



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:06 PM UTC

PDB ID : 4PY1 / pdb_00004py1
Title : Crystal structure of Tyk2 in complex with compound 15, 6-((2,5-dimethoxyphenyl)thio)-3-(1-methyl-1H-pyrazol-4-yl)-[1,2,4]triazolo[4,3-b]pyridazine
Authors : Han, S.; Knafels, J.D.
Deposited on : 2014-03-25
Resolution : 2.16 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

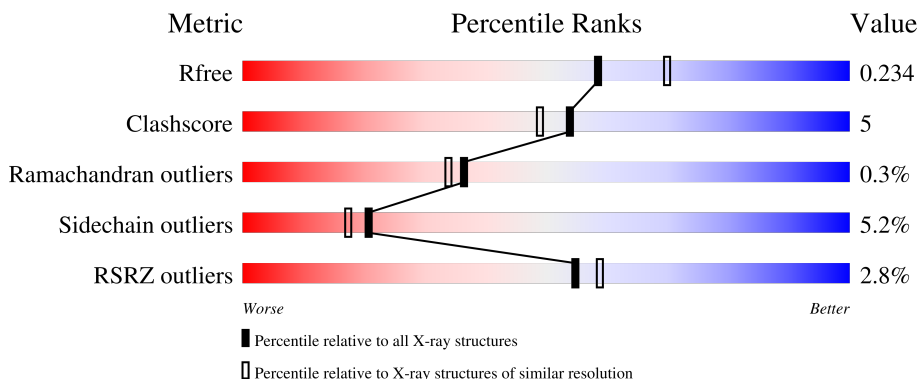
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 of 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 $\leq 5\%$. 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	318	

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	2YK	A	1201	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2493 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 Non-receptor tyrosine-protein kinase TYK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	290	2349	1505	402	428	1	13	0	0	0

There are 29 discrepancies between the modelled and reference sequences:

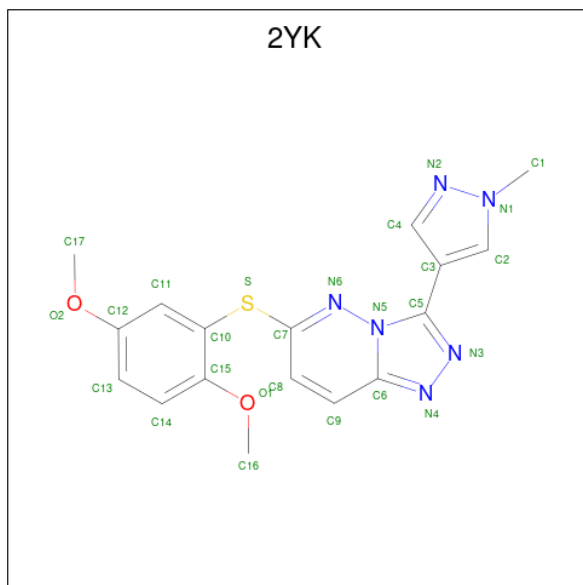
Chain	Residue	Modelled	Actual	Comment	Reference
A	865	MET	-	expression tag	UNP P29597
A	866	ALA	-	expression tag	UNP P29597
A	867	HIS	-	expression tag	UNP P29597
A	868	HIS	-	expression tag	UNP P29597
A	869	HIS	-	expression tag	UNP P29597
A	870	HIS	-	expression tag	UNP P29597
A	871	HIS	-	expression tag	UNP P29597
A	872	HIS	-	expression tag	UNP P29597
A	873	HIS	-	expression tag	UNP P29597
A	874	HIS	-	expression tag	UNP P29597
A	875	HIS	-	expression tag	UNP P29597
A	876	HIS	-	expression tag	UNP P29597
A	877	GLY	-	expression tag	UNP P29597
A	878	ALA	-	expression tag	UNP P29597
A	879	LEU	-	expression tag	UNP P29597
A	880	GLU	-	expression tag	UNP P29597
A	881	VAL	-	expression tag	UNP P29597
A	882	LEU	-	expression tag	UNP P29597
A	883	PHE	-	expression tag	UNP P29597
A	884	GLN	-	expression tag	UNP P29597
A	885	GLY	-	expression tag	UNP P29597
A	886	PRO	-	expression tag	UNP P29597
A	887	GLY	-	expression tag	UNP P29597
A	936	ALA	CYS	engineered mutation	UNP P29597
A	969	ALA	GLN	engineered mutation	UNP P29597
A	971	ALA	GLU	engineered mutation	UNP P29597
A	972	ALA	LYS	engineered mutation	UNP P29597

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1016	SER	ALA	engineered mutation	UNP P29597
A	1142	ALA	CYS	engineered mutation	UNP P29597

- Molecule 2 is 6-[(2,5-dimethoxyphenyl)sulfanyl]-3-(1-methyl-1H-pyrazol-4-yl)[1,2,4]triazolo[4,3-b]pyridazine (CCD ID: 2YK) (formula: C₁₇H₁₆N₆O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	26	17	6	2	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	118	118	118	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	36.47Å 73.51Å 103.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.75 – 2.16 36.75 – 2.16	Depositor EDS
% Data completeness (in resolution range)	97.8 (36.75-2.16) 97.8 (36.75-2.16)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.16Å)	Xtrriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.181 , 0.236 0.190 , 0.234	Depositor DCC
R_{free} test set	1017 reflections (6.68%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtrriage
Anisotropy	0.412	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2493	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% 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: 2YK, PTR

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	0.85	1/2394 (0.0%)	1.31	11/3239 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1148	MET	SD-CE	-7.85	1.59	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1040	GLY	N-CA-C	6.53	128.65	113.18
1	A	1165	LEU	CA-C-N	5.96	125.10	120.33
1	A	1165	LEU	C-N-CA	5.96	125.10	120.33
1	A	1166	ILE	CA-C-O	-5.74	114.85	118.69
1	A	1041	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	1058	ARG	CA-C-N	5.34	129.27	121.31
1	A	1058	ARG	C-N-CA	5.34	129.27	121.31
1	A	1057	VAL	N-CA-C	5.20	116.28	111.45
1	A	1170	LYS	CA-C-N	5.13	127.57	120.29
1	A	1170	LYS	C-N-CA	5.13	127.57	120.29
1	A	1164	ASN	CA-CB-CG	5.02	117.62	112.60

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	2349	0	2307	22	0
2	A	26	0	16	9	0
3	A	118	0	0	2	0
All	All	2493	0	2323	23	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 5.

All (23) 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:930:LYS:HE3	2:A:1201:2YK:H10	1.62	0.80
1:A:1040:GLY:O	2:A:1201:2YK:S	2.55	0.65
1:A:961:LYS:HB2	1:A:979:GLU:HG2	1.81	0.62
1:A:911:VAL:HG21	2:A:1201:2YK:C11	2.30	0.61
1:A:905:GLU:HB3	1:A:910:LYS:HD3	1.85	0.59
1:A:900:ILE:HD11	1:A:915:CYS:HB2	1.85	0.59
1:A:911:VAL:HG23	2:A:1201:2YK:H9	1.87	0.56
1:A:921:ASP:CG	1:A:922:GLY:H	2.15	0.54
1:A:959:ILE:HD12	1:A:1042:PHE:HZ	1.75	0.52
1:A:960:ILE:HD13	1:A:1040:GLY:O	2.11	0.51
2:A:1201:2YK:H15	3:A:1392:HOH:O	2.14	0.48
1:A:979:GLU:HG3	3:A:1348:HOH:O	2.13	0.47
1:A:957:GLU:HG3	1:A:958:HIS:CD2	2.50	0.47
1:A:983:LEU:HD12	1:A:1031:LEU:HD13	1.99	0.45
1:A:1022:ARG:HA	1:A:1078:PHE:CZ	2.52	0.44
1:A:1020:ILE:HD12	1:A:1078:PHE:CD2	2.53	0.44
1:A:911:VAL:HG21	2:A:1201:2YK:H11	1.99	0.43
1:A:1041:ASP:HB2	2:A:1201:2YK:C15	2.48	0.42
1:A:911:VAL:CG2	2:A:1201:2YK:C11	2.97	0.42
1:A:930:LYS:HD2	2:A:1201:2YK:H11	2.02	0.42
1:A:1001:LEU:HD13	1:A:1172:VAL:HG12	2.01	0.42
1:A:1172:VAL:O	1:A:1176:TYR:HD2	2.03	0.41
1:A:1173:HIS:O	1:A:1177:GLN:HB2	2.21	0.41

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	287/318 (90%)	273 (95%)	13 (4%)	1 (0%)	36 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	923	THR

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	249/271 (92%)	236 (95%)	13 (5%)	21 17

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	907	HIS
1	A	910	LYS
1	A	919	THR
1	A	963	LYS
1	A	965	CYS
1	A	1031	LEU
1	A	1036	LEU
1	A	1037	VAL
1	A	1053	GLU
1	A	1100	SER

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Mol	Chain	Res	Type
1	A	1122	LEU
1	A	1147	LEU
1	A	1148	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	920	ASN
1	A	939	GLN
1	A	1005	GLN
1	A	1052	HIS
1	A	1116	GLN
1	A	1146	HIS
1	A	1177	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](#)

1 non-standard protein/DNA/RNA residue 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
1	PTR	A	1054	1	15,16,17	1.48	3 (20%)	17,22,24	1.05	2 (11%)

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
1	PTR	A	1054	1	-	0/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1054	PTR	CE1-CZ	2.45	1.43	1.38
1	A	1054	PTR	CE2-CZ	2.40	1.43	1.38
1	A	1054	PTR	CD2-CG	2.13	1.43	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	PTR	P-OH-CZ	-2.37	115.45	123.88
1	A	1054	PTR	O3P-P-OH	2.05	111.39	105.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	2YK	A	1201	-	26,29,29	2.24	9 (34%)	35,41,41	2.38	16 (45%)

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	2YK	A	1201	-	-	0/10/12/12	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	2YK	C15-C10	4.16	1.45	1.39
2	A	1201	2YK	C5-N3	4.02	1.38	1.32
2	A	1201	2YK	C10-S	3.55	1.81	1.77
2	A	1201	2YK	C11-C12	3.41	1.44	1.39
2	A	1201	2YK	C11-C10	3.37	1.44	1.39
2	A	1201	2YK	C6-N5	3.37	1.44	1.39
2	A	1201	2YK	C2-N1	3.33	1.37	1.34
2	A	1201	2YK	C2-C3	2.94	1.43	1.38
2	A	1201	2YK	N1-N2	2.39	1.38	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	2YK	O1-C15-C10	6.30	122.53	115.83
2	A	1201	2YK	O1-C15-C14	-4.86	116.10	124.30
2	A	1201	2YK	C17-O2-C12	4.05	126.18	117.50
2	A	1201	2YK	C3-C2-N1	-3.80	104.30	107.22
2	A	1201	2YK	C4-C3-C5	-3.73	123.35	128.19
2	A	1201	2YK	C11-C10-C15	-3.50	116.55	119.37
2	A	1201	2YK	C4-N2-N1	2.87	105.99	104.41
2	A	1201	2YK	O2-C12-C13	-2.79	106.57	119.82
2	A	1201	2YK	O2-C12-C11	2.74	133.07	120.00
2	A	1201	2YK	C2-C3-C4	2.67	106.58	104.22
2	A	1201	2YK	C5-N3-N4	2.53	110.76	106.98
2	A	1201	2YK	C3-C4-N2	-2.25	110.30	112.09
2	A	1201	2YK	C10-S-C7	2.17	108.92	102.76
2	A	1201	2YK	C15-C10-S	2.14	123.89	120.05
2	A	1201	2YK	C16-O1-C15	-2.08	114.46	117.51
2	A	1201	2YK	N5-C5-N3	-2.03	106.73	109.03

There are no chirality outliers.

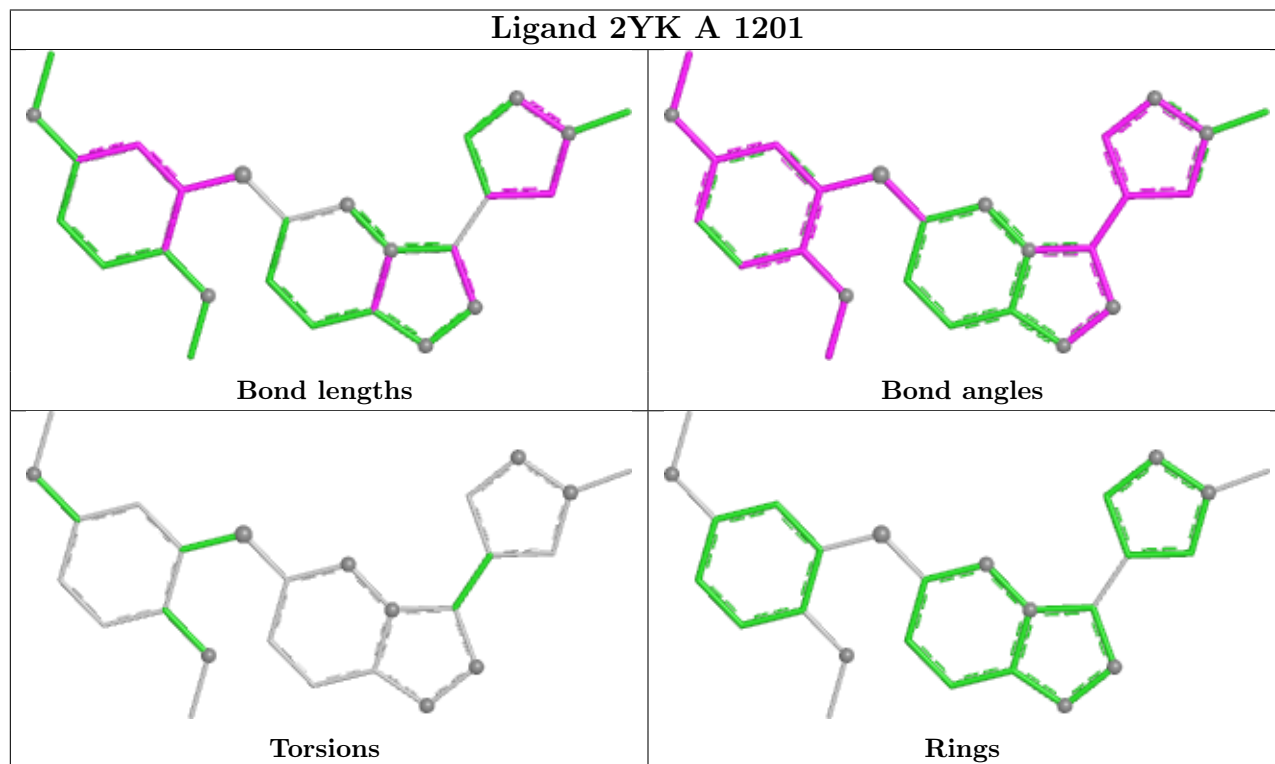
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	2YK	9	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 than 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.



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	289/318 (90%)	0.18	8 (2%) 55 59	20, 42, 80, 98	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	922	GLY	3.3
1	A	972	ALA	3.1
1	A	906	GLY	3.0
1	A	889	PRO	2.9
1	A	965	CYS	2.7
1	A	1057	VAL	2.2
1	A	923	THR	2.1
1	A	1178	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	1054	16/17	0.89	0.09	59,66,80,81	0

6.3 Carbohydrates [i](#)

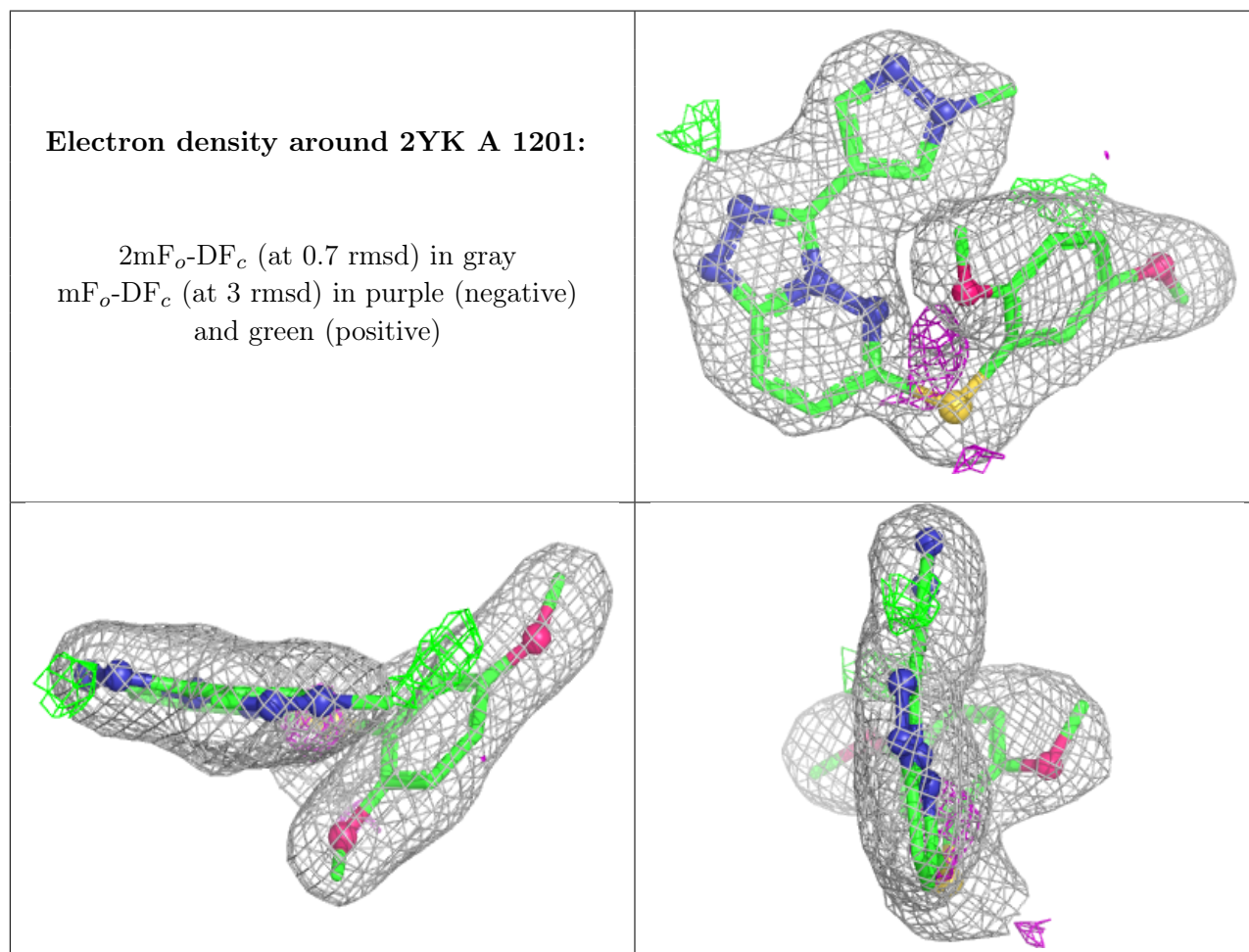
There are no oligosaccharides in this entry.

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	2YK	A	1201	26/26	0.91	0.10	33,38,42,44	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.