Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 03:42 AM UTC

PDB ID	:	6XRN / pdb_00006xrn
Title	:	Crystal structure of human PI3K-gamma in complex with Compound 17
Authors	:	Walker, N.P.; Jeffrey, J.L.
Deposited on	:	2020-07-13
Resolution	:	2.96 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 (i) 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 (i)) were used in the production of this report:

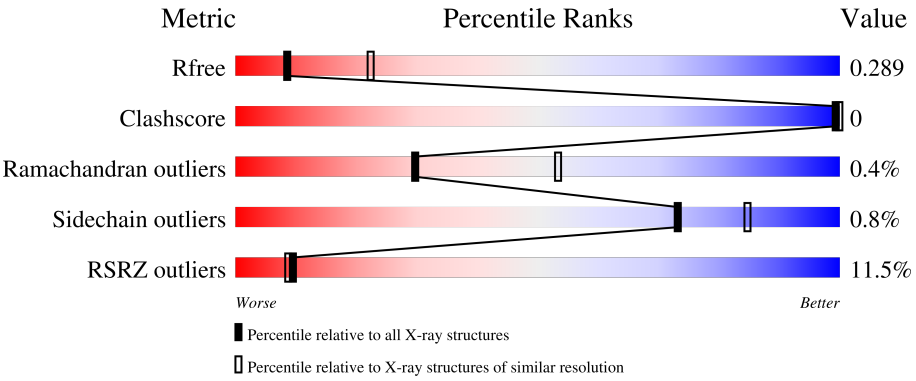
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 <=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	949	10% 86% · 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13537 atoms, of which 6807 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.

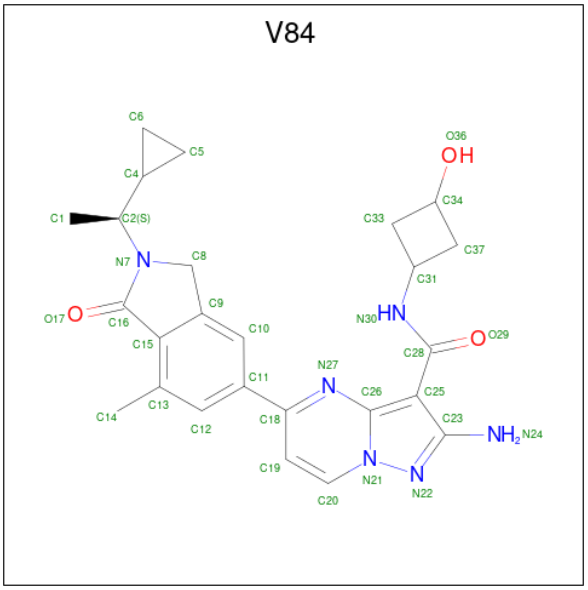
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	824	13475	4306	6779	1138	1217	35	1143	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736

- Molecule 2 is 2-amino-5-{2-[(1S)-1-cyclopropylethyl]-7-methyl-1-oxo-2,3-dihydro-1H-isoindol-5-yl}-N-(trans-3-hydroxycyclobutyl)pyrazolo[1,5-a]pyrimidine-3-carboxamide (CCD ID: V84) (formula: $C_{25}H_{28}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



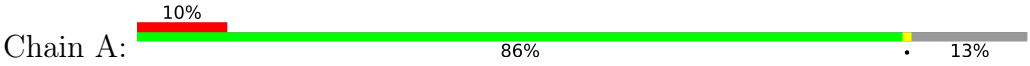
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	62	25	28	6	3	3	0

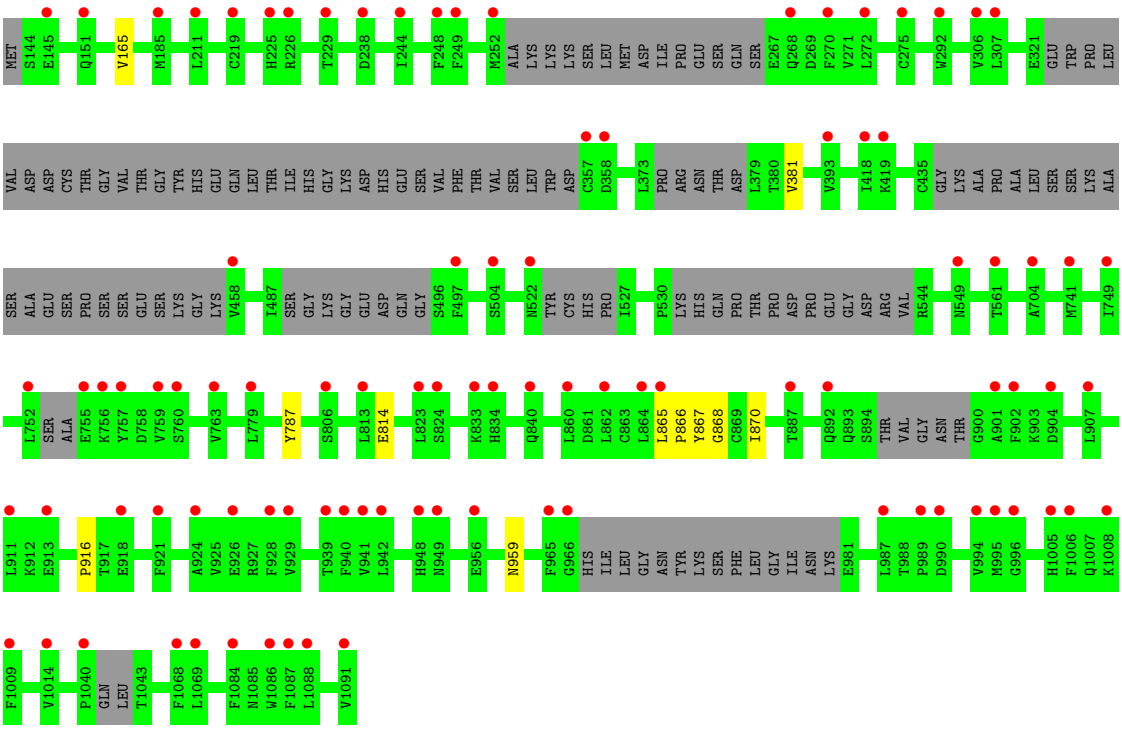
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.21Å 68.17Å 106.80Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	44.78 – 2.96 44.78 – 2.96	Depositor EDS
% Data completeness (in resolution range)	97.3 (44.78-2.96) 97.3 (44.78-2.96)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.224 , 0.270 0.250 , 0.289	Depositor DCC
R_{free} test set	531 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	84.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 103.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13537	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V84

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	0.56	0/6835	0.81	0/9237

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	6696	6779	6744	1	0
2	A	34	28	0	0	0
All	All	6730	6807	6744	1	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 0.

All (1) 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:787:TYR:CD1	1:A:868:GLY:HA3	2.56	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	800/949 (84%)	771 (96%)	26 (3%)	3 (0%)	30 53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	867	TYR
1	A	916	PRO
1	A	866	PRO

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	743/850 (87%)	737 (99%)	6 (1%)	73 85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	VAL
1	A	381	VAL
1	A	814	GLU
1	A	865	LEU
1	A	870	ILE
1	A	959	ASN

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	231	GLN
1	A	411	ASN
1	A	432	GLN
1	A	522	ASN
1	A	609	GLN
1	A	708	HIS
1	A	908	ASN

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 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	V84	A	1101	-	36,39,39	0.95	2 (5%)	43,60,60	2.45	10 (23%)

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	V84	A	1101	-	-	3/20/42/42	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	V84	N21-N22	2.88	1.40	1.37
2	A	1101	V84	C23-N24	2.20	1.39	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	V84	C8-N7-C16	-9.92	108.97	113.15
2	A	1101	V84	C9-C8-N7	7.10	106.08	102.31
2	A	1101	V84	C20-N21-N22	4.34	133.03	124.70
2	A	1101	V84	C18-N27-C26	3.27	121.12	117.78
2	A	1101	V84	C8-C9-C15	-3.13	107.68	109.96
2	A	1101	V84	C37-C34-C33	-2.99	86.84	89.27
2	A	1101	V84	C33-C31-N30	-2.94	112.30	117.76
2	A	1101	V84	O17-C16-C15	-2.68	125.07	129.15
2	A	1101	V84	C13-C15-C16	2.49	134.81	127.09
2	A	1101	V84	C6-C4-C2	-2.23	114.49	119.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	V84	C26-C25-C28-O29
2	A	1101	V84	C26-C25-C28-N30
2	A	1101	V84	C37-C31-N30-C28

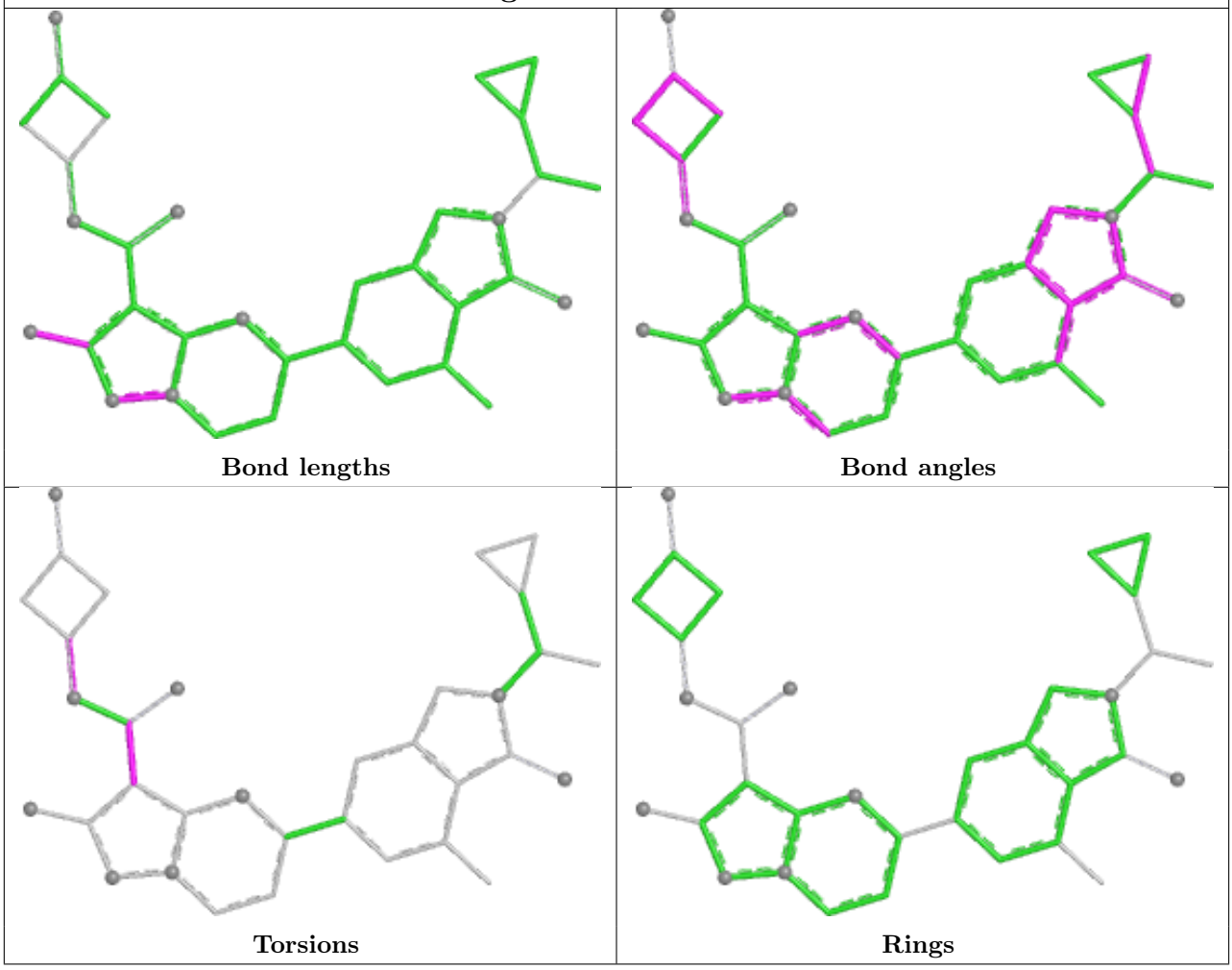
There are no ring outliers.

No monomer is involved in short contacts.

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 V84 A 1101



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, 95^{th} 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	824/949 (86%)	0.89	95 (11%) 9 9	46, 114, 199, 286	138 (16%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	995	MET	4.5
1	A	1084	PHE	4.3
1	A	393	VAL	4.2
1	A	911	LEU	4.2
1	A	823	LEU	4.0
1	A	358	ASP	4.0
1	A	989	PRO	3.8
1	A	749	ILE	3.7
1	A	1091	VAL	3.6
1	A	549	ASN	3.6
1	A	824	SER	3.5
1	A	418	ILE	3.4
1	A	833	LYS	3.4
1	A	966	GLY	3.3
1	A	901	ALA	3.3
1	A	755	GLU	3.2
1	A	248	PHE	3.2
1	A	996	GLY	3.2
1	A	1005	HIS	3.1
1	A	268	GLN	3.0
1	A	840	GLN	3.0
1	A	987	LEU	3.0
1	A	902	PHE	3.0
1	A	924	ALA	2.9
1	A	270	PHE	2.9
1	A	497	PHE	2.9
1	A	307	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	185	MET	2.9
1	A	921	PHE	2.9
1	A	226	ARG	2.8
1	A	1006	PHE	2.8
1	A	763	VAL	2.8
1	A	942	LEU	2.8
1	A	1086	TRP	2.7
1	A	1009	PHE	2.7
1	A	956	GLU	2.7
1	A	272	LEU	2.7
1	A	887	THR	2.7
1	A	948	HIS	2.6
1	A	275	CYS	2.6
1	A	249	PHE	2.6
1	A	813	LEU	2.6
1	A	940	PHE	2.6
1	A	760	SER	2.6
1	A	225	HIS	2.6
1	A	757	TYR	2.6
1	A	357	CYS	2.6
1	A	864	LEU	2.5
1	A	244	ILE	2.5
1	A	252	MET	2.5
1	A	907	LEU	2.5
1	A	939	THR	2.5
1	A	522	ASN	2.4
1	A	865	LEU	2.4
1	A	292	TRP	2.4
1	A	941	VAL	2.3
1	A	1008	LYS	2.3
1	A	892	GLN	2.3
1	A	504	SER	2.3
1	A	752	LEU	2.3
1	A	1087	PHE	2.3
1	A	1069	LEU	2.3
1	A	145	GLU	2.3
1	A	704	ALA	2.3
1	A	219	CYS	2.3
1	A	1014	VAL	2.3
1	A	561	THR	2.2
1	A	1040	PRO	2.2
1	A	949	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	759	VAL	2.2
1	A	1088	LEU	2.2
1	A	929	VAL	2.2
1	A	756	LYS	2.2
1	A	779	LEU	2.1
1	A	913	GLU	2.1
1	A	458	VAL	2.1
1	A	918	GLU	2.1
1	A	229	THR	2.1
1	A	238	ASP	2.1
1	A	904	ASP	2.1
1	A	965	PHE	2.1
1	A	1068	PHE	2.1
1	A	860	LEU	2.1
1	A	926	GLU	2.1
1	A	419	LYS	2.0
1	A	806	SER	2.0
1	A	928	PHE	2.0
1	A	990	ASP	2.0
1	A	741	MET	2.0
1	A	151	GLN	2.0
1	A	834	HIS	2.0
1	A	211	LEU	2.0
1	A	862	LEU	2.0
1	A	306	VAL	2.0
1	A	994	VAL	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 oligosaccharides in this entry.

6.4 Ligands (i)

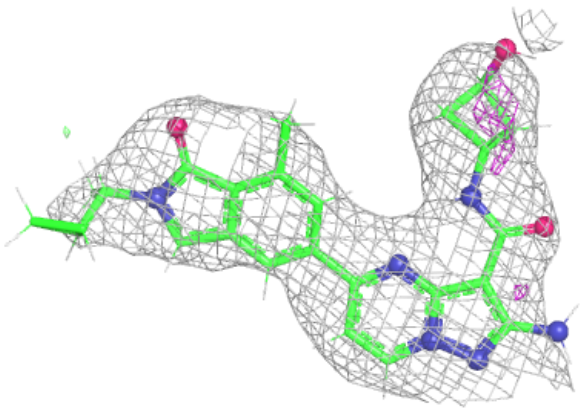
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

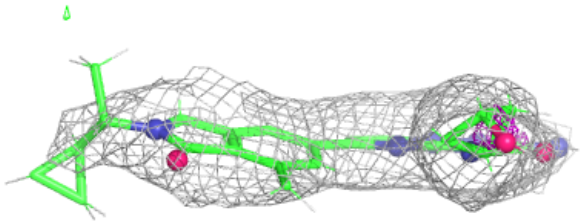
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	V84	A	1101	34/34	0.90	0.12	64,88,134,135	3

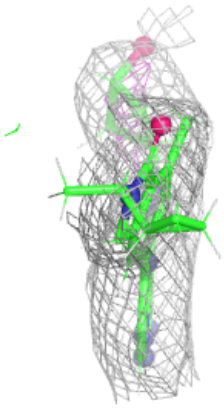
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V84 A 1101:

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







6.5 Other polymers (i)

There are no such residues in this entry.