



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:37 AM UTC

PDB ID : 7K6N / pdb_00007k6n
Title : Crystal structure of PI3Kalpha selective Inhibitor 11-1575
Authors : Chen, P.; Brooun, A.; Deng, Y.L.; Grodsky, N.; Kaiser, S.E.
Deposited on : 2020-09-21
Resolution : 2.77 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

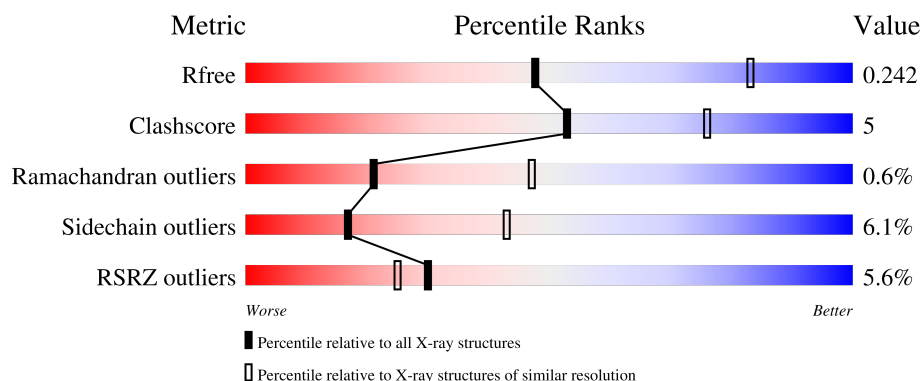
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	946	5% 79% 12% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6926 atoms, of which 34 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.

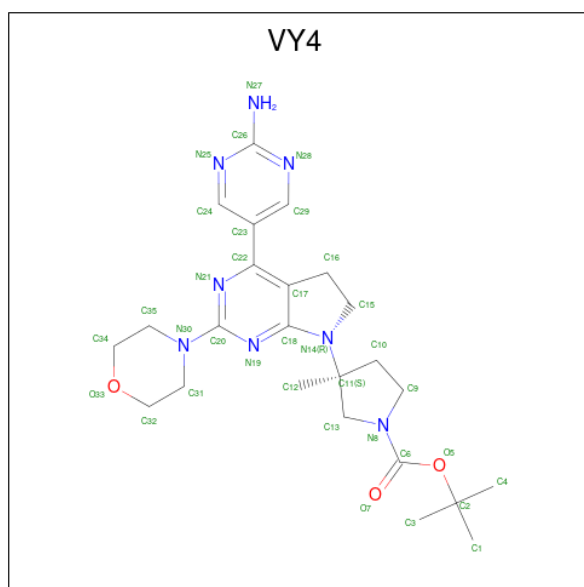
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	875	6685	4290	1123	1218	54	10	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	expression tag	UNP P42336
A	104	SER	-	expression tag	UNP P42336

- Molecule 2 is tert-butyl (3S)-3-[4-(2-aminopyrimidin-5-yl)-2-(morpholin-4-yl)-5,6-dihydro-7H-pyrrolo[2,3-d]pyrimidin-7-yl]-3-methylpyrrolidine-1-carboxylate (CCD ID: VY4) (formula: C₂₄H₃₄N₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	69	24	34	8	3	0	0

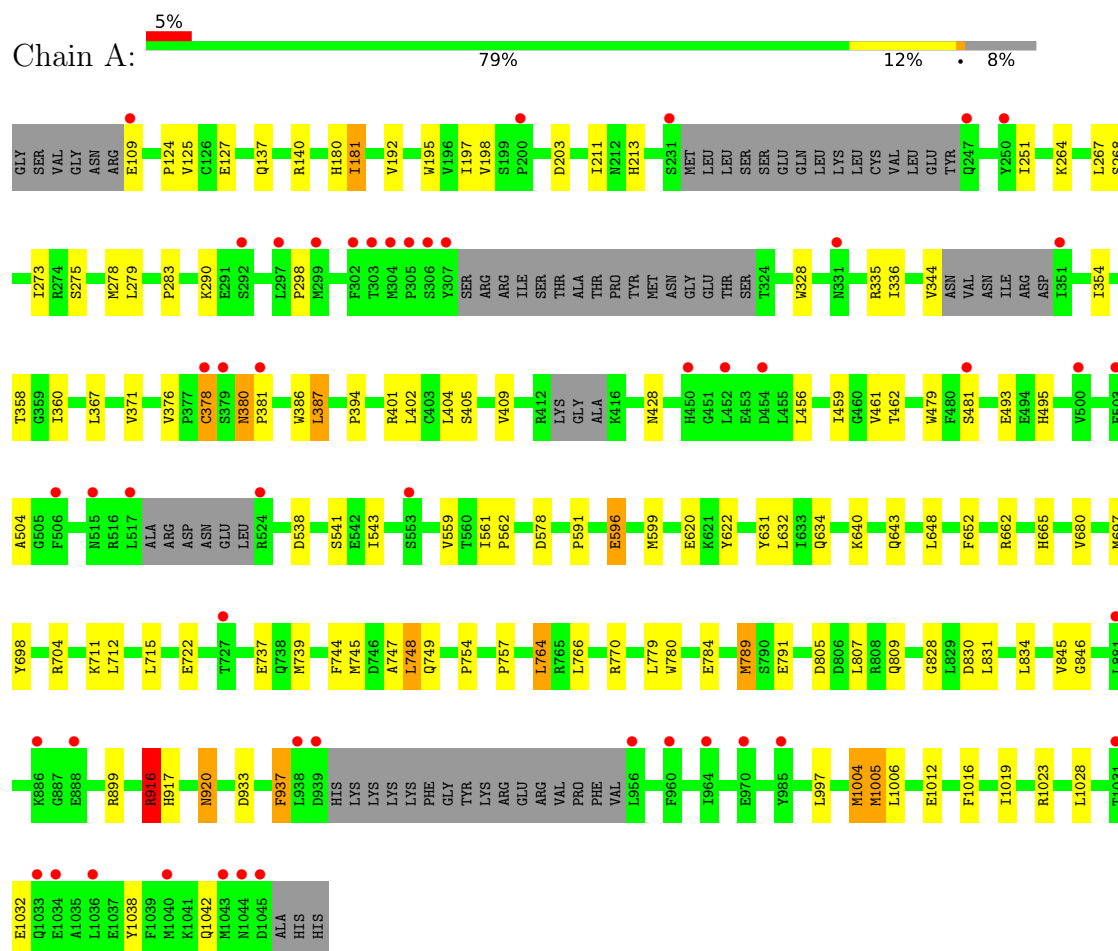
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total 172	O 172	0	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 alpha isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.71Å 137.92Å 144.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.62 – 2.77 99.62 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.62-2.77) 99.9 (99.62-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.200 , 0.235 0.205 , 0.242	Depositor DCC
R_{free} test set	1403 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6926	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: VY4

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	0.75	2/6839 (0.0%)	1.05	3/9312 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1004	MET	SD-CE	-7.63	1.60	1.79
1	A	1005	MET	SD-CE	-5.86	1.65	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	937	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	722	GLU	N-CA-C	5.12	116.55	111.07
1	A	622	TYR	N-CA-C	5.04	120.27	113.72

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	6685	0	6242	64	0
2	A	35	34	0	1	0
3	A	172	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6892	34	6242	65	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 (65) 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:749:GLN:HE21	1:A:764:LEU:H	1.27	0.80
1:A:634:GLN:HG3	1:A:1005:MET:HE3	1.71	0.73
1:A:917:HIS:H	1:A:920:ASN:HD21	1.42	0.68
1:A:599:MET:HE2	1:A:1004:MET:HE1	1.74	0.68
1:A:1023:ARG:HG2	1:A:1028:LEU:HD12	1.78	0.66
1:A:405:SER:HB2	1:A:456:LEU:HD23	1.78	0.66
1:A:335:ARG:HG3	1:A:386:TRP:CE3	2.33	0.64
1:A:495:HIS:NE2	1:A:578:ASP:OD1	2.29	0.63
1:A:275:SER:O	1:A:278:MET:O	2.20	0.59
1:A:916:ARG:HA	1:A:920:ASN:HD21	1.66	0.59
1:A:917:HIS:H	1:A:920:ASN:ND2	2.00	0.59
1:A:807:LEU:HD12	1:A:846:GLY:HA3	1.84	0.59
1:A:195:TRP:HB3	1:A:789:MET:HE1	1.84	0.58
1:A:213:HIS:HD2	1:A:268:SER:OG	1.88	0.57
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.52	0.57
1:A:378:CYS:O	1:A:381:PRO:HD3	2.05	0.56
1:A:739:MET:HE2	1:A:744:PHE:HB3	1.87	0.55
1:A:360:ILE:HG22	1:A:367:LEU:HD12	1.89	0.54
1:A:739:MET:HG3	1:A:766:LEU:HD11	1.90	0.53
1:A:358:THR:HG22	1:A:404:LEU:HD23	1.90	0.53
1:A:665:HIS:HE1	1:A:754:PRO:O	1.90	0.52
1:A:336:ILE:HD13	1:A:402:LEU:HD22	1.93	0.51
1:A:180:HIS:CD2	1:A:828:GLY:HA2	2.46	0.51
1:A:267:LEU:HG	1:A:273:ILE:HG13	1.93	0.51
1:A:124:PRO:HG2	1:A:127:GLU:HG3	1.92	0.50
1:A:180:HIS:CE1	1:A:181:ILE:CD1	2.95	0.50
1:A:634:GLN:HA	1:A:1005:MET:CE	2.42	0.49
1:A:180:HIS:CE1	1:A:181:ILE:HD12	2.47	0.49
1:A:192:VAL:HG12	1:A:283:PRO:HG2	1.94	0.49
1:A:562:PRO:HG3	1:A:591:PRO:HG2	1.94	0.49
1:A:376:VAL:HG21	1:A:381:PRO:HB3	1.95	0.49
1:A:298:PRO:HG2	1:A:697:MET:HG3	1.94	0.49
1:A:599:MET:HE1	1:A:631:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:MET:CE	1:A:748:LEU:HD23	2.43	0.49
1:A:620:GLU:HG2	1:A:652:PHE:CD1	2.49	0.48
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.96	0.48
1:A:920:ASN:HD22	1:A:920:ASN:C	2.21	0.48
1:A:662:ARG:NH1	3:A:9107:HOH:O	2.47	0.48
1:A:371:VAL:HG12	1:A:387:LEU:HG	1.96	0.47
1:A:770:ARG:HG3	1:A:780:TRP:HB3	1.95	0.47
1:A:278:MET:O	1:A:279:LEU:CB	2.62	0.47
1:A:428:ASN:ND2	1:A:643:GLN:HE21	2.13	0.46
1:A:538:ASP:OD2	1:A:1023:ARG:NH1	2.48	0.46
1:A:198:VAL:HG22	1:A:203:ASP:HB2	1.96	0.46
1:A:715:LEU:HD13	1:A:744:PHE:CE1	2.51	0.46
1:A:198:VAL:CG2	1:A:203:ASP:HB2	2.46	0.46
1:A:715:LEU:HD13	1:A:744:PHE:HE1	1.82	0.45
1:A:1016:PHE:HA	1:A:1019:ILE:HD12	1.98	0.45
1:A:197:ILE:HD11	1:A:789:MET:HE2	1.98	0.44
1:A:479:TRP:NE1	1:A:481:SER:HA	2.32	0.44
1:A:830:ASP:O	1:A:899[A]:ARG:HD2	2.18	0.44
1:A:830:ASP:O	1:A:899[B]:ARG:HD3	2.17	0.44
1:A:344:VAL:HG23	1:A:381:PRO:HD2	1.99	0.43
1:A:739:MET:O	1:A:745:MET:HG3	2.18	0.43
1:A:739:MET:HE1	1:A:748:LEU:HD23	2.01	0.42
1:A:328:TRP:HA	1:A:394:PRO:HB3	2.02	0.42
2:A:9001:VY4:C13	2:A:9001:VY4:N19	2.82	0.42
1:A:380:ASN:HD22	1:A:380:ASN:HA	1.60	0.42
1:A:665:HIS:CG	1:A:757:PRO:HG3	2.55	0.41
1:A:180:HIS:HD2	1:A:828:GLY:HA2	1.85	0.41
1:A:596:GLU:HB3	1:A:997:LEU:HD13	2.02	0.41
1:A:1038:TYR:O	1:A:1042:GLN:HG2	2.20	0.41
1:A:711:LYS:HG3	1:A:747:ALA:CB	2.50	0.41
1:A:712:LEU:HG	1:A:748:LEU:HD11	2.02	0.41
1:A:665:HIS:HD2	1:A:698:TYR:OH	2.04	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	862/946 (91%)	836 (97%)	21 (2%)	5 (1%)	21	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	CYS
1	A	264	LYS
1	A	504	ALA
1	A	916	ARG
1	A	933	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	673/860 (78%)	632 (94%)	41 (6%)	17	43

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	125	VAL
1	A	181	ILE
1	A	211	ILE
1	A	251	ILE
1	A	290	LYS
1	A	354	ILE
1	A	380	ASN
1	A	387	LEU
1	A	401	ARG
1	A	409	VAL
1	A	459	ILE

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Mol	Chain	Res	Type
1	A	461	VAL
1	A	462	THR
1	A	493	GLU
1	A	541	SER
1	A	543	ILE
1	A	559	VAL
1	A	561	ILE
1	A	596	GLU
1	A	632	LEU
1	A	648	LEU
1	A	704	ARG
1	A	737	GLU
1	A	748	LEU
1	A	764	LEU
1	A	779	LEU
1	A	784	GLU
1	A	789	MET
1	A	791	GLU
1	A	805	ASP
1	A	809	GLN
1	A	831	LEU
1	A	834	LEU
1	A	845	VAL
1	A	916	ARG
1	A	920	ASN
1	A	937	PHE
1	A	1006	LEU
1	A	1012	GLU
1	A	1032	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	180	HIS
1	A	205	GLN
1	A	213	HIS
1	A	362	HIS
1	A	370	ASN
1	A	380	ASN
1	A	428	ASN
1	A	510	HIS

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Mol	Chain	Res	Type
1	A	637	GLN
1	A	665	HIS
1	A	670	HIS
1	A	703	ASN
1	A	749	GLN
1	A	763	ASN
1	A	797	ASN
1	A	827	GLN
1	A	855	HIS
1	A	878	HIS
1	A	920	ASN
1	A	994	HIS
1	A	1000	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	VY4	A	9001	-	36,39,39	1.67	8 (22%)	50,59,59	0.87	1 (2%)

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	VY4	A	9001	-	-	0/17/51/51	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9001	VY4	O5-C2	-3.45	1.42	1.48
2	A	9001	VY4	C26-N28	3.27	1.40	1.35
2	A	9001	VY4	C23-C22	-3.14	1.45	1.49
2	A	9001	VY4	C26-N25	3.13	1.39	1.35
2	A	9001	VY4	C20-N19	2.91	1.40	1.34
2	A	9001	VY4	C15-N14	2.74	1.50	1.46
2	A	9001	VY4	C20-N30	2.36	1.40	1.35
2	A	9001	VY4	C6-N8	2.10	1.39	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9001	VY4	C17-C18-N14	2.16	111.26	109.83

There are no chirality outliers.

There are no torsion outliers.

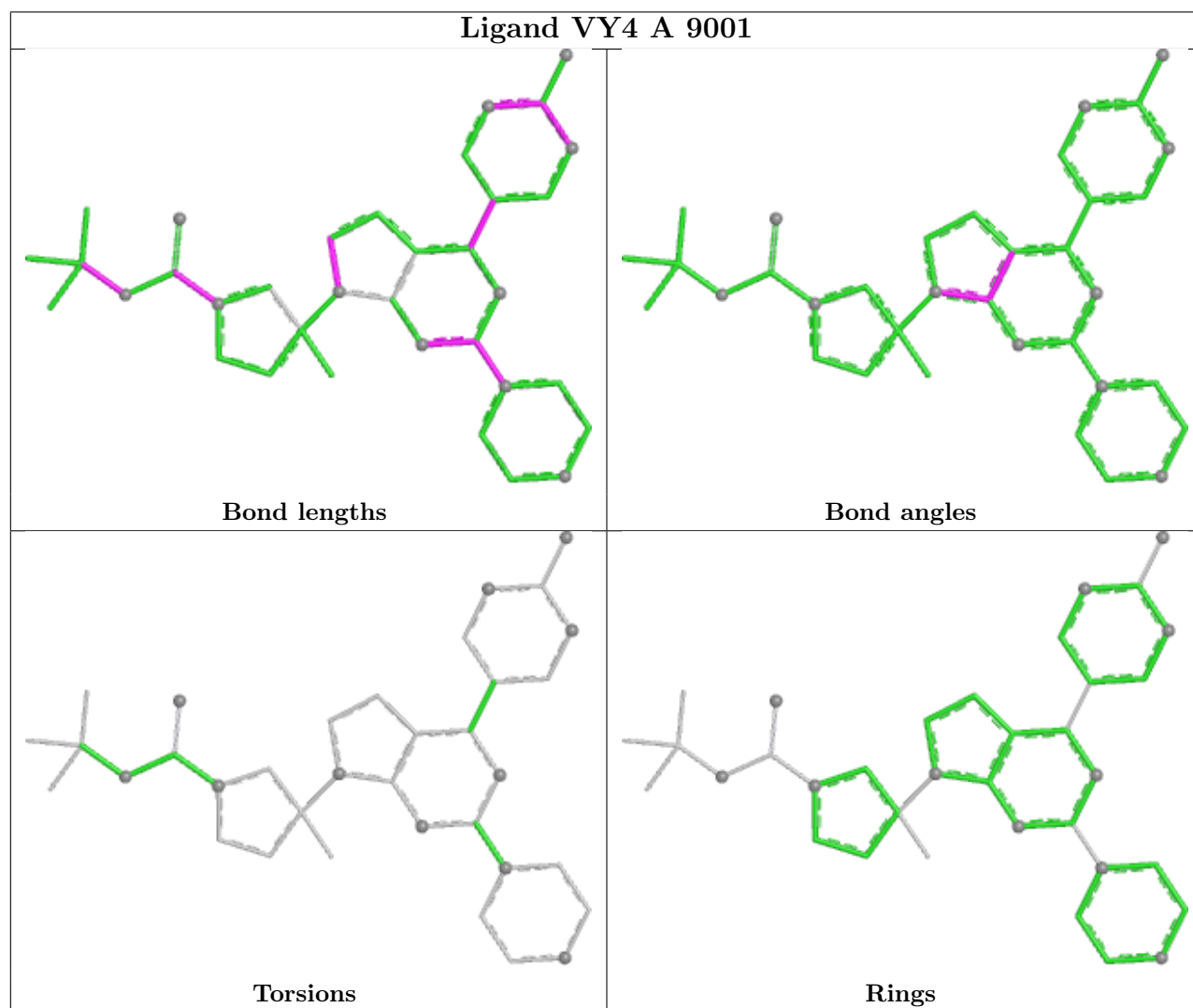
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	VY4	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	873/946 (92%)	0.36	49 (5%) 30 25	31, 54, 81, 107	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	TYR	4.3
1	A	1045	ASP	3.9
1	A	351	ILE	3.8
1	A	1034	GLU	3.6
1	A	303	THR	3.5
1	A	247	GLN	3.5
1	A	956	LEU	3.4
1	A	299	MET	3.1
1	A	379	SER	3.0
1	A	304	MET	3.0
1	A	1044	ASN	3.0
1	A	231	SER	2.9
1	A	553	SER	2.9
1	A	378	CYS	2.9
1	A	517	LEU	2.9
1	A	454	ASP	2.9
1	A	964	ILE	2.9
1	A	302	PHE	2.8
1	A	515	ASN	2.8
1	A	970	GLU	2.7
1	A	727	THR	2.7
1	A	1040	MET	2.7
1	A	500	VAL	2.7
1	A	331	ASN	2.6
1	A	450	HIS	2.6
1	A	524	ARG	2.6
1	A	109	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	886	LYS	2.6
1	A	452	LEU	2.5
1	A	1043	MET	2.4
1	A	985	TYR	2.4
1	A	306	SER	2.4
1	A	1033	GLN	2.3
1	A	506	PHE	2.3
1	A	305	PRO	2.2
1	A	888	GLU	2.2
1	A	939	ASP	2.2
1	A	938	LEU	2.2
1	A	200	PRO	2.2
1	A	292	SER	2.2
1	A	881	LEU	2.2
1	A	1036	LEU	2.2
1	A	481	SER	2.2
1	A	1031	THR	2.1
1	A	960	PHE	2.1
1	A	381	PRO	2.1
1	A	250	TYR	2.1
1	A	503	GLU	2.1
1	A	297	LEU	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](#)

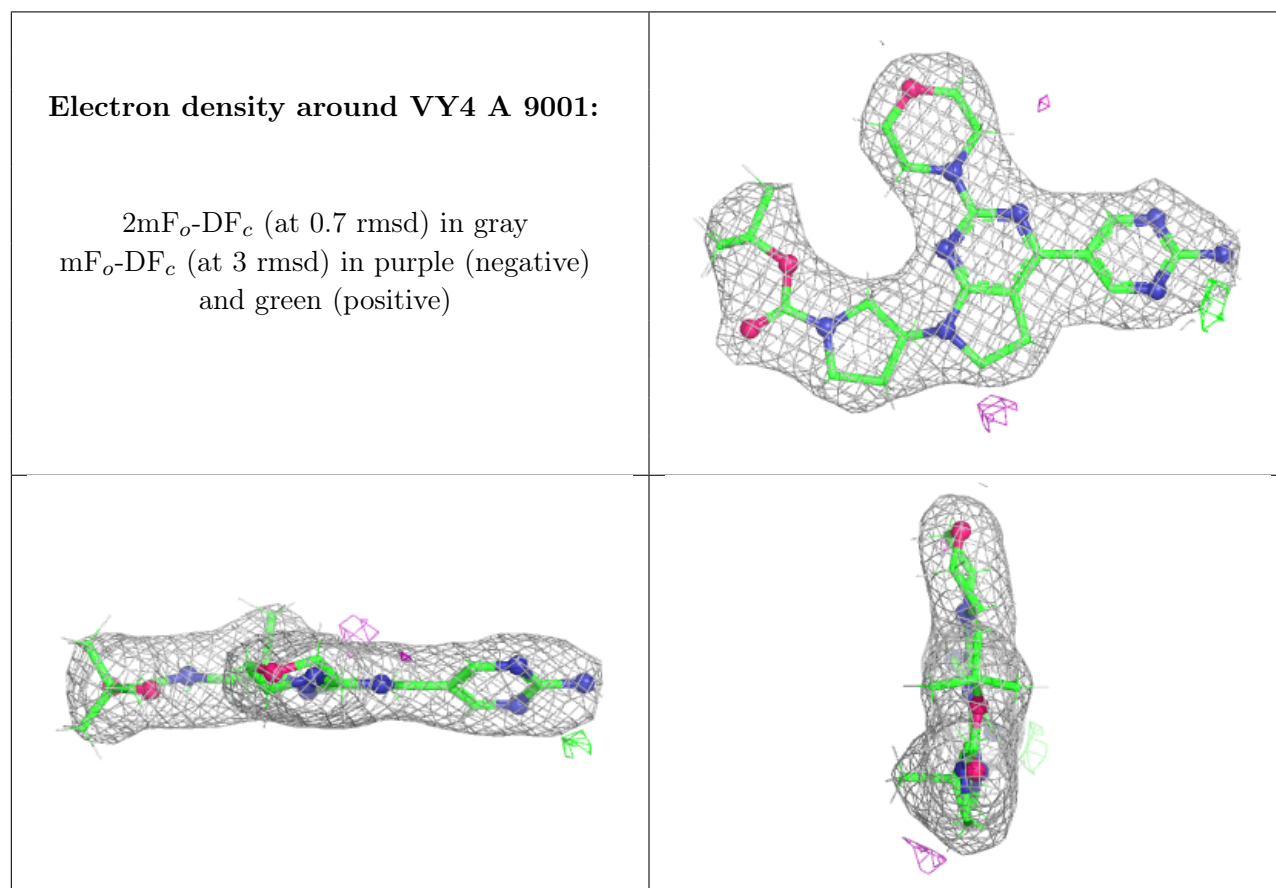
There are no oligosaccharides in this entry.

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, 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($\text{\AA}^2$)	Q<0.9
2	VY4	A	9001	35/35	0.96	0.07	42,46,55,55	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 ⓘ

There are no such residues in this entry.