



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 05:19 PM EDT

PDB ID : 4FUL
Title : PI3 Kinase Gamma bound to a pyrimidine inhibitor
Authors : Gopalsamy, A.; Bennett, E.M.; Shi, M.; Zhang, W.G.; Bard, J.; Yu, K.
Deposited on : 2012-06-28
Resolution : 2.47 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

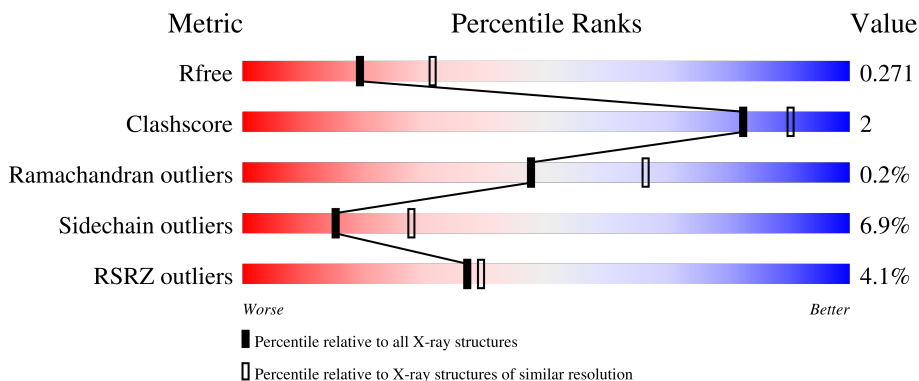
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	966	<div> <div>4%</div> <div>75%</div> <div>11%</div> <div>14%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6846 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.

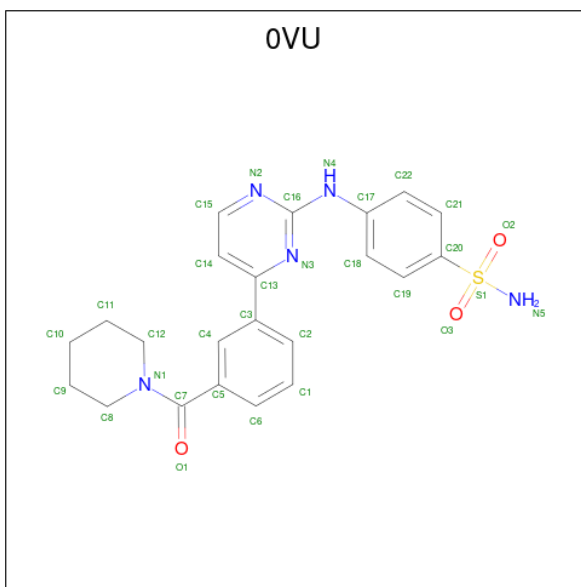
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6698	4303	1145	1214	36			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	459	ARG	GLN	CONFLICT	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 4-({4-[3-(piperidin-1-ylcarbonyl)phenyl]pyrimidin-2-yl}amino)benzenesulfonamide (three-letter code: 0VU) (formula: C₂₂H₂₃N₅O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	22	5	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.04Å 66.90Å 102.82Å 90.00° 97.59° 90.00°	Depositor
Resolution (Å)	33.34 – 2.47 32.24 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.34-2.47) 99.4 (32.24-2.47)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.208 , 0.261 0.207 , 0.271	Depositor DCC
R_{free} test set	1716 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6846	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: 0VU

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	0.49	0/6840	0.70	0/9257

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	6698	0	6696	32	0
2	A	31	0	23	1	0
3	A	117	0	0	0	0
All	All	6846	0	6719	33	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 (33) 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:651:LEU:HD22	1:A:655:ASP:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:LYS:HA	1:A:893:GLN:HG2	1.82	0.61
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.66	0.61
2:A:1201:OVU:H9	2:A:1201:OVU:H20	1.87	0.56
1:A:995:MET:O	1:A:1005:HIS:HB2	2.07	0.55
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.89	0.54
1:A:983:VAL:HG13	1:A:1082:VAL:HG21	1.90	0.54
1:A:639:ASN:O	1:A:643:ILE:HG23	2.09	0.52
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.11	0.50
1:A:497:PHE:HB3	1:A:1042:LEU:HB3	1.94	0.50
1:A:756:LYS:HB2	1:A:807:LYS:HG2	1.94	0.50
1:A:487:ILE:HD12	1:A:1042:LEU:HD11	1.94	0.49
1:A:390:GLY:C	1:A:392:GLN:H	2.16	0.49
1:A:396:GLN:O	1:A:397:ARG:NH1	2.43	0.48
1:A:568:THR:HG22	1:A:570:GLU:H	1.77	0.48
1:A:762:GLN:O	1:A:766:GLN:HG2	2.14	0.48
1:A:696:PHE:CD1	1:A:717:LEU:HD11	2.48	0.48
1:A:624:VAL:HG23	1:A:1026:LEU:HD13	1.97	0.46
1:A:287:ILE:HA	1:A:290:PHE:HD2	1.82	0.45
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.53	0.44
1:A:736:VAL:O	1:A:740:GLU:HB2	2.17	0.44
1:A:802:LYS:HG2	1:A:812:TRP:HB3	1.98	0.44
1:A:756:LYS:H	1:A:807:LYS:HA	1.82	0.44
1:A:226:ARG:HE	1:A:307:LEU:HD23	1.82	0.44
1:A:273:ARG:HG3	1:A:280:TYR:CE1	2.53	0.43
1:A:548:PRO:HD2	1:A:551:LEU:HB2	2.00	0.43
1:A:198:MET:HG2	1:A:311:PRO:HD2	2.01	0.42
1:A:225:HIS:HB2	1:A:306:VAL:HG12	2.00	0.42
1:A:387:ILE:HG22	1:A:394:LEU:HD12	2.02	0.42
1:A:395:CYS:HB3	1:A:416:PHE:CD2	2.50	0.41
1:A:624:VAL:HG21	1:A:659:TYR:CZ	2.56	0.41
1:A:579:ARG:HG2	1:A:610:LEU:HD22	2.04	0.40
1:A:547:MET:HG2	1:A:578:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	814/966 (84%)	779 (96%)	33 (4%)	2 (0%)	47 66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	GLY
1	A	758	ASP

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	734/864 (85%)	683 (93%)	51 (7%)	15 28

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	148	GLN
1	A	164	ASP
1	A	213	LYS
1	A	217	ASN
1	A	222	ILE
1	A	226	ARG
1	A	233	ILE
1	A	271	VAL
1	A	298	LYS
1	A	301	GLU
1	A	305	VAL
1	A	358	ASP
1	A	359	ARG
1	A	364	LYS

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Mol	Chain	Res	Type
1	A	369	ASP
1	A	381	VAL
1	A	391	GLN
1	A	395	CYS
1	A	421	LYS
1	A	461	LEU
1	A	501	LYS
1	A	510	LYS
1	A	521	ASP
1	A	544	ARG
1	A	583	LEU
1	A	601	GLN
1	A	609	GLN
1	A	613	ARG
1	A	647	LYS
1	A	730	HIS
1	A	734	GLN
1	A	739	ILE
1	A	740	GLU
1	A	755	GLU
1	A	770	LYS
1	A	776	ASN
1	A	779	LEU
1	A	823	LEU
1	A	832	PHE
1	A	875	LYS
1	A	883	LYS
1	A	904	ASP
1	A	949	ASN
1	A	959	ASN
1	A	968	ILE
1	A	997	THR
1	A	1036	MET
1	A	1045	LYS
1	A	1052	ARG
1	A	1092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	769	GLN

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 monosaccharides 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	0VU	A	1201	-	34,34,34	1.65	5 (14%)	48,48,48	1.82	11 (22%)

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	0VU	A	1201	-	-	4/22/30/30	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	0VU	S1-N5	5.46	1.71	1.60
2	A	1201	0VU	C7-N1	3.85	1.42	1.34
2	A	1201	0VU	C16-N4	2.69	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	OVU	C4-C3	2.09	1.43	1.39
2	A	1201	OVU	C18-C17	2.01	1.42	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	OVU	N2-C16-N3	-5.03	121.55	126.42
2	A	1201	OVU	C13-N3-C16	4.83	120.53	116.81
2	A	1201	OVU	C20-S1-N5	-4.09	102.71	108.40
2	A	1201	OVU	O1-C7-C5	-3.00	114.35	120.29
2	A	1201	OVU	C15-N2-C16	2.93	117.87	115.42
2	A	1201	OVU	O3-S1-O2	2.86	123.19	118.80
2	A	1201	OVU	O3-S1-C20	-2.47	104.56	107.35
2	A	1201	OVU	C19-C20-S1	2.46	123.06	119.72
2	A	1201	OVU	C5-C7-N1	2.35	121.59	118.66
2	A	1201	OVU	O2-S1-N5	2.19	110.52	107.35
2	A	1201	OVU	C21-C20-S1	-2.11	116.86	119.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	OVU	C19-C20-S1-N5
2	A	1201	OVU	C21-C20-S1-N5
2	A	1201	OVU	C21-C20-S1-O2
2	A	1201	OVU	C19-C20-S1-O2

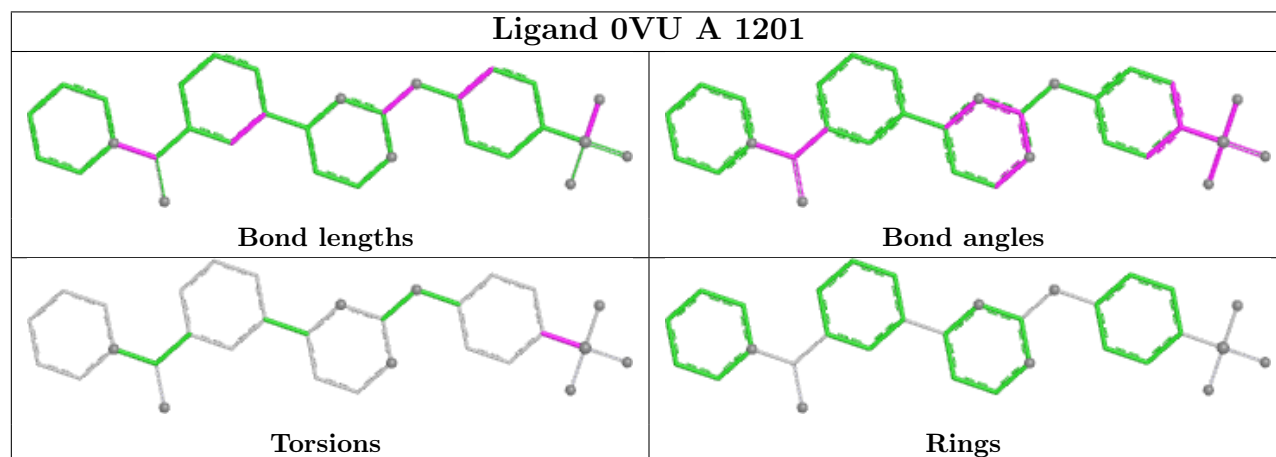
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	OVU	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 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

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	832/966 (86%)	0.05	34 (4%) 37 39	28, 51, 86, 125	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	5.4
1	A	216	ALA	5.4
1	A	612	ALA	4.4
1	A	457	LYS	4.2
1	A	776	ASN	4.2
1	A	269	ASP	3.9
1	A	207	LEU	3.7
1	A	212	TRP	3.7
1	A	215	ILE	3.6
1	A	287	ILE	3.6
1	A	823	LEU	3.5
1	A	1040	PRO	3.5
1	A	1046	GLU	3.5
1	A	747	LEU	3.3
1	A	211	LEU	3.2
1	A	751	SER	3.2
1	A	895	THR	3.1
1	A	825	ASN	3.1
1	A	228	THR	3.0
1	A	488	SER	2.7
1	A	234	LYS	2.6
1	A	1091	VAL	2.6
1	A	461	LEU	2.4
1	A	357	CYS	2.3
1	A	755	GLU	2.3
1	A	148	GLN	2.2
1	A	458	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	2.1
1	A	781	GLU	2.1
1	A	321	GLU	2.1
1	A	897	GLY	2.1
1	A	209	GLU	2.1
1	A	744	LYS	2.0
1	A	241	PRO	2.0

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](#)

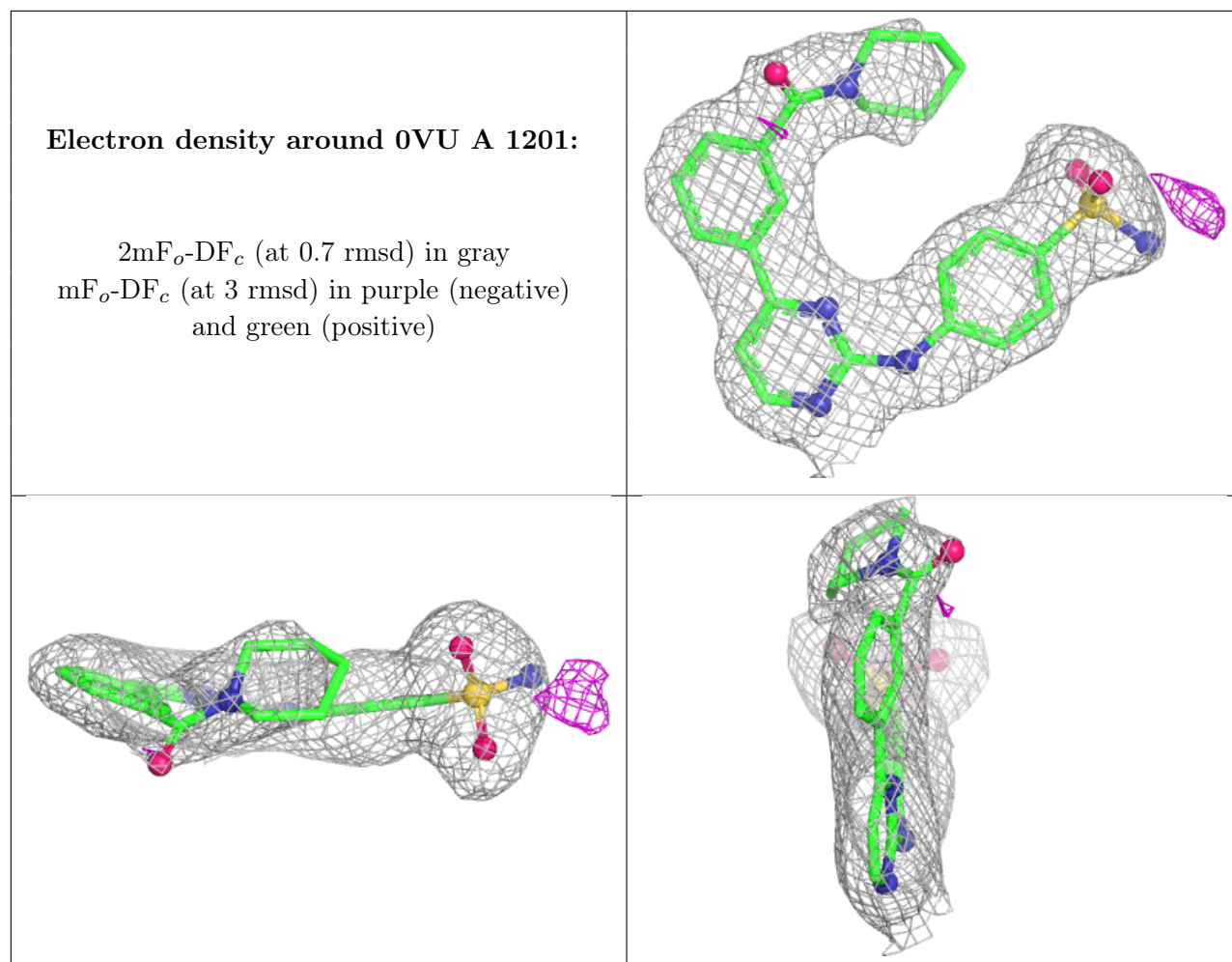
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
2	0VU	A	1201	31/31	0.95	0.14	44,52,71,72	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.