



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:45 AM EDT

PDB ID : 7K6O / pdb_00007k6o
Title : Crystal structure of PI3Kalpha inhibitor 10-5429
Authors : Chen, P.; Brooun, A.; Deng, Y.L.; Grodsky, N.; Kaiser, S.E.
Deposited on : 2020-09-21
Resolution : 2.74 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

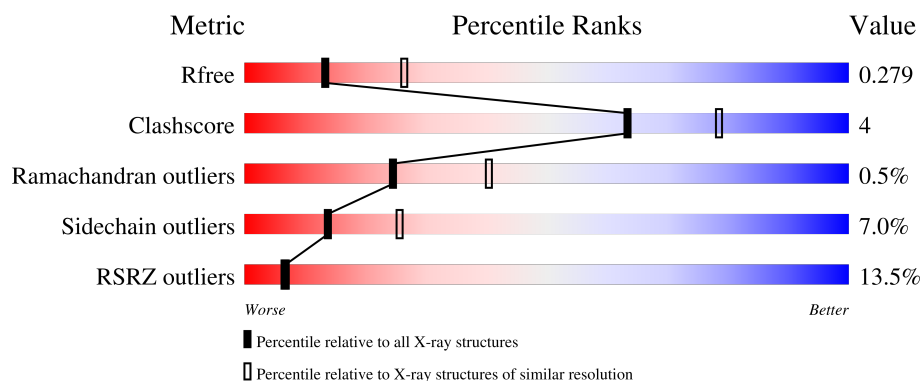
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6469 atoms, of which 27 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.

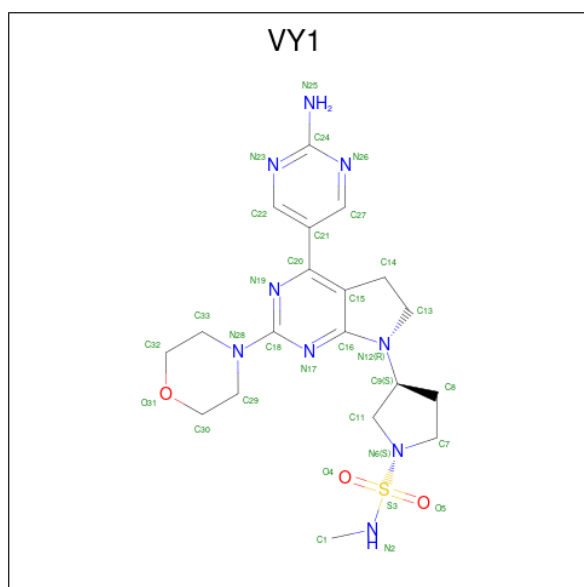
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	852	6339	4043	1071	1175	50	38	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 (3S)-3-[4-(2-aminopyrimidin-5-yl)-2-(morpholin-4-yl)-5,6-dihydro-7H-pyrrolo[2,3-d]pyrimidin-7-yl]-N-methylpyrrolidine-1-sulfonamide (CCD ID: VY1) (formula: C₁₉H₂₇N₉O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
2	A	1	59	19	27	9	3	1	0	0

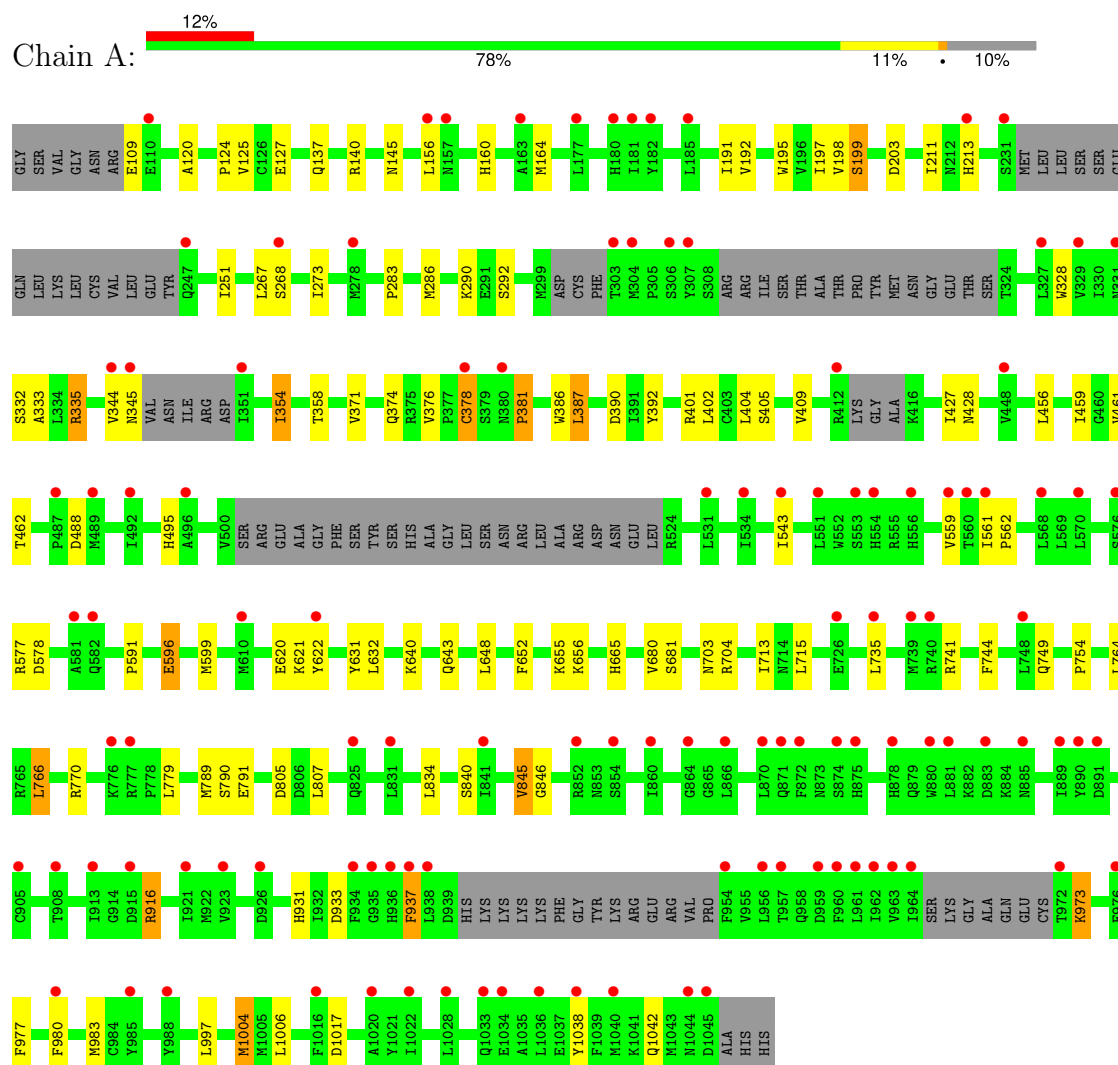
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		

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	57.92Å 135.78Å 141.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.84 – 2.74 97.84 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.9 (97.84-2.74) 99.9 (97.84-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.231 , 0.262 0.248 , 0.279	Depositor DCC
R_{free} test set	1525 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 80.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: VY1

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	1/6477 (0.0%)	1.05	6/8836 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1004	MET	SD-CE	-5.31	1.66	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	937	PHE	CA-CB-CG	8.00	121.80	113.80
1	A	332	SER	N-CA-C	5.82	118.21	110.53
1	A	390	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	840	SER	CA-C-N	5.38	129.19	121.55
1	A	840	SER	C-N-CA	5.38	129.19	121.55
1	A	381	PRO	N-CA-C	5.05	118.80	111.03

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	6339	0	5741	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	32	27	0	0	0
3	A	71	0	0	0	0
All	All	6442	27	5741	48	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 4.

All (48) 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	0.79
1:A:197:ILE:HD11	1:A:789:MET:HE2	1.68	0.74
1:A:599:MET:HE2	1:A:1004:MET:HE1	1.73	0.70
1:A:405:SER:HB2	1:A:456:LEU:HD23	1.79	0.64
1:A:741:ARG:HH21	1:A:744:PHE:HE2	1.48	0.61
1:A:335:ARG:HG3	1:A:386:TRP:CE3	2.38	0.58
1:A:495:HIS:NE2	1:A:578:ASP:OD1	2.34	0.58
1:A:973:LYS:HA	1:A:977:PHE:CB	2.34	0.58
1:A:916:ARG:HE	1:A:931:HIS:HD2	1.52	0.57
1:A:665:HIS:HE1	1:A:754:PRO:O	1.87	0.56
1:A:124:PRO:HG2	1:A:127:GLU:HG3	1.88	0.55
1:A:198:VAL:O	1:A:199:SER:O	2.24	0.55
1:A:195:TRP:HB3	1:A:789:MET:HE1	1.89	0.55
1:A:596:GLU:HB3	1:A:997:LEU:HD13	1.88	0.54
1:A:137:GLN:HE22	1:A:140:ARG:HH11	1.54	0.53
1:A:267:LEU:HG	1:A:273:ILE:HG13	1.90	0.53
1:A:764:LEU:HB3	1:A:766:LEU:HD23	1.90	0.53
1:A:807:LEU:HD12	1:A:846:GLY:HA3	1.91	0.52
1:A:599:MET:HE1	1:A:631:TYR:HB3	1.90	0.52
1:A:620:GLU:HG2	1:A:652:PHE:CD1	2.45	0.51
1:A:160:HIS:CD2	1:A:164:MET:HE2	2.46	0.51
1:A:333:ALA:HA	1:A:392:TYR:HA	1.93	0.50
1:A:713:ILE:HG12	1:A:845:VAL:HG11	1.94	0.49
1:A:192:VAL:HG12	1:A:283:PRO:HG2	1.95	0.49
1:A:328:TRP:CE2	1:A:577:ARG:HD2	2.49	0.48
1:A:213:HIS:HD2	1:A:268:SER:OG	1.96	0.48
1:A:345:ASN:O	1:A:378:CYS:SG	2.72	0.47
1:A:371:VAL:HG12	1:A:387:LEU:HG	1.96	0.47
1:A:378:CYS:O	1:A:381:PRO:HD3	2.14	0.47
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.97	0.47
1:A:749:GLN:HE21	1:A:764:LEU:N	2.06	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG21	1:A:381:PRO:HB3	1.96	0.46
1:A:402:LEU:HD23	1:A:427:ILE:HD12	1.98	0.45
1:A:376:VAL:CG2	1:A:381:PRO:HB3	2.47	0.45
1:A:428:ASN:ND2	1:A:643:GLN:HE21	2.16	0.44
1:A:916:ARG:HE	1:A:931:HIS:CD2	2.34	0.44
1:A:562:PRO:HG3	1:A:591:PRO:HG2	1.99	0.43
1:A:621:LYS:NZ	1:A:622:TYR:CE2	2.79	0.43
1:A:358:THR:HG22	1:A:404:LEU:HD23	2.01	0.43
1:A:354:ILE:HG21	1:A:381:PRO:HG3	2.01	0.43
1:A:344:VAL:HG23	1:A:381:PRO:HD2	2.01	0.42
1:A:198:VAL:HG22	1:A:203:ASP:HB2	2.03	0.41
1:A:120:ALA:HB2	1:A:703:ASN:HD21	1.85	0.41
1:A:764:LEU:HB3	1:A:766:LEU:CD2	2.49	0.41
1:A:1038:TYR:O	1:A:1042:GLN:HG2	2.21	0.41
1:A:286:MET:HG3	1:A:789:MET:HE3	2.04	0.40
1:A:980:PHE:HA	1:A:983:MET:HE2	2.03	0.40
1:A:345:ASN:C	1:A:378:CYS:SG	3.04	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	835/946 (88%)	803 (96%)	28 (3%)	4 (0%)	24	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	A	378	CYS
1	A	973	LYS
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	617/860 (72%)	574 (93%)	43 (7%)	14	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	125	VAL
1	A	145	ASN
1	A	156	LEU
1	A	191	ILE
1	A	211	ILE
1	A	251	ILE
1	A	290	LYS
1	A	292	SER
1	A	335	ARG
1	A	354	ILE
1	A	374	GLN
1	A	387	LEU
1	A	401	ARG
1	A	409	VAL
1	A	459	ILE
1	A	461	VAL
1	A	462	THR
1	A	488	ASP
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	655	LYS
1	A	656	LYS
1	A	681	SER
1	A	704	ARG
1	A	715	LEU

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Mol	Chain	Res	Type
1	A	735	LEU
1	A	766	LEU
1	A	770	ARG
1	A	779	LEU
1	A	790	SER
1	A	791	GLU
1	A	805	ASP
1	A	834	LEU
1	A	845	VAL
1	A	916	ARG
1	A	937	PHE
1	A	1006	LEU
1	A	1017	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	180	HIS
1	A	189	GLN
1	A	205	GLN
1	A	213	HIS
1	A	370	ASN
1	A	384	ASN
1	A	428	ASN
1	A	637	GLN
1	A	665	HIS
1	A	703	ASN
1	A	749	GLN
1	A	763	ASN
1	A	797	ASN
1	A	826	ASN
1	A	931	HIS
1	A	994	HIS

5.3.3 RNA ⓘ

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	VY1	A	9001	-	32,36,36	1.52	6 (18%)	43,53,53	1.05	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	VY1	A	9001	-	-	4/18/47/47	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9001	VY1	C24-N26	3.23	1.40	1.35
2	A	9001	VY1	C24-N23	3.20	1.39	1.35
2	A	9001	VY1	C18-N17	3.18	1.40	1.34
2	A	9001	VY1	C21-C20	-3.03	1.45	1.49
2	A	9001	VY1	C18-N19	2.23	1.38	1.34
2	A	9001	VY1	C13-N12	2.20	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9001	VY1	C13-N12-C9	-4.06	116.94	123.43

There are no chirality outliers.

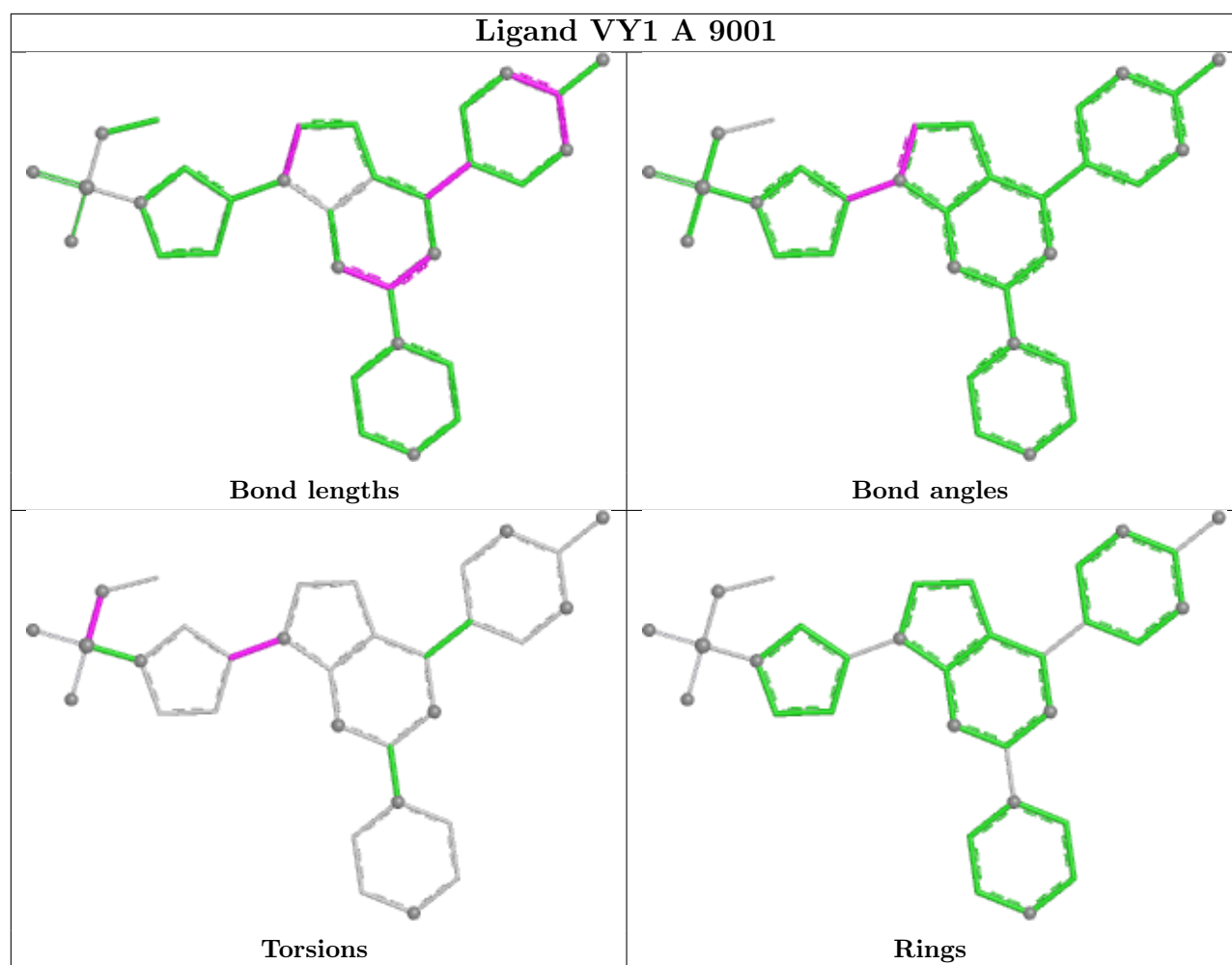
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	VY1	C1-N2-S3-O4
2	A	9001	VY1	C1-N2-S3-O5
2	A	9001	VY1	C8-C9-N12-C16
2	A	9001	VY1	C11-C9-N12-C16

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 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	844/946 (89%)	0.92	114 (13%) 7 6	39, 80, 131, 153	1 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	875	HIS	4.8
1	A	959	ASP	4.5
1	A	496	ALA	4.3
1	A	1036	LEU	4.3
1	A	915	ASP	4.3
1	A	1045	ASP	4.2
1	A	878	HIS	4.2
1	A	957	THR	4.1
1	A	874	SER	3.9
1	A	880	TRP	3.9
1	A	913	ILE	3.8
1	A	964	ILE	3.7
1	A	885	ASN	3.7
1	A	739	MET	3.7
1	A	582	GLN	3.5
1	A	231	SER	3.5
1	A	872	PHE	3.5
1	A	1034	GLU	3.4
1	A	960	PHE	3.3
1	A	871	GLN	3.2
1	A	921	ILE	3.2
1	A	534	ILE	3.1
1	A	860	ILE	3.1
1	A	351	ILE	3.1
1	A	954	PHE	3.1
1	A	934	PHE	3.1
1	A	303	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	278	MET	3.1
1	A	972	THR	3.0
1	A	985	TYR	3.0
1	A	1044	ASN	3.0
1	A	378	CYS	2.9
1	A	831	LEU	2.9
1	A	331	ASN	2.9
1	A	268	SER	2.9
1	A	554	HIS	2.9
1	A	740	ARG	2.8
1	A	307	TYR	2.8
1	A	905	CYS	2.8
1	A	938	LEU	2.8
1	A	531	LEU	2.8
1	A	890	TYR	2.8
1	A	962	ILE	2.8
1	A	551	LEU	2.8
1	A	182	TYR	2.7
1	A	157	ASN	2.7
1	A	448	VAL	2.7
1	A	961	LEU	2.7
1	A	776	LYS	2.7
1	A	980	PHE	2.7
1	A	1022	ILE	2.6
1	A	380	ASN	2.6
1	A	935	GLY	2.6
1	A	908	THR	2.5
1	A	726	GLU	2.5
1	A	1020	ALA	2.5
1	A	177	LEU	2.5
1	A	556	HIS	2.5
1	A	489	MET	2.5
1	A	306	SER	2.4
1	A	1040	MET	2.4
1	A	870	LEU	2.4
1	A	956	LEU	2.4
1	A	610	MET	2.4
1	A	923	VAL	2.4
1	A	988	TYR	2.4
1	A	327	LEU	2.4
1	A	881	LEU	2.4
1	A	180	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	976	GLU	2.4
1	A	926	ASP	2.4
1	A	487	PRO	2.4
1	A	543	ILE	2.3
1	A	936	HIS	2.3
1	A	883	ASP	2.3
1	A	963	VAL	2.3
1	A	1016	PHE	2.3
1	A	1028	LEU	2.3
1	A	864	GLY	2.3
1	A	181	ILE	2.3
1	A	777	ARG	2.3
1	A	247	GLN	2.2
1	A	553	SER	2.2
1	A	156	LEU	2.2
1	A	213	HIS	2.2
1	A	622	TYR	2.2
1	A	1038	TYR	2.2
1	A	345	ASN	2.2
1	A	492	ILE	2.2
1	A	841	ILE	2.2
1	A	937	PHE	2.2
1	A	560	THR	2.2
1	A	561	ILE	2.2
1	A	852	ARG	2.2
1	A	825	GLN	2.2
1	A	891	ASP	2.2
1	A	854	SER	2.1
1	A	866	LEU	2.1
1	A	576	SER	2.1
1	A	412	ARG	2.1
1	A	304	MET	2.1
1	A	889	ILE	2.1
1	A	581	ALA	2.1
1	A	1033	GLN	2.1
1	A	568	LEU	2.1
1	A	735	LEU	2.1
1	A	329	VAL	2.1
1	A	110	GLU	2.0
1	A	570	LEU	2.0
1	A	344	VAL	2.0
1	A	559	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	2.0
1	A	185	LEU	2.0
1	A	748	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](#)

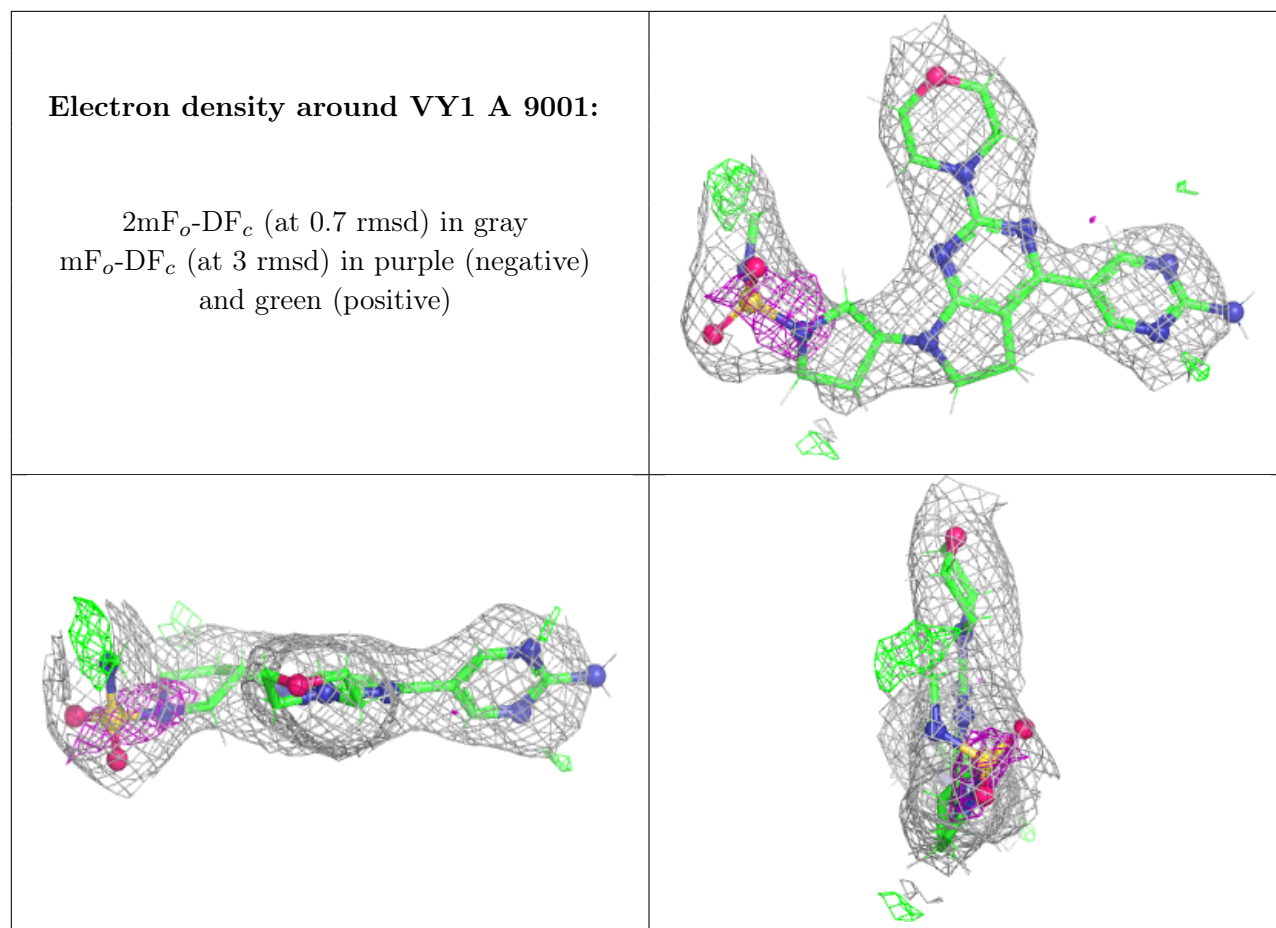
There are no oligosaccharides in this entry.

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	VY1	A	9001	32/32	0.82	0.17	97,107,128,128	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.