45	1.39
2	A	1501	45Q	C24-N23	-2.57	1.39	1.46
2	A	1501	45Q	C08-N12	-2.36	1.31	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	45Q	C27-N26-C25	6.97	119.28	109.52
2	A	1501	45Q	C19-C22-N23	4.80	122.45	113.12
2	A	1501	45Q	C07-C06-C08	-4.12	114.78	121.28
2	A	1501	45Q	C28-N23-C24	3.75	117.26	108.83
2	A	1501	45Q	C05-C06-C08	3.57	125.75	120.59
2	A	1501	45Q	C06-C08-N12	3.00	125.76	120.96
2	A	1501	45Q	C29-N26-C25	2.95	115.07	110.66
2	A	1501	45Q	C09-C08-C06	-2.44	126.05	129.44
2	A	1501	45Q	C09-C10-N11	-2.23	107.28	110.47
2	A	1501	45Q	C28-C27-N26	2.21	113.30	110.80
2	A	1501	45Q	C22-N23-C28	2.18	115.91	111.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	45Q	C07-C06-C08-C09

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Mol	Chain	Res	Type	Atoms
2	A	1501	45Q	C19-C22-N23-C28
2	A	1501	45Q	C07-C06-C08-N12
2	A	1501	45Q	C05-C06-C08-C09

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	45Q	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 45Q A 1501

Bond lengths

Bond angles

Torsions

Rings
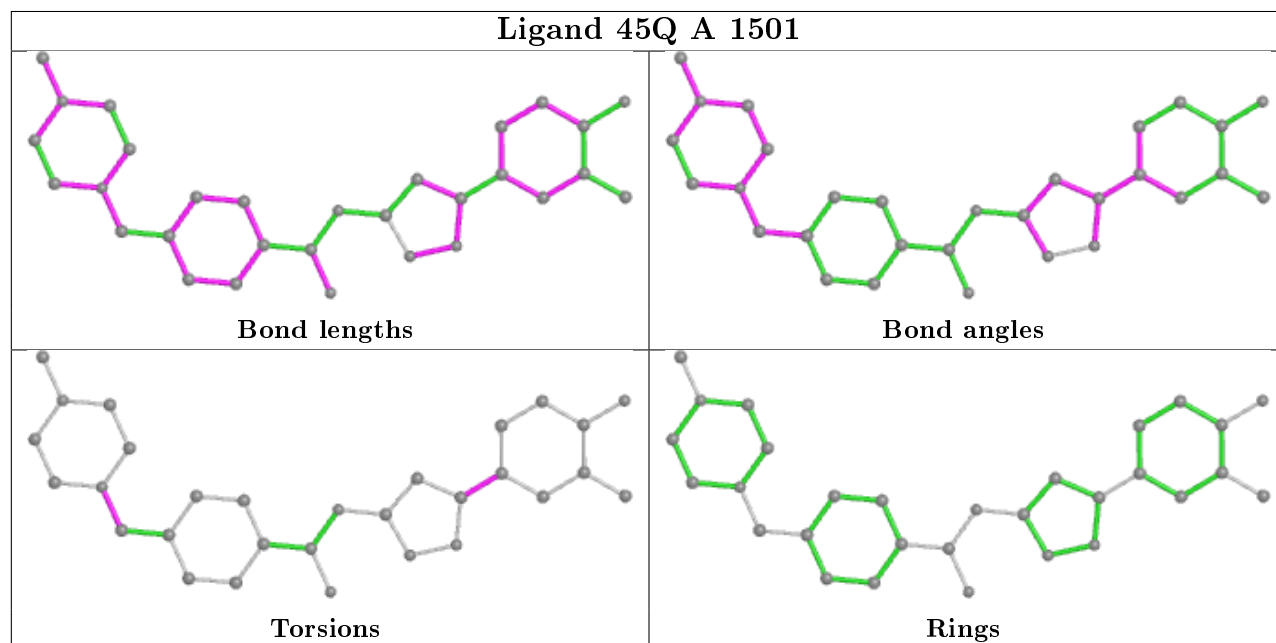
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	303/327 (92%)	0.41	29 (9%)	8 8	14, 27, 60, 86	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1280	ALA	6.2
1	A	1090	THR	6.1
1	A	1126	ALA	5.4
1	A	1091	ASP	4.6
1	A	1286	GLY	4.5
1	A	1123	GLY	4.3
1	A	1124	HIS	3.9
1	A	1137	GLY	3.9
1	A	1216	SER	3.8
1	A	1218	PRO	3.8
1	A	1092	TYR	3.5
1	A	1143	SER	3.3
1	A	1302	MET	3.3
1	A	1093	ASN	3.1
1	A	1089	MET	2.9
1	A	1094	PRO	2.8
1	A	1277	ILE	2.8
1	A	1158	GLU	2.8
1	A	1217	GLN	2.6
1	A	1301	PHE	2.6
1	A	1385	TYR	2.5
1	A	1194	ILE	2.5
1	A	1142	PRO	2.5
1	A	1101	LYS	2.5
1	A	1332	SER	2.5
1	A	1318	LEU	2.4
1	A	1136	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1100	GLY	2.2
1	A	1319	LEU	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.
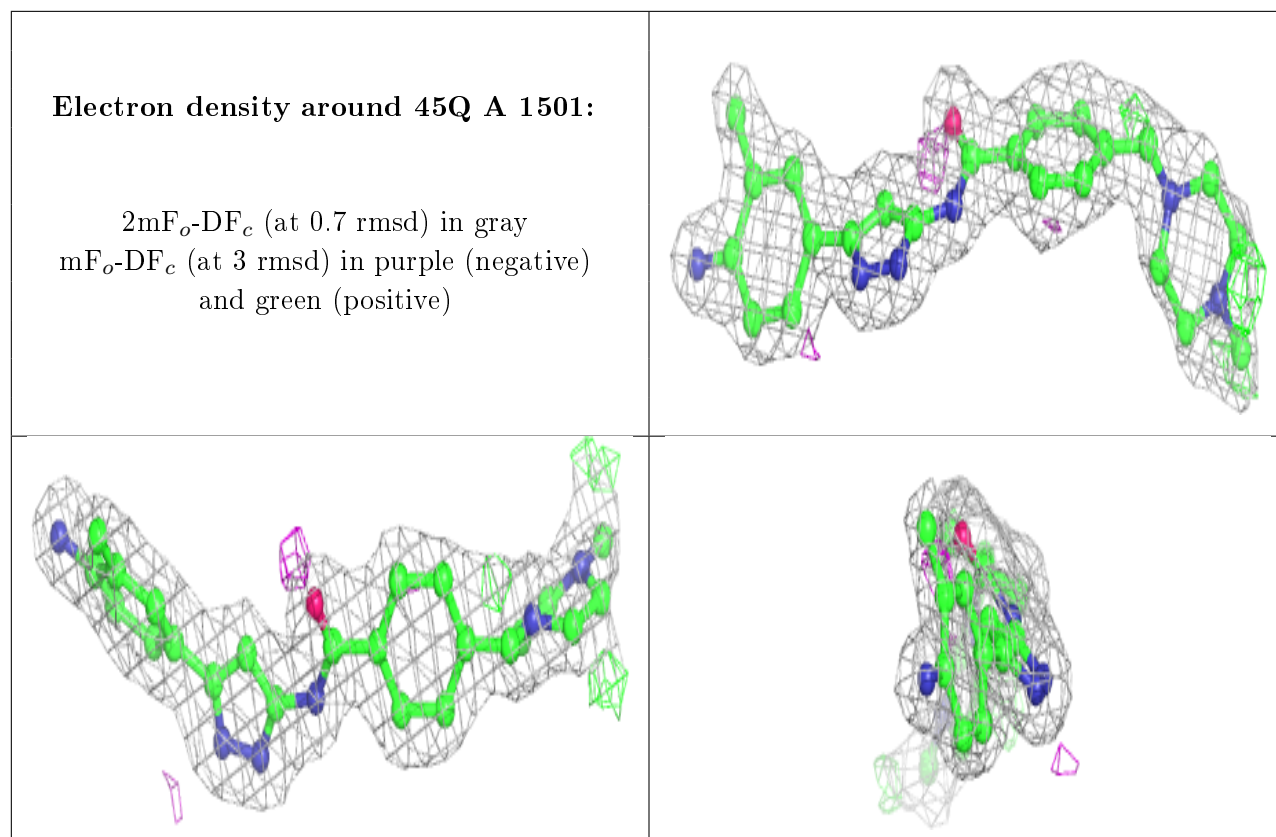
6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. 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($Å^2$)	Q<0.9
2	45Q	A	1501	30/30	0.91	0.12	19,26,57,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 45Q A 1501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.